BORN-OPPENHEIMER APPROXIMATION APPLIED TO SOME SINGULAR SYSTEMS

by

Kaya Güven Akbaş

B.S., Physics, Boğaziçi University, 2013

M.S., Physics, Boğaziçi University, 2016

Submitted to the Institute for Graduate Studies in
Science and Engineering in partial fulfillment of
the requirements for the degree of
Doctor of Philosophy

Graduate Program in Physics

Boğaziçi University

2024

ACKNOWLEDGEMENTS

First of all, I would like to express my endless gratitude to my supervisor Prof. Teoman Turgut for agreeing to work with me and for his endless efforts in helping me to complete my master's and PhD degrees. Even though he knew how difficult it was to work and get along with me, he never complained about it and was ready to provide any support. I will always be grateful to him for his endless patience and belief in me.

I am extremely grateful to Assoc. Prof. Fatih Erman For generously sharing her intelligence with us and providing endless help throughout our work.

I would also like to thank my thesis committee, Prof. Aybike Özer, Assoc. Prof. Levent Akant, Assist. Prof. Can Kozçaz for their interest and comments.

I would also like to express my sincere gratitude to my dearest friend Dr. Sema Seymen for her valuable assistance during the writing process of my thesis, productive discussions we had about our studies and never ending support in my life.

ABSTRACT

BORN-OPPENHEIMER APPROXIMATION APPLIED TO SOME SINGULAR SYSTEMS

In this thesis, we examine the spectral properties of a Schrödinger operator H_0, which has been modified by introducing δ interactions. Our analysis explicitly demonstrates the reconfiguration of poles in the new Green's function concerning those present in the original Green's function of H_0 by demonstrating the energies of new bound states are interleaved between the existing ones. Notably, the ground state energy consistently decreases when the δ interaction is attractive. We develop an alternative perturbative approach for determining the bound state energies and wave functions, assuming a small coupling constant. We extend our findings to cases requiring a renormalization. Our study also explores the applicability of these outcomes to more complex situations, such as multi-center configurations, δ interactions localized along curves, and the movement of particles within a compact two-dimensional manifold affected by δ interactions. We explicitly investigate the semi-relativistic extension of the problem. Next, we add a heavy particle to the classical kink system in one dimension. Within the Born-Oppenheimer approach, we notice that this heavy particle behaves akin to a repulsive delta potential within the kink equation of motion. Understanding how this delta potential affects the wave function within the system, we obtain a new phase and the change in the kink's mass. We can also determine this change through perturbation. Finally, we analyze how the energy of the heavy particle changes. The last part is about a basic singular system in a two-dimensional space which involves two heavy particles interacting with a light particle through an attractive contact interaction. With careful application of the Born-Oppenheimer approximation, we demonstrate its applicability to this specific scenario. Consequently, we determine the dominant term within the approximation and provide insights into obtaining higher-order corrections.

ÖZET

BORN-OPPENHEIMER YAKLAŞIMININ BAZI TEKİL SİSTEMLERE UYGULAMASI

Bu tezde, Schrödinger operatörü H_0'ın spektral özelliklerini, bu operatörde δ potansiyeli etkileşimleriyle oluşan değişiklikleri inceledik ve yeni Green fonksiyonunun kutuplarının, H_0'ın orijinal kutuplarına kıyasla yeniden düzenlendik. Yeni bağlı durum enerjilerinin eskilerin arasına giriftlendiğini ve δ etkileşimi çekici olduğunda temel durum enerjisinin hep düştüğünü kanıtladık. Bağlama sabitinin küçük olması varsayımında bağlı durum enerjilerini ve dalga fonksiyonlarını bulmanın alternatif bir pertürbatif yöntemini türettik. Bu sonuçların renormalizasyon gerektiren farklı durumlara da genişletilebileceğini gösterdik. Sonuçlarımızı çoklu merkezli duruma, eğrilere dayalı δ etkileşimlerine ve bir parçacığın δ etkileşimi etkisi altında kompakt bir iki boyutlu manifoldda hareket ettiği durumlara genişletmenin mümkün olabileceğini gördük. Son problemimizin yarı-relativistik durumunu inceledik. Sonra, ilk kısımdakileri ve Born-Oppenheimer yaklaşımını kullanarak bir boyuttaki kink modele ağır parçacık ekledik ve kink kütlesindeki değişimi inceledik. Ağır parçacığın iten bir delta potansiyeli gibi davrandığını ve bunun sonucunda da kinkin dalga fonksiyonunda bir değişim olduğunu gördük. Delta potansiyelin dalga fonksiyonunu nasıl değiştirdiğini bildiğimizden, yeni dalga fonksiyonunu kullanarak yeni bir faz kayması hesapladık. Daha sonra da kink kütlesindeki değişimi bulmaya çalıştık. Kink sisteminin ağır parçacığın enerjisini ne kadar değiştirdiğini gösterdik. Son olarak iki boyutta, iki ağır parçacığın bir hafif parçacıkla çekici bir temas etkileşimiyle etkileştiği basit bir tekil sistem üzerine çalıştık. Normalizasyon gerektiren bu tekil problem için gerekli özeni gösterip hesapları dikkatlice yaptıktan sonra problemin bu yaklaşımı kullanma konusunda tutarlı olduğunu ortaya çıkardık. Son kısımda Born-Oppenheimer yaklaşımının baskın terimini hesapladık ve yüksek dereceden düzeltmelerin nasıl bulunabileceği hakkında bilgi verdik.

TABLE OF CONTENTS

ACKNOWLEDGEMENTS iii
ABSTRACT iv
ÖZET v
LIST OF FIGURES viii
LIST OF SYMBOLS ix
1. INTRODUCTION 1
1.1. Preliminary Expressions 1
2. ON SCHRÖDINGER OPERATORS MODIFIED BY δ INTERACTIONS . 11
2.1. Modifications by δ Interactions in Regular Cases 11
2.1.1. A Different Perspective for the Perturbative Estimates on the Bound State Energies 20
2.1.2. A Different Perspective for the Perturbative Estimates on the Bound State Wave Function 22
2.2. Singular Modifications by δ Interactions 25
2.3. Possible Generalizations 35
2.3.1. N Center Case 35
2.3.2. δ Interaction Supported on Curves in Plane 36
2.3.3. A Particle in a Compact Manifold under the Influence of a $\delta-$Interaction 39
2.3.4. A Semi-relativistic Model on a 2-Dimensional Compact Manifold 42
2.4. Degenerate Case 50
3. BORN-OPPENHEIMER APPROXIMATION APPLIED TO KINK MODEL IN ONE DIMENSION 53
3.1. A Brief Summary About the One-Dimensional Kink Model 53
3.2. Quantum Corrections to the Kink Solution in the Presence of a Heavy Non-relativistic Scalar Particle 60
4. BORN OPPENHEIMER APPROXIMATION FOR A SIMPLE SYSTEM WHICH IS RENORMALIZABLE 73

4.1. Two heavy particles interacting with a light one 73
4.2. Effective Potential for the Heavy Degrees of Freedom 81
4.3. Energy Levels of the System 90
5. CONCLUSION 94
REFERENCES 96
APPENDIX A: Some Properties of Green's Function 107
APPENDIX B: Small Distance Expansions 111
APPENDIX C: Perturbative Corrections 120

LIST OF FIGURES

Figure 2.1. The graph of $1/\alpha$ and a typical behavior of the term $\sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{E_n - E} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda)$ versus E for $\alpha > 0$. The intersection points give the bound state energies. Here $E_0, E_1, E_2, \ldots$ represents the bound state energies of H_0 and $E_0^*, E_1^*, E_2^*, \ldots$ represents the bound state energies of the Hamiltonian modified by δ interaction. 17

Figure 2.2. Graphical solution E of the equation $\frac{1}{\alpha} = G_0(a, a|E)$, where the Green's function of the form $G_0(a, a|E)$ is given as $\frac{1}{\hbar}\left(\frac{m}{-2E}\right)^{1/2} - \frac{\kappa}{2\cosh^2(\kappa a)(E + \frac{\hbar^2\kappa^2}{2m})}\left(\frac{\hbar\kappa}{\sqrt{-2mE}}\right)$. Here we have chosen $\alpha = 1/2$, $\hbar = 2m = 1$, $\kappa = 1$, and $a = 1$. Here the vertical asymptotes correspond to the bound state energies of the initial Hamiltonian H_0 or the point where the continuous spectrum of H_0 begins. 19

LIST OF SYMBOLS

A	Normalization constant of light particle wave function
$D(H_0)$	Some dense domain on which we define H_0
E_g	Heavy particle ground state energy
E_k	The bound state energy of ϕ_k
E_k^*	The bound state energy of the modified Hamiltonian
E_n	Eigenvalues corresponding to the eigenfunction ϕ_n
${}_2F_1$	Hypergeometric function
$f_i(x)$	Normal modes functions of the kink differential equation
$f_n(x)$	The eigenfunctions of the Laplace Beltrami operator
$f_k^+(x)$	Even wave solution of the kink model
$f_k^-(x)$	Odd wave solution of the kink model
$\hat{f}_k^+(x)$	Even wave solution of the modified kink model
f_s	Orthonormal normal modes functions of the fluctuations
g^{ij}	Inverse metric
$G_0(x, y\|E)$	Original Hamiltonian green's function
$G(x, y\|E)$	Green's function associated with the modified Hamiltonian
H	Modified Hamiltonian by the δ interaction
H_0	Self-adjoint Schrödinger operator or Hamiltonian
$\hat{H}_0$	Original Hamiltonian of the kink model
K_0	Modified Bessel function of the second kind
K_1	Modified Bessel function of the second kind
$K_t(x, y)$	Heat kernel
$K_\nu(z)$	Modified Bessel function
$l_n^{2\beta}(r)$	Two dimensional associated Laguerre polynomials
$L(\Gamma)$	Length of the curve
$L^2(\mathbb{R}^{\not\vDash})$	Hilbert space
M_{cl}	Total energy of the static solution
M_{kink}	Kink mass

m	Field mass
m_*	Reduced mass of heavy and light particle
M	Heavy particle mass
N	Normalization constant of light particle wave function
$P_\nu^\mu(x)$	Associated Legendre polynomials
$\mathbb{P}_k$	Projection operator onto the eigenspace of E_k^*
$R_{H_0}(z)$	Integral kernel of the resolvent for H_0
$\mathbb{R}^2$	Real number space in 2-dimension
R_n	Heavy particle wave function
x^i	The local coordinates
X	Center of mass coordinates between heavy particles
V	General potential
z	Relative coordinates between heavy particles
α_R	Renormalized coupling constant
γ	Euler's constant
$\gamma(s)$	A curve along normal direction
Γ_k	The closed contour around each simple pole E_k^*
δ_Γ	Dirac delta function supported by the curve Γ
δE_k	The change in the bound state energy E_k
δE	Heavy particle energy
$\delta(k)$	Phase shift
Δ	Laplacian operator
ΔE_{cl}	Energy shift from the classical solutions
ΔE_{cl}	Shifts of the oscillator zero-point energies
ΔE_{ct}	Energy contribution from the counter terms
ϵ^2	Renormalization parameter
ζ_0	Length scale
$\eta(x,t)$	Periodic solutions of the kink differential equation
κ	A constant whose dimension is mass
λ	Eigenvalue for the continuous spectrum

μ^2	Renormalization parameter
ν^2	Light particle binding energy
$\sigma_d(H)$	A discrete or point spectrum
$\sigma_c(H)$	A purely absolutely continuous real spectrum
$\phi^{(+)}(x)$	The positive frequency part of the bosonic field
$\phi^{(-)}(x)$	The negative frequency part of the bosonic field
$\phi(x\|x_1, x_2)$	Light particle particle wave function
Φ_R	Renormalized principle operator
ϕ_n	Eigenfunctions of H_0
$\Phi(E)$	Principle operator
ϕ_k	The bound state wave function of H_0
$\Psi(x; x_1, x_2)$	Three particle wave function
$\psi(x_1, x_2)$	Two heavy particle particle wave function
Ψ	Heavy particle field
ψ	Test functions
Φ_{ij}	Principle operator matrix element
ω_i	Normal frequencies
ω_n	Frequency corresponding to the Laplace Beltrami operator
ω_s^2	Frequencies of the modified kink Hamiltonian
∇_g^2	Laplace Beltrami operator ∇_g^2

1. INTRODUCTION

The δ potential interaction is used in many areas of theoretical physics. This model is used in scattering theory to describe the strong nuclear force between protons and neutrons in nuclear physics or to describe electron-ion interactions in solid state physics. Therefore, a comprehensive understanding of the δ potential interaction will provide significant assistance to physicists when dealing with complex models, facilitating research and analysis processes. In this thesis, we tried to calculate clearly and understandably how the bound state energy and wave functions in the system change when we add a δ interaction to a Hamiltonian for both the classical case and the situations requiring renormalization. We then used the information we obtained to solve two different physics problems by combining it with the Born-Oppenheimer approach used to solve multi-particle systems.

1.1. Preliminary Expressions

First, we work on a self-adjoint Schrödinger operator, $H_0 = -\frac{\hbar^2}{2m}\Delta + V$, which is defined on a dense domain $D(H_0)$. We make assumptions about its spectra: it possesses both a discrete or point spectrum $\sigma_d(H)$ and a purely continuous real spectrum $\sigma_c(H)$. These spectra don't overlap, i.e., there are no embedded eigenvalues between them. Additionally, we suppose that the discrete spectrum doesn't have accumulation points and it is limited from below. These conditions impose some limitations on the regularity of the potentials, but they are common in most quantum mechanics problems involving physically reasonable potentials.

Let ϕ_n, where $\phi_n \in L^2$, be an eigenvector or eigenfunction associated with the eigenvalue E_n in the discrete spectrum of the operator H_0, such that it satisfies the equation $H_0\phi_n = E_n\phi_n$ and simultaneously, when considering the continuous spectrum of the operator H_0, if χ_λ, which is outside of L^2 is considered as the generalized eigenfunction representing this spectrum and its associated generalized eigenvalue as λ, then

the Hamiltonian must satisfy the equation $H_0\chi_\lambda = \lambda\chi_\lambda$. We point out that the proper meaning of the generalized eigenfunctions has been understood in the context of so-called Rigged Hilbert spaces [1–3]. The function $\chi_\lambda(x) = \frac{1}{\sqrt{2\pi}}e^{i\lambda x/\hbar}$ is the well-known generalized eigenfunction of the momentum operator $(P\psi)(x) = -i\hbar\frac{d}{dx}\psi(x)$ in $L^2(\mathbb{R})$. Under relatively mild assumptions on the potential V for dimensions $d \leq 3$ case, it is known that the generalized eigenfunctions of a Schrödinger operator can actually be selected as continuous functions [5,6]. This is extremely valuable for our computations as we either evaluate them at a point or integrate them over a curve in this work.

According to a fundamental premise in quantum mechanics, it is possible to formally expand any function $\psi \in L^2(\mathbb{R})$, as detailed in, for example, page 48 in [7]):

$$\psi(x) = \sum_n a_n\phi_n(x) + \int_\Lambda a(\lambda)\chi_\lambda(x)\, d\mu(\lambda)\ , \tag{1.1.1}$$

where

$$a_n = \int_{\mathbb{R}} \overline{\phi_n(x)}\psi(x)dx\ , \qquad a(\lambda) = \int_{\mathbb{R}} \overline{\chi_\lambda(x)}\psi(x)dx\ . \tag{1.1.2}$$

In the Equation (1.1.1), the range of integration denoted by Λ refers to a parameter space, typically a subset of $\mathbb{R}$ or, more generally, $\mathbb{R}^n$. This space is constructed based on the absolutely continuous spectrum $\sigma_c(H_0)$, detailed in references such as [8] and recent studies [9]. The term $d\mu(\lambda)$ in the expansion represents a spectral measure associated with the self-adjoint operator H_0. In many quantum mechanical scenarios, the absence of a singular continuous spectrum allows us to express this measure simply as $d\mu(\lambda) = d\lambda$. This simplification involves absorbing any possible positive measurable function into the definition of eigenfunctions. This approach is particularly feasible when interpreting the integration as a direct integral, a concept discussed in [7]. In cases where there is degeneracy, summation over those indices becomes necessary. To put it differently, the Fourier transform acts as a formal expansion of a function ψ in terms of generalized eigenfunctions χ_λ associated with the momentum operator P.

The effect of the operator P on the function ψ is described as:

$$(P\psi)(x) = \int_{-\infty}^{\infty} \lambda \left(\int_{-\infty}^{\infty} \psi(\xi)\overline{\chi_\lambda(\xi)}d\xi \right) \chi_\lambda(x)d\lambda \, . \tag{1.1.3}$$

The concept of eigenfunction expansions was initially introduced by Weyl [10] for ordinary differential equations. Its further development occurred through contributions from Titchmarsh [11], Kodaira [12], and the extension to multidimensional cases for self-adjoint elliptic differential operators, as elaborated in [5]. The rigorous construction of such expansions using generalized eigenfunctions is achieved, particularly when imposing the condition of uniformly locally square integrable potential energy in the Schrödinger operator $H_0 = -\frac{\hbar^2}{2m}\Delta + V$. This condition is stated as Theorem 3 in [13]. Throughout this work, we implicitly assume the validity of these prerequisites for the eigenfunction expansions.

We are exploring Schrödinger operators, specifically H_0 operators modified by a δ interaction. The aim is to explicitly illustrate changes in eigenvalues and eigenfunctions using the eigenfunction expansions found in the Green's function for such generic H_0. Grosche's influential work [70] has extensively studied the modification of bound state spectra in one dimension and in d dimensional radial cases, particularly focusing on exactly solvable potentials V using path integral frameworks. Among the fundamental choices for H_0 is the well-studied one-dimensional harmonic oscillator problem, including its extension to radial symmetry. Various researchers [15–17] have investigated the impact of introducing a δ interaction to these harmonic oscillator Hamiltonians. The statistical properties of this system have been thoroughly examined in [18]. Moreover, its relevance to Bose-Einstein condensation has been explored in [19].

The treatment of point-like δ interactions in two and three dimensions is a well-studied topic that necessitates renormalization. Rigorous mathematical analyses have been carried out in [22,23], while in works such as [24,26–28,81], these interactions serve as useful models for comprehending various quantum field theory concepts. The extension of the harmonic oscillator Hamiltonian with a δ potential to higher dimensions also demands renormalization, explored in discussions such as [29], and more recent

investigations like [30–32]. An intriguing example of exact solvability that exhibits both discrete and continuous spectra is the reflectionless potential [33, 70]. We aim to illustrate how the spectral characteristics of this potential evolve when influenced by the presence of δ interactions, presenting it as a case study.

The impact of δ interactions on the eigenvalues of H_0 leads to a transformation described by either algebraic or transcendental equations. The eigenvalues of H_0 vanish unless specific wave functions vanish at the δ interaction's support or when the Dirac delta function's support aligns with the nodes of the initial Hamiltonian's wave function, H_0. This finding was demonstrated primarily for specific solvable instances rather than a comprehensive range of Hamiltonians, as detailed in references [29, 70]. In these scenarios, the modified system's complete Green's function, denoted as G, comprises the original G_0 of H_0 and an additional term derived from G_0. It isn't immediately evident whether the poles of G_0 cancel out with those of this extra term, where G_0 appears non-trivially in its expression. The cancellation was explicitly highlighted only for cases such as the one-dimensional harmonic oscillator Hamiltonian (discussed in [15]) and for higher-dimensional harmonic and linear potentials (referenced in [32]). This thesis aims to explicitly prove this cancellation by employing the eigenfunction expansion of the complete Green's function. It considers the pole structure of the generalized eigenfunction expansion across a broader spectrum of potentials. Additionally, it establishes that when the δ interaction's support doesn't align with the node of the bound state eigenfunction of H_0, the new eigenvalues E_k^* for an attractive δ interaction lie between E_{k-1} and E_k. The methodology introduces a perturbative approach from an alternate perspective to calculate, in an iterative manner, the new eigenvalues and wave functions under the assumption of a small coupling. This is then compared with the standard approach. These findings are extendable to multi-center cases and instances requiring renormalization. Notably, the perturbative method, when applied to problems requiring renormalization, produces divergent results from the standard approach that substitutes the bare coupling constant α with the renormalized one α_R, as anticipated. Moreover, analogous conclusions can be drawn for modifications induced by δ interactions supported on curves in the plane and for scenarios where a particle

inherently moves within a compact manifold under the influence of a δ interaction.

This thesis is structured as follows: Section 2.1 begins by utilizing the eigenfunction expansion of the Green's function. We explicitly demonstrate that the poles of the Green's function of H_0, modified by the δ interaction in one dimension, nullify the poles of the Green's function of H_0 under certain mild conditions. Additionally, we establish proof that the new bound state energies are interleaved between the pre-existing ones. Furthermore, we discuss these outcomes by presenting an explicit example involving an exactly solvable reflectionless potential. Following this, we introduce a novel perturbative method for determining the bound state energies and wavefunctions up to the second order, comparing them with established classical results. In Section 2.2, we extend these findings to the singular case, necessitating the problem's renormalization. This section addresses the adjustments required to accommodate singularities. Finally, Section 2.3 delves into potential extensions of our results. This includes exploring scenarios such as the N-center case, δ interaction situated on a curve within a plane, interaction of a particle on a compact manifold with a point center, and the adaptation of our arguments to a possible semi-relativistic version of singular interaction.

The initial article thoroughly examined the influence of the δ potential interaction on the H_0 Hamiltonian, a crucial topic in the physics literature, especially in theoretical physics. It provided in-depth analysis regarding changes in the Green's function and the appearance of new poles, offering clear illustrations for various scenarios that necessitate normalization as well as those where normalization isn't required. Our current strategy is to apply the information and formulas obtained from this article, which are very useful in understanding the δ interaction, to two different systems using the Born-Oppenheimer approach. One of these systems is a kink model described by a potential like $\lambda\phi^4$. The other is a three-particle singular model which consists of two heavy particles carrying attractive delta potentials and a light particle interacting with them in two dimension. The Born-Oppenheimer approximation is a historically significant model extensively used not only in understanding the motion of heavy particles but also in multiple-particle models. This approximation separates the behavior of heavy

particles, typically atomic nuclei, from lighter particles like electrons. It assumes that the movement of atomic nuclei is significantly slower compared to the rapid motion of electrons within a molecule or a system. Let me give some information about this approach.

Born-Oppenheimer approximation [72] is the basic tool of molecular physics [73–75]. When all the particles interact via Coulomb forces, as is the typical case of molecular physics, the Born-Oppenheimer vibrational energy levels go with $(m/M)^{1/2}$, where m/M refers to the light mass to heavy mass ratio. One can consider rotational energy levels as well as unharmonic vibrations as higher order corrections, since they turn out to be of order (m/M). In the usual approach the relevant expansion parameter is thought to be $(m/M)^{1/4}$, yet only even powers seem to show up in the expansions. There is a large literature on the stationary level calculations in the Born-Oppenheimer approximation, we will not be able to cover most of it, we only mention some of the more rigorous works, since in our present work, we also aim to get an approximation scheme in which we can control the errors that we make in a self-consistent way. The time-dependent Born-Oppenheimer approximation is a very interesting and closely related subject, the reader can consult the review articles [76–78] for more information. However, our system is highly singular and requires renormalization as is well known in the literature [79–86]. Therefore, one does not expect the existing results on well-behaved potentials to hold in this regime.

An interesting toy model in which two heavy and one light particle all interact via harmonic oscillator potentials is presented by R. Seiler in [87], where the assumptions of the Born-Oppenheimer approach is carefully tested. Following this, some rigorous aspects of Born-Oppenheimer approximation is presented in [88]. It is not at all clear that the eigenvalues of the light degrees of freedom, that one computes, under the influence of potentials when the heavy centers are clamped, actually define well-behaved non-intersecting surfaces when one considers the heavy degrees of freedoms as parameters. This difficult problem is solved by Hunziker in [89], where even for Coulomb type potentials energy eigenfunctions are shown to be essentially analytic

functions of the heavy coordinates. These problems further investigated in a series of papers by Hagedorn [90–92]. In the usual potentials, higher order corrections to the Born-Oppenheimer approximation are rigorously investigated by Hagedorn in a series of papers [93,94]. Further investigations along similar lines are presented in [95]. They typically correspond to higher order corrections to the effective potentials generated by the light degrees of freedom. The reader can find a large collection of references and various mathematically precise statements on Born-Oppenheimer approximation in a recent review by Jecko [78].

A different attempt to include higher order corrections to Born-Oppenheimer approximation is given by Weingert and Littlejohn [96] as an example of their diagonalization technique in the deformation quantization approach. They discover derivative terms in the higher order corrections. As our problem concerns a highly singular system, we get kinetic energy corrections, very similar to the ones found in [96], even at the leading order.

In a similar spirit to [87], a slightly simpler model for its pedagocial value was proposed by G. Gangopadhyay and B. Dutta-Roy in [97] where the authors consider a light particle coupled to a heavy particle via a delta function potential and the whole system is confined to a box in one dimension. This system has a distributional potential yet it is not truly singular, since an analytical treatment is still possible one can test the Born-Oppenheimer approximation. We propose to consider a toy model in a highly nontrivial situation, which requires a coupling constant renormalization. Recently, we considered a simpler version of this problem in one dimension, in which there is no renormalization, consequently we could analyse this case in much more detail [98].

The kink model is a concept used in quantum field theory to describe a phenomenon where quantum fields become unstable in a particular state, leading to energy transitions. Kinks are a type of topological structure that arises in the vacuum structure of quantum fields. These kinks are typically modeled in one-dimensional space-time systems and are utilized to explain the behavior of various types of parti-

cles within quantum field theory. Specifically, in one-dimensional field theories, they appear as transition regions between minimum-energy states of different field configurations. Quantum kinks represent configurations of fields transitioning between different states, signifying changes in energy levels during these transitions. These structures are studied in quantum field theories and cosmology, particularly in the early stages of the universe or during various phase transitions. Kink models serve as a tool to understand phase transitions, topological structures, and behaviors of quantum fields in physics. They play a crucial role in exploring complex systems and understanding transformations in specific conditions.

In our study, we introduced a heavy particle to the established kink model and employed the Born-Oppenheimer approach to examine its influence on the system. During certain computations, we observed that the addition of this massive particle introduces a repulsive delta potential to the system. In our initial paper [71], we calculated how the Green's function and wave function change when the delta potential is incorporated into the system. Using the outcomes from that paper, we computed a new wave function and phase shift. From this foundation, we can readily calculate the alterations in the kink mass. Furthermore, employing perturbation methods enables us to determine changes in the kink mass. Lastly, we computed the impact of the kink system on the energy of the heavy particle.

Using the Born-Oppenheimer approach in a two-dimensional system with three particles allowed us to calculate the distance between heavy particles and their energies. This has enabled us to find out surprising results that contribute to a deeper understanding of the Born-Oppenheimer approach. These results were very recent, and no calculation had been made before such a singular case requiring renormalization. The existing literature on Born-Oppenheimer approximation is tailored to deal with interaction potentials which are sufficiently regular. It is not obvious that these methods would suffice to deal with somewhat more singular cases, especially the problems which require renormalization. In view of the fact that most quantum field theories require renormalization this is an especially important problem which has direct physi-

cal implications. The insight that one may gain even from some simple models is likely to shed light on the methods to be developed for more realistic systems. The model we have in mind looks very simple, we consider two heavy particles in two dimensions interacting via a contact term with a third light particle. To make the calculations tractable we use a non-relativistic approach (nevertheless, see the remark below), a more interesting version would be to treat the light particle as a relativistic one. The relativistic model may be relevant for understanding the following problem, just as in the case of nucleons interacting with each other via exchange of mesons, the interaction of two heavy quarks may be energetically more favorable by exchange of glue balls, which are to be modeled as light relativistic particles.

In any case, we see that the basic idea of separating heavy (slow) and light (fast) modes does indeed work, yet in a rather nontrivial manner. One does not find a simple expansion scheme, where corrections manifest themselves easily. It has to be worked out carefully, and even the leading term requires a delicate set of computations. We see that the leading term is actually also large, this is an effect due to the nonlinear nature of renormalization, the light degree of freedom also has very large energy. What is then the relevant expansion parameter? It turns out that the separation between the heavy particles is very small, as compared to single center binding length scale. This length scale is determined by the binding energy of the light particle to a single heavy center, this is our input parameter for renormalization, coupling constant is traded off with this binding energy. The ratio of these two length scales is our expansion parameter in a very subtle way as we see below. One may compute some of the lower order terms as well, a few contain the logarithm of the large parameter M/m, there are also next lower order terms one can in principle compute. A many body approach could be more natural to develop a systematic expansion but this seems to be much more challenging at the moment.

Having completed the present work, we learned through the work of D. S. Rosa *et.al.* [99] (and references therein) that three particle problem within the Born-Oppenheimer approximation was originally introduced by Fonseca, Reddish and Stanley as an ana-

lytic model to study the Effimov effect, they use regular separable potentials between the heavy and light particles [100]. Our delta-function potential model is essentially worked in the Jacobi type coordinates within the Born-Oppenheimer approximation in [101], in the main part they assume some reasonable potential between the heavy centers. Moreover these ideas are further elaborated in [99] mainly for large separation of the heavy centers, with such atomic systems in mind. In the limit of large separation, in which the large z expansion becomes important, the correction terms that we compute are actually small and they can be neglected. These ideas are further developed in arbitrary dimensions in the recent work [102] using the Born-Oppenheimer approximation, albeit in this work corrections due to small distance are not taken into account. When there is no repulsive potential between the heavy centers, we see that it is crucial to develop an improved expansion.

2. ON SCHRÖDINGER OPERATORS MODIFIED BY δ INTERACTIONS

2.1. Modifications by δ Interactions in Regular Cases

In this study, we make use of some well-known characteristics of Green's function. To make it easier for the reader, we present them here with our chosen notation. For instance, the integral kernel of the resolvent $R_{H_0}(z)$ for the Schrödinger operator $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ or simply Green's function is defined as follows

$$\left(R_{H_0}(E)\psi\right)(x) = \left(R_0(E)\psi\right)(x) = \left((H_0 - E)^{-1}\psi\right)(x) = \int_{\mathbb{R}} G_0(x, y|E)\psi(y)dy \ , \quad (2.1.1)$$

can be represented using the following bilinear expansion.

$$G_0(x, y|E) = \sum_{n=0}^{\infty} \frac{\phi_n(x)\overline{\phi_n(y)}}{E_n - E} + \int_{\Lambda} \frac{\chi_\lambda(x)\overline{\chi_\lambda(y)}}{\lambda - E}\, d\mu(\lambda) \ . \quad (2.1.2)$$

The Green's function $G_0(x, y|E)$ is a square integrable function of x for almost all y and vice versa [34]. These equations given above continue to remain applicable in higher dimensions.

Let's start by considering one dimensional problem where H_0 is modified by a δ function interaction supported at the origin

$$H = H_0 - \alpha\delta \ , \quad (2.1.3)$$

where $\alpha \in \mathbb{R}$. It is possible to say that there are many different ways to make sense of the formal expression provided above of H. the first one of these ways is to consider the δ interaction as a self-adjoint extension of H_0. The recent book, which offers a modern introduction to this subject, was written by Gallone and Michelangeli [35] and the classic reference elaborating this point of view is the monograph by Albeverio et all [22]. δ interactions can also be defined through the strong limit of the resolvent of Hamiltonians with δ interaction replaced by some scaled function, see [23, 36] for the

details. The formulation of the problem in this section can be generalized to higher dimensions as long as the co-dimension is preserved. this means that dimension of the space - dimension of the support of the δ interaction is one. We will return to this issue at a later time for possible generalizations of the problem.

As is well-known that Green's function for the Hamiltonian (2.1.3) is expressed with Krein's type of formula stated below

$$G(x,y|E) = G_0(x,y|E) + \frac{G_0(x,0|E)G_0(0,y|E)}{\Phi(E)} \ . \tag{2.1.4}$$

This formula can be easily derived as follows,

$$\begin{aligned}(H_0 - E - \alpha\delta(x))G(x,y|E) &= (H_0 - E - \alpha\delta(x))\left(G_0(x,y|E) + \frac{G_0(x,0|E)G_0(0,y|E)}{\Phi(E)}\right) \\ &= \delta(x-y) - \alpha G_0(0,y|E)\delta(x) + \frac{G_0(0,y|E)\delta(x)}{\Phi(E)} - \alpha\frac{G_0(0,0|E)G_0(0,y|E)\delta(x)}{\Phi(E)} \\ &= \delta(x-y) - \alpha G_0(0,y|E)\delta(x) + \frac{G_0(0,y|E)\delta(x)}{\Phi(E)}\Big[1 - \alpha G_0(0,0|E)\Big] = \delta(x-y)\end{aligned} \tag{2.1.5}$$

where $G_0(x,y|E)$ is the Green's function for H_0 and

$$\Phi(E) := \frac{1}{\alpha} - G_0(0,0|E) \ . \tag{2.1.6}$$

Although some books use notation Γ instead of Φ in the context of point interactions, we will always use notation Φ throughout the study. As we emphasized in the introduction, here and in the subsequent parts, it is assumed that $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ satisfies some conditions. These conditions are; H_0 is self-adjoint on some dense domain $D(H_0) \subset L^2(\mathbb{R})$, Spectrum of H_0 is a disjoint union of discrete $\sigma_d(H_0)$ (set of eigenvalues) and (absolutely) continuous spectrum $\sigma_c(H_0)$, The discrete spectrum has no accumulation point, For stability, we assume H_0 has spectrum bounded below, and it is assumed that these assumptions will continue to be valid in higher dimensions as well. These conditions on the spectrum put some mild restrictions on the potential V. The classical work of Reed and Simon [37] contains a list of possible potential classes that are assumed to satisfy for the conditions mentioned above.

We then claim our first result regarding the spectral properties of the Hamiltonian (2.1.3) as follows: Let us define $\phi_k(x)$ as the bound state wave function of H_0 associated with the bound state energy E_k. Then, the bound state energy E_k^*, when H_0 is modified (perturbed) with a δ function interaction $(-\alpha\delta(x))$, satisfies the equation

$$\Phi(E) = \frac{1}{\alpha} - G_0(0,0|E) = 0 \,, \tag{2.1.7}$$

if $\phi_k(0) \neq 0$ for this particular k. If for this choice of k we have $\phi_k(0) = 0$, the bound state energy does not change, $E_k^* = E_k$. Moreover, the continuous spectrum of the Hamiltonian modified with δ interaction is the same as that of H_0.

First, we start the proof by showing how the pole structure of the full Green's function $G(x,y|E)$ is rearranged and the poles of $G_0(x,y|E)$, which explicitly appears as an additive factor in $G(x,y|E)$ actually are cancelled and new poles appear. Note that from the explicit expression of the full Green's function (2.1.4), one may expect that the poles of the full Green's function may contain the poles of G_0 as well as the zeroes of the function $\Phi(E)$.

Using the eigenfunction expansion of the Green's function (2.1.2) and splitting the term in the summation associated with the isolated simple eigenvalue E_k of H_0, we obtain

$$\begin{aligned}
G(x,y|E) = {} & \frac{\phi_k(x)\overline{\phi_k(y)}}{E_k - E}\left(1 - \left(1 - \frac{(E_k - E)}{|\phi_k(0)|^2}D(\alpha,E)\right)^{-1}\right) + g(x,y|E) + h(x,y|E) \\
& + \frac{(E_k - E)}{(E_k - E)D(\alpha,E) - |\phi_k(0)|^2}\Big(g(x,0|E)g(0,y|E) + g(x,0|E)h(x,0|E) \\
& + g(x,0|E)h(0,y|E) + h(x,0|E)h(0,y|E)\Big) \\
& + \frac{1}{(E_k - E)D(\alpha,E) - |\phi_k(0)|^2}\Big(g(x,0|E)\phi_k(0)\overline{\phi_k(y)} + g(0,y|E)\phi_k(x)\overline{\phi_k(0)} \\
& + h(x,0|E)\phi_k(0)\overline{\phi_k(y)} + h(0,y|E)\phi_k(x)\overline{\phi_k(0)}\Big) \,.
\end{aligned} \tag{2.1.8}$$

The equation demonstrating the polar structure of the Green's function mentioned above is quite long and complex. To facilitate comprehension, we have represented this equation using certain letter expressions. Now, let's provide explicit definitions for

these expressions:

$$g(x,y|E) := \sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(y)}}{E_n - E} , \tag{2.1.9}$$

$$h(x,y|E) := \int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(y)}}{\lambda - E}\, d\mu(\lambda) , \tag{2.1.10}$$

$$D(\alpha,E) := \frac{1}{\alpha} - \sum_{n\neq k} \frac{|\phi_n(0)|^2}{E_n - E} - \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda) . \tag{2.1.11}$$

As you can see these are regular near E_k, for simplicity.

The functions g, h at $x = 0$ and $y = 0$, and it is possible to define the function D very well thanks to the fact that continuous representations of the generalized eigenfunctions χ_λ exist in here [5, 6]. Except for the first term in Equation (2.1.8), It is very clear that all terms have an analytical behavior in a sufficiently small disk around $E = E_k$. If we choose E close enough to E_k, i.e., if $\frac{|E_k - E|}{|\phi_k(0)|^2}\,|D(\alpha,E)| < 1$, the first term in the above equation becomes

$$-\frac{\phi_k(x)\overline{\phi_k(y)}}{|\phi_k(0)|^2}\left(\frac{1}{\alpha} - \sum_{n\neq k}\frac{|\phi_n(0)|^2}{E_n - E} - \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda)\right) + O(1) , \tag{2.1.12}$$

so that $G(x,y|E)$ is regular (no poles) near $E = E_k$ as long as $\phi_k(0) \neq 0$. Hence, the pole $E = E_k$ of $G_0(x,y|E)$ is not a pole of $G(x,y|E)$ if $\phi_k(0) \neq 0$. So what we want to say is that the only poles of $G(x,y|E)$ must come from the zeroes of the function $\Phi(E)$.

Finally, According to the Weyl's theorem [37] the continuous spectrum of the problem coincides with the initial Hamiltonian. This is due to the fact that the difference between the resolvent of the Hamiltonian and the resolvent of the initial Hamiltonian has a finite rank and this is made possible by the explicit formula given as

$$R(E) = R_0(E) + (\Phi(E))^{-1}\langle\overline{G(\cdot,0|E)},\cdot\rangle G(\cdot,0|E) \tag{2.1.13}$$

which is defined on its resolvent set. This formula should be understood by its action

on a vector ψ, i.e.,

$$(R(E)\psi)(x) = (R_0(E)\psi)(x) + (\Phi(E))^{-1}\left(\int_{-\infty}^{\infty} G(y,0|E)\psi(y)\,dy\right)G(x,0|E)\,. \tag{2.1.14}$$

The use of Dirac's braket notation provides a more natural representation of this formula (2.1.13),

$$R(E) = R_0(E) + (\Phi(E))^{-1}R_0(E)|0\rangle\langle 0|R_0(E)\,. \tag{2.1.15}$$

Now, we will look at how much change there is between the ground state energy of the modified Hamiltonian and the ground state energy of the original Hamiltonian according to the sign of the coupling constant. To begin with, let's focus on the attractive case where the coupling constant is positive.

To begin with, let's focus on the attractive case where the coupling constant is positive. If $\alpha > 0$ and $\phi_k(0) \neq 0$ for some $k \geq 1$, then the new bound state energies E_k^* are interlaced between the eigenvalues of H_0:

$$E_{k-1} < E_k^* < E_k\,. \tag{2.1.16}$$

From here, when we look at the case where k is zero ($k = 0$), it is clear that we conclude that the ground state energy of the modified Hamilton system will be smaller than its original value. $E_0^* < E_0$. Since the Green's function G_0 has poles at the eigenvalues $E = E_n$ of H_0 in the complex E plane and has a branch cut along the generalized eigenvalues of H_0, This function is differentiable everywhere except at its poles and along the branch cut. Then, when we calculate the derivative of $G_0(0,0|E)$ with respect to E, considering both summation and integration, we formally obtain the following equation

$$\frac{dG_0(0,0|E)}{dE} = \sum_{n=0}^{\infty}\frac{|\phi_n(0)|^2}{(E_n-E)^2} + \int_{\Lambda}\frac{|\chi_\lambda(0)|^2}{(\lambda-E)^2}\,d\mu(\lambda) > 0\,. \tag{2.1.17}$$

This shows us that $G_0(0,0|E)$ is a monotonically increasing function of E between its poles as well as between the largest eigenvalue below the continuum branch cut and

the infimum of the branch cut which is typically zero. Moreover, by separating the $n = k$ term within the summation, it becomes clear that.

$$\lim_{E\to E_k^-} \sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{E_n - E} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda) \;=\; \infty\,, \tag{2.1.18}$$

$$\lim_{E\to E_k^+} \sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{E_n - E} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda) \;=\; -\infty\,, \tag{2.1.19}$$

for all $k = 0, 1, 2, \cdots$, and when we calculate the limit, taking into account both the summation and the integral, we obtain the following result

$$\lim_{E\to -\infty} \sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{E_n - E} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda) \;=\; 0^+\,. \tag{2.1.20}$$

Then, if $\alpha > 0$ from the above results it becomes clear that the roots say: E_k^*, of the Equation (2.1.7) must be located at the points of intersection of $1/\alpha$ and $G_0(0, 0|E)$, as shown in Figure 2.1. This indicates that the energies of the newly found bound states E_k^* are shifted downwards and interlaced between E_{k-1} and E_k. Let E_0 be the ground state energy of H_0. Unlike excited states, the new ground state energy can be minimized to the greatest extent by selecting a sufficiently large value for α. Given the positivity of the wave functions associated with the ground state of Schrödinger operators according to Kato's inequality [37], having no nodes $\phi_0(0) \neq 0$, as we clearly stated above that new ground state energy E_0^* is always smaller than the ground state energy of the original Hamiltonian.

Now let's consider the case where $\alpha < 0$ (repulsive case), then the bound state energies of H_0 are shifted upward and interlaced as $E_k < E_k^* < E_{k+1}$ if $\phi_k(0) \neq 0$. As seen in the Figure 2.1 by moving the line $1/\alpha$ below the E axis. Otherwise, bound state energies of H_0 remain the same. The statements mentioned earlier still hold if we consider the support of the delta potential at $x = a$. In this case, we have

$$G(x, y|E) = G_0(x, y|E) + \frac{G_0(x, a|E)G_0(a, y|E)}{\frac{1}{\alpha} - G_0(a, a|E)}\,, \tag{2.1.21}$$

and the bound state energies remain unchanged when the δ interaction is added to the system if a is at one of the nodes of the bound state wave function of H_0, that is, $\phi_k(a) = 0$. Otherwise, we can obtain the bound state energies from this equation $\Phi(E) = \frac{1}{\alpha} - G_0(a, a|E) = 0$.

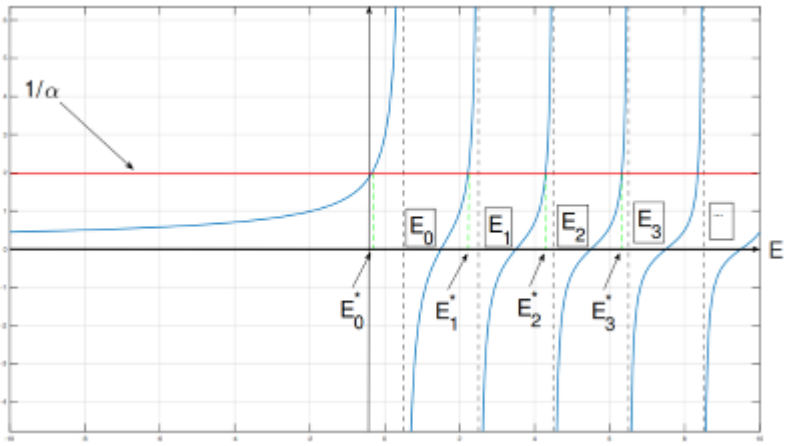

Figure 2.1. The graph of $1/\alpha$ and a typical behavior of the term $\sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{E_n - E} + \int_{\Lambda} \frac{|\chi_\lambda(0)|^2}{\lambda - E}\, d\mu(\lambda)$ versus E for $\alpha > 0$. The intersection points give the bound state energies. Here $E_0, E_1, E_2, \ldots$ represents the bound state energies of H_0 and $E_0^*, E_1^*, E_2^*, \ldots$ represents the bound state energies of the Hamiltonian modified by δ interaction.

The Figure 2.1 shows us that the addition of the δ interaction to H_0 leads to an increase in the number of bound states by one. An extra pole appears below the ground state energy of H_0 and all the other eigenvalues are interlaced. Moreover, for the Hamiltonian H_0, the energy of the bound state remains unchanged when a particular configuration of the delta δ interaction is introduced into the Hamiltonian. that is, the bound state energy E_k of the system remains the same when a delta *delta*interaction is placed at a point where the bound state wave function associated with the energy E_k of the unperturbed Hamiltonian H_0 has a mode.

We can provide a clearer understanding of our points by examining a precisely solvable instance for H_0, the unperturbed Hamiltonian, where its spectrum includes both discrete and continuous components. Exploring this particular scenario will enable us to illustrate the previously discussed concepts more clearly. Express the Schrödinger operator related to the reflectionless interaction potential V given by

$$(H_0\psi)(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - \frac{\hbar^2}{2m}\kappa^2 \frac{N(N+1)}{\cosh^2(\kappa x)}\psi(x)\,, \tag{2.1.22}$$

where $N \in \mathbb{N}$. In this case, the discrete spectrum consists of the following eigenvalues $E_n = -\frac{\hbar^2\kappa^2}{2m}(N-n)^2$, where $n = 0, 1, 2, \ldots N-1$. The system has finite number of bound states denoted as N, with corresponding eigenfunctions specified as follows

$$\phi_n^{(N)}(x) = \sqrt{\kappa}\left((N-n)\frac{(2N+1-n)!}{n!}\right)^{1/2} P_N^{n-N}(\tanh(\kappa x)) \,, \tag{2.1.23}$$

where $P_\mu^\nu(x)$ is Legendre function, expressed by $P_\nu^\mu(x) = \frac{1}{\Gamma(1-\mu)}\left(\frac{1+x}{1-x}\right)^{1/2} {}_2F_1(-\nu, \nu+1; 1-\mu; \frac{1-x}{2})$ in terms of hypergeometric functions ${}_2F_1$. In this case, the continuous spectrum is the positive real axis, i.e, $\sigma_c(H_0) = [0, \infty)$ and the generalized eigenfunctions are given by $\chi_k^{(N)}(x) = \left(\frac{k}{2\sinh(\pi k/\kappa)}\right)^{1/2} P_N^{ik/\kappa}(\tanh(\kappa x))$ with the generalized eigenvalues $E_k = \frac{\hbar^2 k^2}{2m}$, with $k \in \mathbb{R}$.

To simplify the analysis, let's set $N = 1$. In this specific case, there exists only one bound state, and the corresponding normalized eigenfunction is outlined as follows

$$E_0 = -\frac{\hbar^2\kappa^2}{2m} \,, \tag{2.1.24}$$

$$\phi_0(x) = \sqrt{\frac{\kappa}{2}}\frac{1}{\cosh(\kappa x)} \,. \tag{2.1.25}$$

The specific eigenfunction corresponding to this case ($N = 1$) can be defined by

$$\chi_E(x) = \sqrt{\frac{\kappa}{2\pi}} e^{ikx}\left(\frac{ik - \kappa\tanh(\kappa x)}{\kappa + ik}\right) \,, \tag{2.1.26}$$

with the generalized eigenvalues $E = \frac{\hbar^2 k^2}{2m}$. The Green's function for this specific potential problem in appropriate units has been thoroughly discussed and presented in the referenced article [70] and the exact formula, following the conventions and units that we use here is presented as

$$\begin{aligned} G_0(x, y|E) =& \frac{1}{\hbar}\left(\frac{m}{-2E}\right)^{1/2} \exp\left(-\frac{|x-y|\sqrt{-2mE}}{\hbar}\right) \\ &- \frac{\kappa}{2\cosh(\kappa x)\cosh(\kappa y)(E + \frac{\hbar^2\kappa^2}{2m})} \\ &\times \left[1 - \left(1 - \frac{\hbar\kappa}{\sqrt{-2mE}}\right)\cosh\left(\kappa|x-y|\left(1 + \frac{\sqrt{-2mE}}{\kappa\hbar}\right)\right)\right] . \end{aligned} \tag{2.1.27}$$

In our convention for the Green's function, there is an additional factor of $\hbar$ compared to the one introduced in this article [70].

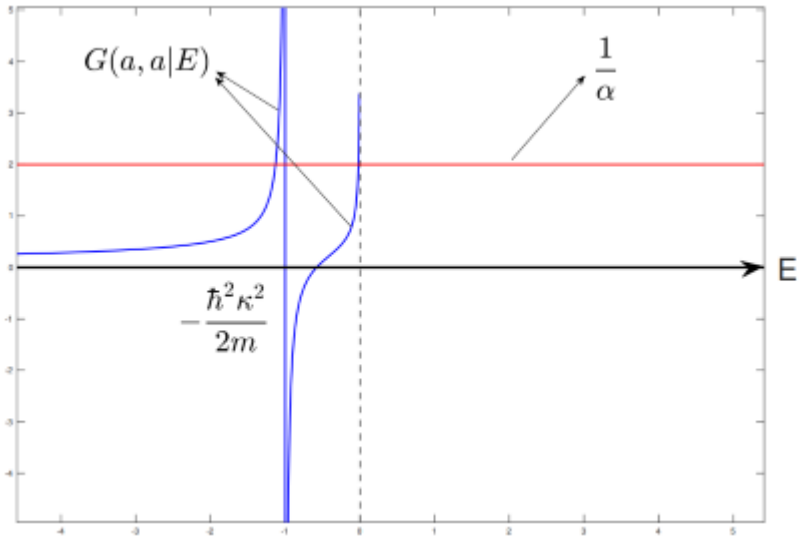

Figure 2.2. Graphical solution E of the equation $\frac{1}{\alpha} = G_0(a,a|E)$, where the Green's function of the form $G_0(a,a|E)$ is given as $\frac{1}{\hbar}\left(\frac{m}{-2E}\right)^{1/2} - \frac{\kappa}{2\cosh^2(\kappa a)(E+\frac{\hbar^2\kappa^2}{2m})}\left(\frac{\hbar\kappa}{\sqrt{-2mE}}\right)$. Here we have chosen $\alpha = 1/2$, $\hbar = 2m = 1$, $\kappa = 1$, and $a = 1$. Here the vertical asymptotes correspond to the bound state energies of the initial Hamiltonian H_0 or the point where the continuous spectrum of H_0 begins.

Since ϕ_0 has no node, as mentioned above that the new eigenvalue resulting from the addition of δ interaction at the point a into H_0 must satisfy the subsequent equation

$$\begin{aligned}\frac{1}{\alpha} - G(a,a|E) =& \frac{1}{\alpha} - \frac{1}{\hbar}\left(\frac{m}{-2E}\right)^{1/2} \\ &+ \frac{\kappa}{2\cosh^2(\kappa a)(E+\frac{\hbar^2\kappa^2}{2m})}\left(\frac{\hbar\kappa}{\sqrt{-2mE}}\right) \\ =& 0\ . \end{aligned} \tag{2.1.28}$$

It can be seen from here that G_0 has a simple pole at

$$E = -\frac{\hbar^2\kappa^2}{2m}$$

and it becomes singular around the energy value $E = 0$, where the continuous spectrum of this problem begins. As can be easily understood from the Figure 2.2 that if a is chosen non-zero $a \neq 0$, we will always observe two bound state energies, one above $-\frac{\hbar^2\kappa^2}{2m}$ and one below $-\frac{\hbar^2\kappa^2}{2m}$, as we expected from the analysis above. It is very important to point out the following fact here that the Green function $G_0(a,a|E)$ blows up near its branch point at $E = 0$ where the continuous spectrum begins, which leads

to the existence of two additional bound states when the δ interaction is added to the original problem. However, if we set the value of a to zero $a = 0$, then $G_0(0,0|E)$ vanishes at $E = 0$. This shows us that there is only one root and a single bound state energy below $-\frac{\hbar^2\kappa^2}{2m}$. This is not a typical case, as previously described and illustrated in the Figure 2.1. It is quite possible to explain this case with the following symmetry argument. Initially, let's examine the reflectionless potential system, which has $\mathbb{Z}_2$ symmetry, and a single bound state.with even parity. When we add the δ interaction to this potential, it becomes clear that $\mathbb{Z}_2$ symmetry continues to be preserved if $a = 0$. Then, the excited state is required to have an odd parity since the systems with such symmetries must have a definite symmetry and this distinct symmetry requirement ensures that the excited state is orthogonal to the ground state, which has even parity by the positivity [37]. The fact that the excited state has odd parity means that the wave function associated with this state must vanish at $x = 0$, which eliminates the δ interaction term from the formal Hamiltonian. However, in the case where the initial system H_0 has only one bound state, specifically the ground state, then the modified system influenced by the δ interaction must also have a single bound state energy level when $a = 0$.

When $a \neq 0$,the energies of the bound states can be explicitly calculated and are expressed as follows:

$$E_0^* = -\left(\sqrt{\frac{\hbar^2\kappa^2}{2m} + \frac{m\alpha^2}{8\hbar^2}} + \sqrt{\frac{m\alpha^2}{8\hbar^2}}\right)^2 , \tag{2.1.29}$$

$$E_1^* = -\left(\sqrt{\frac{\hbar^2\kappa^2}{2m} + \frac{m\alpha^2}{8\hbar^2}} - \sqrt{\frac{m\alpha^2}{8\hbar^2}}\right)^2 . \tag{2.1.30}$$

2.1.1. A Different Perspective for the Perturbative Estimates on the Bound State Energies

We are taking a different approach to develop a perturbative approximation for determining the eigenvalues of $H_0 - \alpha\delta$. In the context of standard perturbation theory [33, 38], our approach begins by using the so-called Rayleigh-Schrödinger series

expansion for both the bound state energies and wave functions and subsequently, these expansions are inserted into the Schrödinger equation, and each term of the expansion is solved recursively, which has been discussed more rigorously in [37, 39].

Here, to make things a little clearer and easier we take a more heuristic approach, assuming $\alpha << 1$ and $\phi_k(0) \neq 0$. As discussed earlier, the addition of δ interaction to H_0 is expected to lead to a shift in the new bound state energies. Assuming $E = E_k^* = E_k + \delta E_k$, where E_k denote the bound state energies of H_0 and δE_k represents the change in the bound state energy E_k. Then, the solutions for the new bound state energies E_k^* can be obtained from the following expression:

$$\begin{aligned}
&\frac{1}{\alpha} - \sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{E_n - (E_k + \delta E_k)} - \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - (E_k + \delta E_k)}\, d\mu(\lambda) \\
&= \frac{1}{\alpha} - \sum_{n\neq k} \frac{|\phi_n(0)|^2}{E_n - (E_k + \delta E_k)} + \frac{|\phi_k(0)|^2}{\delta E_k} - \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - (E_k + \delta E_k)}\, d\mu(\lambda) = 0\ . \qquad (2.1.31)
\end{aligned}$$

The given equation, which precisely determines bound state energies, but involves eigenfunctions at $x = 0$. By expanding the terms in the summation and integral using powers of δE_k and subsequently multiplying the equation by $\alpha\, \delta E_k$, we arrive at an expression that shows the fluctuations in the eigenvalues.

$$\begin{aligned}
&\delta E_k - \alpha\, \delta E_k \sum_{n\neq k} \frac{|\phi_n(0)|^2}{E_n - E_k} \left(1 + \frac{\delta E_k}{E_n - E_k} + O(\delta E_k^2)\right) \\
&-\alpha\, \delta E_k \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E_k} \left(1 + \frac{\delta E_k}{\lambda - E_k} + O(\delta E_k^2)\right) d\mu(\lambda) + \alpha|\phi_k(0)|^2 + O(\delta E_k^3) = 0\ . \qquad (2.1.32)
\end{aligned}$$

Suppose δE_k is written as a power series in terms of α, that is, $\delta E_k = E_k^{(1)} + E_k^{(2)} + \cdots$, now if we define $E_k^{(n)}$ as the change in the bound state energy of order α^n. Then, solve $E_k^{(1)}$ and $E_k^{(2)}$ term by term, we obtain two independent equations for $E_k^{(1)}$ and $E_k^{(2)}$ as shown below.

$$E_k^{(1)} = -\alpha|\phi_k(0)|^2\ , \qquad (2.1.33)$$

$$E_k^{(2)} = -\alpha^2|\phi_k(0)|^2 \left(\sum_{n\neq k} \frac{|\phi_n(0)|^2}{E_n - E_k} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E_k} d\mu(\lambda)\right)\ , \qquad (2.1.34)$$

Looking at the above equations it can easily be said that they are consistent with the first and second order formulas in non-degenerate perturbation theory that has discussed in [7, 33], given by

$$E_k^{(1)} = \langle \phi_k, -\alpha\delta\phi_k \rangle \tag{2.1.35}$$

$$E_k^{(2)} = -\sum_{n\neq k} \frac{|\langle \phi_k, -\alpha\delta\phi_n \rangle|^2}{E_n - E_k} - \int_\Lambda \frac{|\langle \chi_\lambda, -\alpha\delta\phi_k \rangle|^2}{\lambda - E_k} d\mu(\lambda) \, . \tag{2.1.36}$$

Here the crucial point to emphasize is our aim to express the solution δE_k for (2.1.32) as the formal power series with respect to α. This choice is made under the assumption that both α and δE_k are sufficiently small, enabling the use of standard perturbation theory [40]. Let's summarize our results with the following paragraph.

Consider ϕ_k as the eigenfunctions corresponding to the eigenvalues E_k of H_0 and let χ_λ denote the generalized eigenfunctions of H_0. When we add δ interaction with the coupling constant $-\alpha$ into H_0, the Equations (2.1.33) and (2.1.34) formally express the changes in bound state energies up to the first and second order in α.

2.1.2. A Different Perspective for the Perturbative Estimates on the Bound State Wave Function

In this section, using the contour integral method, we will try to look at the perturbative estimation of the wave function from a different perspective. First, we can start the solution by defining the projection operator for the case concerned. One can determine the projection operator onto the eigenspace corresponding to a given eigenvalue E_k^* by using a contour integral of the resolvent $R(E) = (H - E)^{-1}$ around each simple eigenvalue E_k^*,

$$\mathbb{P}_k = -\frac{1}{2\pi i} \oint_{\Gamma_k} R(E) \, dE \, , \tag{2.1.37}$$

where Γ_k denotes the closed contour surrounding each simple pole E_k^*, or equivalently

$$\psi_k(x)\overline{\psi_k(y)} = -\frac{1}{2\pi i} \oint_{\Gamma_k} G(x, y|E) \, dE \, . \tag{2.1.38}$$

Starting with the explicit representation of the Green's function (2.1.4) and applying the residue theorem, we can obtain

$$\psi_k(x) = \frac{G_0(x,0|E_k^*)}{\left(\frac{dG_0(0,0|E)}{dE}\Big|_{E=E_k^*}\right)^{1/2}} \,. \tag{2.1.39}$$

When we use the eigenfunction expansion of G_0 under this form of energy $E_k^* = E_k + \delta E_k$, we arrive at the following formula of the wave function

$$\psi_k(x) = \frac{\left(\sum_{n=0}^{\infty} \frac{\phi_n(x)\overline{\phi_n(0)}}{E_n-(E_k+\delta E_k)} + \int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{\lambda-(E_k+\delta E_k)} d\mu(\lambda)\right)}{\left(\sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2}{(E_n-(E_k+\delta E_k))^2} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{(\lambda-(E_k+\delta E_k))^2} d\mu(\lambda)\right)^{1/2}} \,. \tag{2.1.40}$$

By separating the $n = k$ term in both the sums and integrals, and subsequently expanding the above terms in powers of δE_k, then the resulting wave function takes the form as seen below

$$\begin{aligned}
\psi_k(x) =& \left[1 + \frac{\delta E_k^2}{|\phi_k(0)|^2} \sum_{n\neq k} \frac{|\phi_n(0)|^2}{(E_n-E_k)^2} + \frac{\delta E_k^2}{|\phi_k(0)|^2} \int_\Lambda \frac{|\chi_\lambda(0)|^2}{(\lambda-E_k)^2} d\mu(\lambda) + O(\delta E_k^3)\right]^{-1/2} \\
&\times \left(- \frac{\phi_k(x)\overline{\phi_k(0)}}{|\phi_k(0)|} + \left(\sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(0)}}{(E_n-E_k)|\phi_k(0)|} \left(\delta E_k + \frac{\delta E_k^2}{(E_n-E_k)} + O(\delta E_k^3) \right) \right) \right. \\
&\left. + \left(\int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{(\lambda-E_k)|\phi_k(0)|} \left(\delta E_k + \frac{\delta E_k^2}{(\lambda-E_k)} + O(\delta E_k^3) \right) d\mu(\lambda) \right) + O(\delta E_k^3) \,,
\end{aligned} \tag{2.1.41}$$

under the assumption that $|\frac{\delta E_k}{(E_n-E_k)}| < 1$ and $|\frac{\delta E_k}{(\lambda-E_k)}| < 1$ then by considering the terms in δE_k up to the second order, we arrive at the following expressions

$$\begin{aligned}
\psi_k(x) =& \phi_k(x)e^{-i\theta_k+i\pi} + \sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(0)}}{|\phi_k(0)|} \frac{E_k^{(1)}}{E_n-E_k} + \int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{|\phi_k(0)|} \frac{E_k^{(1)}}{\lambda-E_k} d\mu(\lambda) \\
&- \frac{1}{2}\phi_k(x)e^{-i\theta_k+i\pi} \left(\sum_{n\neq k} \frac{|\phi_n(0)|^2}{|\phi_k(0)|)^2} \frac{(E_k^{(1)})^2}{(E_n-E_k)^2} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{|\phi_k(0)|^2} \frac{(E_k^{(1)})^2}{(\lambda-E_k)^2} d\mu(\lambda) \right) \\
&+ \sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(0)}}{(E_n-E_k)|\phi_k(0)|} \left(E_k^{(2)} + \frac{(E_k^{(1)})^2}{(E_n-E_k)} \right) \\
&+ \left(\int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{(\lambda-E_k)|\phi_k(0)|} \left(E_k^{(2)} + \frac{(E_k^{(1)})^2}{(\lambda-E_k)} \right) d\mu(\lambda) \right) + O(\delta E_k^3) \,,
\end{aligned} \tag{2.1.42}$$

given that $\phi_k(0) = |\phi_k(0)|e^{i\theta_k}$, we obtain the corresponding bound state wave functions for each order by using the first order and second order results, as expressed in (2.1.35) and (2.1.36) for the bound state energies,

$$\psi_k^{(0)}(x) = e^{-i\theta_k + i\pi}\phi_k(x) \tag{2.1.43}$$

$$\begin{aligned}\psi_k^{(1)}(x) =& \alpha\ \phi_k(0)e^{-i\theta_k+i\pi}\sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(0)}}{E_n - E_k} \\ &+ \alpha\ \phi_k(0)e^{-i\theta_k+i\pi}\int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{\lambda - E_k}d\mu(\lambda)\end{aligned} \tag{2.1.44}$$

$$\begin{aligned}\psi_k^{(2)}(x) =& -\frac{\alpha^2}{2}\phi_k(x)e^{-i\theta_k+i\pi}|\phi_k(0)|^2\left(\sum_{n\neq k}\frac{|\phi_n(0)|^2}{(E_n - E_k)^2} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{(\lambda - E_k)^2}d\mu(\lambda)\right) \\ &+ \alpha^2\phi_k(0)e^{-i\theta_k+i\pi}\sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(0)}}{(E_n - E_k)} \\ &\left(\sum_{m\neq k}\frac{|\phi_m(0)|^2}{E_m - E_k} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{\lambda - E_k}d\mu(\lambda) - \frac{|\phi_k(0)|^2}{(E_n - E_k)}\right) \\ &+ \alpha^2\phi_k(0)e^{-i\theta_k+i\pi}\int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{(\lambda - E_k)} \\ &\left(\sum_{m\neq k}\frac{|\phi_m(0)|^2}{E_m - E_k} + \int_\Lambda \frac{|\chi_{\lambda'}(0)|^2}{\lambda' - E_k}d\mu(\lambda') - \frac{|\phi_k(0)|^2}{\lambda - E_k}\right)d\mu(\lambda)\ .\end{aligned} \tag{2.1.45}$$

Following the results of standard regular perturbation theory, the normalized wave functions for bound states, expanded up to second order in the parameter α, can be expressed as:

$$\psi_k^{(0)}(x) = \phi_k(x) \tag{2.1.46}$$

$$\begin{aligned}\psi_k^{(1)}(x) =& \sum_{n\neq k}\frac{\langle\phi_n, -\alpha\delta\phi_k\rangle}{E_k - E_n}\phi_n(x) \\ &+ \int_\Lambda \frac{\langle\chi_\lambda, -\alpha\delta\phi_k\rangle}{\lambda - E_k}\chi_\lambda(x)d\mu(\lambda)\end{aligned} \tag{2.1.47}$$

$$\psi_k^{(2)}(x) = \sum_{n\neq k}\sum_{m\neq k}\frac{\langle\phi_n,-\alpha\delta\phi_m\rangle\langle\phi_m,-\alpha\delta\phi_k\rangle}{(E_k-E_n)(E_k-E_m)}\phi_n(x) - \sum_{n\neq k}\frac{\langle\phi_n,-\alpha\delta\phi_k\rangle\langle\phi_k,-\alpha\delta\phi_k\rangle}{(E_k-E_n)^2}\phi_n(x)$$
$$- \frac{1}{2}\sum_{n\neq k}\frac{\langle\phi_k,-\alpha\delta\phi_n\rangle\langle\phi_n,-\alpha\delta\phi_k\rangle}{(E_k-E_n)^2}\phi_k(x)$$
$$+ \int_\Lambda\left(\sum_{n\neq k}\frac{\langle\phi_n,-\alpha\delta\chi_\lambda\rangle\langle\chi_\lambda,-\alpha\delta\phi_k\rangle}{(E_k-E_n)(E_k-\lambda)}\phi_n(x)\right)d\mu(\lambda)$$
$$+ \int_\Lambda\left(\sum_{m\neq k}\frac{\langle\chi_\lambda,-\alpha\delta\phi_m\rangle\langle\phi_m,-\alpha\delta\phi_k\rangle}{(E_k-E_m)(E_k-\lambda)}\chi_\lambda(x)\right)d\mu(\lambda)$$
$$+ \int_\Lambda\left(\int_\Lambda\frac{\langle\chi_\lambda,-\alpha\delta\chi_{\lambda'}\rangle\langle\chi_{\lambda'},-\alpha\delta\phi_k\rangle}{(E_k-\lambda)(E_k-\lambda')}\chi_\lambda(x)d\mu(\lambda')\right)d\mu(\lambda)$$
$$- \int_\Lambda\frac{\langle\chi_\lambda,-\alpha\delta\phi_k\rangle\langle\phi_k,-\alpha\delta\phi_k\rangle}{(E_k-\lambda)^2}d\mu(\lambda)\ \chi_\lambda(x)$$
$$- \frac{1}{2}\int_\Lambda\frac{\langle\phi_k,-\alpha\delta\chi_\lambda\rangle\langle\chi_\lambda,-\alpha\delta\phi_k\rangle}{(E_k-\lambda)^2}d\mu(\lambda)\ \phi_k(x)\ . \tag{2.1.48}$$

What we have found above seems completely consistent with our results up to a phase factor $e^{-i\theta_k+i\pi}$. It's important to note that although the second-order perturbation result for the normalized wave function only in discrete cases has been discussed in [41], our results clearly show us that it can be generalized.

If we want to briefly summarize what we have done so far: The wave functions $\psi_k(x)$, associated with the bound states of the Hamiltonian H_0 modified by the δ interaction are expressed in the Equation (2.1.39). These wave functions are associated with the bound state energies E_k^*, which satisfy the equation $\frac{1}{\alpha} - G_0(0,0|E) = 0$. Expanding the bound state wave function $\psi_k(x)$ in terms of the coupling constants α up to second order brings us to the following Equations (2.1.43), (2.1.44), and (2.1.45).

2.2. Singular Modifications by δ Interactions

In this section, we will consider δ interaction cases in higher dimensions. Under the condition of the co-dimension, which means equi-dimensionality, let's examine the case where the dimensions of the space and the dimension of the support of the δ interaction are greater then one for example, point δ interaction in two and three

dimensions, or δ interaction supported by a curve in three dimensions, it is necessary to define δ interaction using a renormalization procedure. We can explain the reason for this mainly by the fact that the Green's function associated with the free Hamiltonians H_0 has the singularity in both two and three dimensions. The historical background of this subject is quite extensive and there is a lot of material available in the physics literature, see e.g., [24, 26–28, 81]. The mathematical aspects of this subject have been thoroughly explored in classic monographs such as [22, 23] and more recent perspective is presented in the work [35]. In this context, we now consider the Schrödinger operators H_0 under the same assumption mentioned earlier and our primary aim is to analyze how the spectrum of H_0 is affected by the addition of the δ interactions.

We mentioned that Green's function G_0 has a singularity in higher dimensions. Therefore, when working at high dimensions it can be highly advantageous for us to express the Green's function G_0 in terms of the heat kernel $K_t(x, y)$ associated with the operator $H_0 = -\frac{\hbar^2}{2m}\Delta + V$, given by

$$G_0(x, y|E) = \int_0^\infty K_t(x, y)e^{tE}dt \ , \tag{2.2.1}$$

in regions where the real part of the energy $\mathrm{Re}(E) < 0$ and the Hamiltonian H_0 must satısfy the following equation $H_0K_t(x, y) = \frac{\partial}{\partial t}K_t(x, y)$. This definition extends to other values of E in the complex E plane through analytical continuation. It's important to note that the first term in the short time asymptotic expansion of the diagonal heat kernel associated with any self-adjoint elliptic second order differential operator, as discussed in [42] in d dimensions, is given as follows,

$$K_t(x, x) \sim t^{-d/2} \ . \tag{2.2.2}$$

From the above equation, in higher dimensions it is evident that the condition where the heat kernel $K_t(x, x)$ is diagonal, leads to a divergence near $t = 0$ in the diagonal part $G_0(x, x|E)$:

$$\int_0^\infty \frac{e^{-t|E|}}{t^{d/2}} \ dt \ , \tag{2.2.3}$$

for $d = 2, 3$. In order to make sense of such singular interactions, it is necessary to

introduce a cut-off parameter, denoted as $\epsilon > 0$ and subsequently proceed to regularize the Hamiltonian. One way to achieve this is to replace the δ interaction with the heat kernel $K_{\epsilon/2}(x, 0)$. As $\epsilon \to 0$, the heat kernel converges distributionally to the δ function. Then, we parameterize the coupling constant α depending on the cut-off, ensuring the regularized Hamiltonian convergences to a non-trivial limit in the norm resolvent sense as the cut-off is removed. A natural choice for this coupling constant can be described as follows

$$\frac{1}{\alpha(\epsilon)} = \frac{1}{\alpha_R(M)} + \int_{\epsilon}^{\infty} K_t(0,0)e^{tM}dt \ , \tag{2.2.4}$$

where M is defined as the renormalization scale and one can remove it in favor of a physical parameter by imposing the renormalization condition. For instance, it would be correct to claim that both M, and by extension α_R, are related to the ground state energy of the particle, which is affected by the addition of δ interaction to H_0, say $-\mu^2$ this requirement, in general, leads to a flow in the space of coupling constants α_R [43]. The most advantageous decision would be to set $\frac{1}{\alpha_R} = 0$ while demanding $M = -\mu^2$, as it provides a more convenient way to perform the bound state calculations. For our purposes, we make use of α_R and additionally set $M = -\mu^2$, considering a bound state below E_0 to ensure the clarity of our notation. In order to facilitate understanding of this subject. Now we will give you a more detailed and clear discussion on the single parameter dependence of the model.

Let's try to explain the single parameter dependency for the Renormalized Theory that we have mentioned above a little more here.

It is worth noting that although it appears to accommodate two parameters α_R and μ^2, the renormalized theory actually exhibits a single-parameter dependence in our equations. it's a well-known concept from the theory of self-adjoint extensions, we aim to explicitly confirm that the zeros of $\Phi(E)$ remain unchanged, even under the consideration of a specific dependence between α_R and μ^2. Consider a compact two-dimensional manifold. We aim to maintain the invariance of the function $\Phi(E)$ when we modify μ^2 by adjusting α_R accordingly. Moreover, by ensuring that the zeros

of Φ do not change despite changes in μ^2, we observe that, as a meromorphic function with a fixed pole structure, Φ stays invariant. This will lead to a differential equation;

$$\mu\frac{\partial}{\partial\mu}\frac{1}{\alpha_R} = 2\mu^2\sum_{n=0}^{\infty}\frac{|\phi_n(a)|^2}{(E_n-E)(E_n+\mu^2)} - (E+\mu^2)\sum_{n=0}^{\infty}\frac{2\mu^2|\phi_n(a)|^2}{(E_n-E)(E_n+\mu^2)^2} \quad (2.2.5)$$

$$= 2\mu^2\sum_{n=0}^{\infty}\frac{|\phi_n(a)|^2}{(E_n+\mu^2)^2} = 2\mu^2\int_0^{\infty} dt\; t\; K_t(a,a)e^{-\mu^2 t} \quad (2.2.6)$$

This explicitly demonstrates the independence of the left-hand side from E and its explicit functional relationship with μ^2, facilitating the integration to derive α_R as a function of μ. This representation resembles a form of flow equation. Interestingly, a similar flow equation for the beta function has previously discussed in [59] for a restricted region of E values. Likewise, our relativistic model depends on a single parameter, which can be adjusted in accordance with the flux of α_R. If we were to perform the computation:

$$\frac{\partial}{\partial\mu}\frac{1}{\alpha_R} = \sum_{n=0}^{\infty}\frac{|f_n(a)|^2}{\omega_n(\omega_n+\mu)^2}. \quad (2.2.7)$$

The expression on the right gives a positive finite quantity and indicates a similar flow expression, which illustrates single parameter dependence of the theory. One can establish its correlation with the heat kernel using the method provided at the end of the Section 2.3.4.

Then, we go back to the problem and take the formal limit as $\epsilon \to 0$. This leads us to the following expression for the integral kernel of the resolvent or Green's function,

$$G(x,y|E) = G_0(x,y|E) + \frac{G_0(x,0|E)G_0(0,y|E)}{\frac{1}{\alpha_R} - \sum_{n=0}^{\infty}\frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)} - \int_\Lambda \frac{|\chi_\lambda(0)|^2(E+\mu^2)}{(\lambda+\mu^2)(\lambda-E)}\,d\mu(\lambda)}\,. \quad (2.2.8)$$

We can clearly see that this has exactly the same form as the Krein's formula given by (2.1.4), where the form of the function Φ is expressed as follows:

$$\begin{aligned}\Phi(E) &= \frac{1}{\alpha_R} + \int_0^{\infty} K_t(0,0)\left(e^{-t\mu^2} - e^{tE}\right)\,dt \\ &= \frac{1}{\alpha_R} - \sum_{n=0}^{\infty}\frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)} - \int_\Lambda \frac{|\chi_\lambda(0)|^2(E+\mu^2)}{(\lambda+\mu^2)(\lambda-E)}\,d\mu(\lambda)\,. \quad (2.2.9)\end{aligned}$$

Here we have used the eigenfunction expansion of the heat kernel. The work presented by [29] extensively examines specific cases within the context of path integrals, focusing particularly on two or three dimension. However, it is important to note that this study does not include explicit derivation, showing that the cancellation of the poles of the free resolvent in the final expression.

Continuing the same logical progression as in the one-dimensional case, we can now explicitly show the disappearance of the poles in the Hamiltonian H_0 with the addition δ interaction. This holds true under the same assumptions about the spectrum of H_0 as those considered in the one-dimensional case.

To make our arguments simpler and more understandable, let's assume a fully discrete spectrum, the generalization to include a continuum with generalized eigenfunctions is a straightforward step in our analysis. We once more separate the term within the eigenfunction expansion of the Green's function related to the isolated single eigenvalue E_k of H_0:

$$\begin{aligned} G(x,y|E) = &\sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(y)}}{E_n - E} + \frac{\phi_k(x)\overline{\phi_k(y)}}{E_k - E} \\ &+ \frac{\left(\sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(0)}}{E_n - E}\right)\left(\sum_{n\neq k} \frac{\phi_n(0)\overline{\phi_n(y)}}{E_n - E}\right)}{\frac{1}{\alpha_R} - \sum_{n\neq k} \frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)} - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k-E)(E_k+\mu^2)}} \\ &+ \frac{\left(\sum_{n\neq k} \frac{\phi_n(x)\overline{\phi_n(0)}}{E_n - E}\right)\left(\frac{\phi_k(0)\overline{\phi_k(y)}}{E_k - E}\right)}{\frac{1}{\alpha_R} - \sum_{n\neq k} \frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)} - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k-E)(E_k+\mu^2)}} \\ &+ \frac{\left(\frac{\phi_k(x)\overline{\phi_k(0)}}{E_k - E}\right)\left(\sum_{n\neq k} \frac{\phi_n(0)\overline{\phi_n(y)}}{E_n - E}\right)}{\frac{1}{\alpha_R} - \sum_{n\neq k} \frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)} - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k-E)(E_k+\mu^2)}} \\ &+ \frac{\left(\frac{\phi_k(x)\overline{\phi_k(0)}}{E_k - E}\right)\left(\frac{\phi_k(0)\overline{\phi_k(y)}}{E_k - E}\right)}{\frac{1}{\alpha_R} - \sum_{n\neq k} \frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)} - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k-E)(E_k+\mu^2)}} \,. \end{aligned} \tag{2.2.10}$$

If we combine the second and the last term in the above expression, we obtain

$$G(x,y|E) = \frac{\phi_k(x)\overline{\phi_k(y)}}{E_k - E}\left(1 - \left(1 - \frac{(E_k-E)}{|\phi_k(0)|^2}\left(\frac{1}{\alpha_R} - \sum_{n\neq k}\frac{|\phi_n(0)|^2}{E_n - E} + \frac{|\phi_k(0)|^2}{E_k+\mu^2}\right)\right)^{-1}\right)$$
$$+ \sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(y)}}{E_n - E} + (E_k - E)\frac{\left(\sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(0)}}{E_n-E}\right)\left(\sum_{n\neq k}\frac{\phi_n(0)\overline{\phi_n(y)}}{E_n-E}\right)}{(E_k-E)\left(\frac{1}{\alpha_R} - \sum_{n\neq k}\frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)}\right) - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k+\mu^2)}}$$
$$+ \frac{\left(\sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(0)}}{E_n-E}\right)\left(\phi_k(0)\overline{\phi_k(y)}\right)}{(E_k-E)\left(\frac{1}{\alpha_R} - \sum_{n\neq k}\frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)}\right) - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k-E)(E_k+\mu^2)}}$$
$$+ \frac{\left(\phi_k(x)\overline{\phi_k(0)}\right)\left(\sum_{n\neq k}\frac{\phi_n(0)\overline{\phi_n(y)}}{E_n-E}\right)}{(E_k-E)\left(\frac{1}{\alpha_R} - \sum_{n\neq k}\frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)}\right) - \frac{|\phi_k(0)|^2(E+\mu^2)}{(E_k+\mu^2)}}\,. \tag{2.2.11}$$

It is very clear that except the first term, all subsequent terms show regular behavior near $E = E_k$. For the first term, if we choose E sufficiently close to E_k, i.e., if $\frac{|E_k-E|}{|\phi_k(0)|^2}\left|\frac{1}{\alpha_R} - \sum_{n\neq k}\frac{|\phi_n(0)|^2}{E_n-E} + \frac{|\phi_k(0)|^2}{E_k+\mu^2}\right| < 1$, under the assumptions we mentioned, the first term of the above equation becomes:

$$-\frac{\phi_k(x)\overline{\phi_k(y)}}{|\phi_k(0)|^2}\left(\frac{1}{\alpha_R} - \sum_{n\neq k}\frac{|\phi_n(0)|^2}{E_n - E} + \frac{|\phi_k(0)|^2}{E_k+\mu^2}\right) + O(|E_k - E|^2) \tag{2.2.12}$$

so that $G(x,y|E)$ is regular near $E = E_k$ as long as $\phi_k(0) \neq 0$. Assuming the presence of a continuous spectrum, this part of the spectrum remains unchanged, following the same logic as previously mentioned.

Consider the wave function $\phi_k(x)$ corresponding to a bound state with energy E_k for the unperturbed Hamiltonian H_0. When H_0 is perturbed by attractive δ interactions, the resulting modified bound state energies E_k^* is obtained by solving the equation:

$$\frac{1}{\alpha_R} - \sum_{n=0}^{\infty}\frac{|\phi_n(0)|^2(E+\mu^2)}{(E_n - E)(E_n+\mu^2)} - \int_\Lambda \frac{|\chi_\lambda(0)|^2(E+\mu^2)}{(\lambda - E)(\lambda+\mu^2)}\,d\mu(\lambda) = 0\,, \tag{2.2.13}$$

if $\phi_k(0) \neq 0$ for some this particular k. In the case where $\phi_k(0) = 0$ for the given value of k the bound state energies stay the same, $E_k^* = E_k$. Additionally, it's crucial to emphasize that the continuous spectrum of the Hamiltonian, when subjected to the δ interaction, stays the same as that of H_0.

In the renormalized case, the interlacing of the energy eigenvalues is exactly the same as observed in the case, where renormalization is not necessary, and if $\alpha_R < 0$, then it leads to a further downward shift in all the bound state energies. This result may sometimes not be obvious. Additionally, when $\alpha_R \to 0^-$ it is considered an infinitely strong coupling case, making $\frac{1}{\alpha_R}$ the true coupling constant. This interpretation arises from the behavior of the Green's function, which increases with energy E and as $E \to -\infty$, the renormalized sum goes to $-\infty$ as well. Allowing $E \to -\infty$ guarantees the existence of a solution below $-\mu^2$, where the sum converges to zero. The results mentioned above will be conclusively demonstrated for a manifold at the end of the Section 2.3.4.

Note that these findings can be viewed as a generalization of the well-known Sturm comparison theorems to cases involving singular δ interactions, It is noteworthy that e the same property holds true even in the renormalized case.

Continuing our discussion along the same logical line as in the regular problem, we now construct a perturbative approximation for the eigenvalues of H_0 by introducing the singular δ interaction. We make the assumption that $\alpha_R << 1$. Let $E = E_k^* = E_k + \delta E_k$, where E_k represent the bound the bound state energies of H_0. The poles of the Green's function $G(x, y|E)$ are then obtained by solving the following equation:

$$\begin{aligned}
&\frac{1}{\alpha_R} - \sum_{n=0}^{\infty} \frac{|\phi_n(0)|^2(E_k + \delta E_k + \mu^2)}{(E_n + \mu^2)(E_n - (E_k + \delta E_k))} \\
&- \int_\Lambda \frac{|\chi_\lambda(0)|^2(E_k + \delta E_k + \mu^2)}{(\lambda + \mu^2)(\lambda - (E_k + \delta E_k))}\, d\mu(\lambda) \\
&= \frac{1}{\alpha_R} - \sum_{n \neq k} \frac{|\phi_n(0)|^2(E_k + \delta E_k + \mu^2)}{(E_n + \mu^2)(E_n - (E_k + \delta E_k))} + \frac{|\phi_k(0)|^2(E_k + \delta E_k + \mu^2)}{(E_k + \mu^2)(\delta E_k)} \\
&- \int_\Lambda \frac{|\chi_\lambda(0)|^2(E_k + \delta E_k + \mu^2)}{(\lambda + \mu^2)(\lambda - (E_k + \delta E_k))}\, d\mu(\lambda) = 0\ . \qquad (2.2.14)
\end{aligned}$$

Expanding the given expressions in the powers of δE_k and subsequently multiplying

the equation by the product of $\alpha_R \delta E_k$, the resulting expression is as follows

$$\begin{aligned}
&\delta E_k + \alpha_R |\phi_k(0)|^2 + \frac{\alpha_R |\phi_k(0)|^2}{E_k + \mu^2} \delta E_k - \alpha_R \delta E_k \sum_{n \neq k} \frac{|\phi_n(0)|^2 (E_k + \mu^2)}{(E_n - E_k)(E_n + \mu^2)} \\
&\times \left(1 + \frac{\delta E_k}{E_n - E_k} + O(\delta E_k^2) \right) \\
&- \alpha_R \delta E_k \sum_{n \neq k} \frac{|\phi_n(0)|^2 \delta E_k}{(E_n - E_k)(E_n + \mu^2)} \left(1 + \frac{\delta E_k}{E_n - E_k} + O(\delta E_k^2) \right) \\
&- \alpha_R \delta E_k \int_\Lambda \frac{|\chi_\lambda(0)|^2 (E_k + \mu^2)}{(\lambda - E_k)(\lambda + \mu^2)} \left(1 + \frac{\delta E_k}{\lambda - E_k} + O(\delta E_k^2) \right) \, d\mu(\lambda) \\
&- \alpha_R \delta E_k \int_\Lambda \frac{|\chi_\lambda(0)|^2 \delta E_k}{(\lambda - E_k)(\lambda + \mu^2)} \left(1 + \frac{\delta E_k}{\lambda - E_k} + O(\delta E_k^2) \right) \, d\mu(\lambda) + O(\delta E_k^3) = 0 \, .
\end{aligned} \tag{2.2.15}$$

Suppose we can express δE_k as a power series in terms of the parameter α_R, that is, $\delta E_k = E_k^{(1)} + E_k^{(2)} + \cdots$. In this expansion, each term $E_k^{(n)}$ represents the change in the bound state energy of order α_R^n. When we solve the equation systematically term by term, we can obtain the following results for $E_k^{(1)}$ and $E_k^{(2)}$

$$E_k^{(1)} = - \alpha_R |\phi_k(0)|^2 \, , \tag{2.2.16}$$

$$\begin{aligned}
E_k^{(2)} = \alpha_R^2 |\phi_k(0)|^2 \Bigg(&\frac{|\phi_k(0)|^2}{E_k + \mu^2} - \sum_{n \neq k} \frac{|\phi_n(0)|^2 (E_k + \mu^2)}{(E_n - E_k)(E_n + \mu^2)} \\
&- \int_\Lambda \frac{|\chi_\lambda(0)|^2 (E_k + \mu^2)}{(\lambda - E_k)(\lambda + \mu^2)} d\mu(\lambda) \Bigg) \, .
\end{aligned} \tag{2.2.17}$$

It is crucial to emphasize that the equations we found regarding first- and second-order perturbed energy changes tell us this: There is no change in the first order result of the bound state energy compared to the case where renormalization is not necessary, except for the replacement of α with the renormalized coupling constant α_R. However, as can be seen, the bound state energy obtained from the second-order result is completely different from the case where the renormalization is not required.

When examining the wave function, we formally obtain the same formula with the perturbative perspective on the bound state wave function, which is in Equation (2.1.42) for the expansion of the wave function in terms of the contribution coming to the bound state energy, i.e. in terms of δE_k. By substituting the previously stated

results for the first and second-order eigenvalues, we arrive at the following formula:

$$\psi_k^{(0)}(x) = e^{-i\theta_k + i\pi}\phi_k(x) \ , \tag{2.2.18}$$

$$\psi_k^{(1)}(x) = \alpha_R \phi_k(0) e^{-i\theta_k + i\pi}\left(\sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(0)}}{E_n - E_k} + \int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{\lambda - E_k}d\mu(\lambda)\right) \ , \tag{2.2.19}$$

and

$$\begin{aligned}\psi_k^{(2)}(x) = &-\frac{\alpha_R^2}{2}\phi_k(x)e^{-i\theta_k+i\pi}|\phi_k(0)|^2\left(\sum_{n\neq k}\frac{|\phi_n(0)|^2}{(E_n-E_k)^2} + \int_\Lambda \frac{|\chi_\lambda(0)|^2}{(\lambda-E_k)^2}d\mu(\lambda)\right)\\
&+\alpha_R^2\sum_{n\neq k}\frac{\phi_n(x)\overline{\phi_n(0)}}{(E_n-E_k)}\phi_k(0)e^{-i\theta_k+i\pi}\left[\sum_{m\neq k}\frac{|\phi_m(0)|^2(E_k+\mu^2)}{(E_m-E_k)(E_m+\mu^2)}\right.\\
&\left.+\int_\Lambda \frac{|\chi_\lambda(0)|^2(E_k+\mu^2)}{(\lambda-E_k)(\lambda+\mu^2)}d\mu(\lambda) - \frac{|\phi_k(0)|^2(E_n+\mu^2)}{(E_n-E_k)(E_k+\mu^2)}\right]\\
&+\alpha_R^2\int_\Lambda \frac{\chi_\lambda(x)\overline{\chi_\lambda(0)}}{(\lambda-E_k)}\phi_k(0)e^{-i\theta_k+i\pi}\left[\sum_{m\neq k}\frac{|\phi_m(0)|^2}{E_m-E_k} + \int_\Lambda \frac{|\chi_{\lambda'}(0)|^2}{\lambda'-E_k}d\mu(\lambda')\right.\\
&\left.-\frac{|\phi_k(0)|^2(\lambda+\mu^2)}{(\lambda-E_k)(E_k+\mu^2)}\right]d\mu(\lambda) \ .\end{aligned} \tag{2.2.20}$$

It is important to note that We observe that the results of perturbation theory for the renormalized problem can be derived using a method influenced by field theory. To simplify the discussion, let's consider a Hamiltonian H_0 characterized by a purely discrete spectrum, such as a free particle moving on a manifold or a harmonic oscillator subject to perturbation by the addition of a delta interaction. This approach is applicable to the other cases discussed in this thesis in a similar way.

We add a cut-off for the eigenvalues of H_0, denoted as N and define $\delta_N(x,a)$ as the regularization function for our delta interaction on a manifold. Here

$$\delta_N(x,a) = \sum_n e^{-n/N}\overline{\phi_n(x)}\phi_n(a) \ . \tag{2.2.21}$$

It turns out that as $N \to \infty$ we can clearly see that $\delta_N(x,a)$ converges to $\delta(x,a)$ in the weak sense. Let us define

$$\frac{1}{\alpha} = \frac{1}{\alpha_R} + G_0(a,a|-\mu^2;N) \ , \tag{2.2.22}$$

where

$$G_0(a,a|-\mu^2;N)=\sum_n \frac{e^{-n/N}|\phi_n(a)|^2}{E_n+\mu^2}\ , \tag{2.2.23}$$

or equivalently,

$$\alpha=\frac{\alpha_R}{1+\alpha_R G_0(a,a|-\mu^2;N)}\ . \tag{2.2.24}$$

Now, in the usual perturbative approach, we consider α_R as a formal parameter, that can be taken to be arbitrarily small. This allows us to systematically organize our expansions by ordering terms according to powers of f α_R and formally expand, which gives

$$\alpha=\alpha_R-\alpha_R^2 G_0(a,a|-\mu^2;N)+O(\alpha_R^3)\ . \tag{2.2.25}$$

The formal δ-interaction term in the Hamiltonian now fives us the following equation,

$$-\left[\alpha_R-\alpha_R^2 G_0(a,a|-\mu^2;N)+O(\alpha_R^3)\right]\delta_N(x,a)\ . \tag{2.2.26}$$

Therefore, in a standard perturbative expansion organized by the powers of α_R, mixed terms will appear, because the interaction term is now formulated as a series involving the small parameter α_R.

We can consider α_R to be significantly smaller than any other quantity in a way that allows us to employ analytic continuation arguments. This enables us to take the limit as $N\to\infty$ while keeping the formulae intact. First order perturbation now keeps only the first term of the interaction,

$$E^{(1)}_{N;k}=-\alpha_R\int_{\mathbb{R}^d} d^dx\ \overline{\phi_k(x)}\delta_N(x,a)\phi_k(x)\ , \tag{2.2.27}$$

where $d=2$ or $d=3$. The limit $N\to\infty$ reproduces the answer (2.2.16). The second-order term consists of two parts, the first one, originating from interaction, is treated as a first-order term due to its dependence on α_R^2 and then the leading term of the

second order:

$$E_k^{(2)} = \alpha_R^2 \sum_{m\neq k} \frac{\int_{\mathbb{R}^d} d^d x \overline{\phi_k(x)}\delta_N(x,a)\phi_m(x) \int_{\mathbb{R}^d} d^d x' \overline{\phi_m(x')}\delta_N(x',a)\phi_k(x')}{E_k - E_m}$$
$$+ \alpha_R^2 \sum_m \frac{e^{-m/N}|\phi_m(a)|^2}{E_m+\mu^2} \int_{\mathbb{R}^d} d^d x\ \overline{\phi_k(x)}\delta_N(x,a)\phi_k(x)\ . \tag{2.2.28}$$

As $N \to \infty$ if we ignore the convergence issues, we observe that

$$\begin{aligned} E_k^{(2)} &= \alpha_R^2 \sum_{m\neq k} \frac{\overline{\phi_k(a)}\phi_m(a)\overline{\phi_m(a)}\phi_k(a)}{E_k - E_m} + \alpha_R^2 \sum_m \frac{|\phi_m(a)|^2}{E_m+\mu^2}\overline{\phi_k(a)}\phi_k(a) \\ &= \alpha_R^2\Big(|\phi_k(a)|^2(E_k+\mu^2)\sum_{m\neq k}\frac{|\phi_m(a)|^2}{(E_k-E_m)(E_m+\mu^2)} + \frac{|\phi_k(a)|^2|\phi_k(a)|^2}{E_k+\mu^2}\Big), \end{aligned}$$

where the last term of the above equation is obtained by isolating the $m = k$ term from the expression $G_N(a, a|-\mu^2)$. So the direct approach we developed essentially forms a sound basis for the cancellations and expansions associated with regularized perturbation theory.

2.3. Possible Generalizations

2.3.1. N Center Case

We can extend our approach to the case of N point-like δ interactions. In situations where renormalization is not required, we will assume that all couplings are positive, indicating an attractive case. Let's enumerate these points as $a_1, a_2, ..., a_N$ with $a_i \neq a_j$ whenever $i \neq j$ and the associated couplings with $\alpha_1, \alpha_2, ...\alpha_N$. Continuing recursively, let's assume that that H_0 has the same spectral properties detailed in Section 2.1. In the case where $\phi_k(a_1) \neq 0$ for some set of eigenfunctions then, they cause a shift in the corresponding eigenvalue to a new value E_k^{*1} located between E_{k-1} and E_k. Consequently, the eigenfunctions change to $\mathcal{N}_0 G_0(x, a_1|E_k^{*1})$ where $\mathcal{N}_0$ is the normalization constant. So, we have a new Hamiltonian H_1, which has a new set of discrete states represented by $\phi_k^{(1)}$. and additionally, there is the possibility of a new set of continuum states, that we do not try to calculate. Now let's try to expand the problem by adding a new delta interaction to the system that already has a single

delta interaction. When we introduce the δ interaction at a point a_2, the same process repeats, and new eigenvalues $E_k^{*_2}$ corresponding to $\phi_k^{(1)}(a_2) \neq 0$ fall between $E_{k-1}^{*_1}$ and $E_k^{*_1}$. The poles associated with the old eigenvalues are removed, and there are new wave functions given by $\mathcal{N}_1 G_1(x, a_2|E_k^{*_2})$. Proceeding with a recursive approach, we can define $H_N = H_{N-1} - \alpha_N \delta(x, a_N)$, allowing us to determine the Green's function according to [44, 45]

$$G_N(x, y|E) = G_{N-1}(x, y|E) + G_{N-1}(x, a_N|E)\Phi^{-1}(E)G_{N-1}(a_N, y|E), \tag{2.3.1}$$

with $\Phi(E) = \frac{1}{\alpha_N} - G_{N-1}(a_N, a_N|E)$. Using this recursive argument, it can be concluded that the new eigenvalues $E_k^{*_N}$ fall between the eigenvalues $E_{k-1}^{*_{N-1}}$ and $E_k^{*_{N-1}}$. The resulting eigenfunction $\phi_k^{(N)}(x)$ is given by $\mathcal{N}_{N-1} G_{N-1}(x, a_N|E_k^{*_N})$, note that $G_{N-1}(x, a_N|E_k^{*_N}) = G_0(x, a_N|E_k^{*_N}) + \sum_{i,j=1}^{N-1} G_0(x, a_i|E_k^{*_N})\Phi_{ij}^{-1}(E_k^{*_N})G_0(a_j, a_N|E_k^{*_N})$, where $\Phi_{ij}(E) = \frac{1}{\alpha_i}\delta_{ij} - G_0(a_i, a_j|E)$ is the matrix formed by the point centers $a_1, ...a_{N-1}$.

By the way, the preceding derivation does not rely on the finiteness of the matrix Φ. Even if the matrix $\Phi(E)$ needs renormalization, our derivation remains valid.

2.3.2. δ Interaction Supported on Curves in Plane

Take into account that none of the derivations rely on interactions localized at a particular point. We can easily extend our analysis to include cases where the interaction is distributed along a curve. Continuing from the previous discussion, we can easily accommodate situations involving multiple non-intersecting curves and points. To simplify the discussion, let's concentrate initially on a single rectifiable curve, denoted as Γ in the plane. We make the assumption that the spectrum of the operator H_0 is only discrete.

The Hamiltonian mentioned above can be mathematically defined in different ways. One of these ways is to interpret the above formal interaction by using the

quadratic form

$$\int_{\mathbb{R}^2} |\nabla\psi|^2 d^2x - \alpha \int_\Gamma |\psi|^2 ds \ , \tag{2.3.2}$$

in the case where H_0 is the Laplacian. Then, it can be demonstrated that there exists a self-adjoint Hamiltonian associated with this quadratic form. [46–48]. Another possible way is to impose conditions that guarantee both continuity and jump discontinuity in the normal derivatives on the curve Γ. Γ in [46] and [49]). Other strategies include the use of scaled potentials, as presented in the research [50], or the direct construction of the resolvent operator, as discussed in the works of [46, 51]. The examination of such Hamiltonians is motivated by the intention to create a practical model that accurately represents the behavior of trapped electrons at interfaces between two distinct semiconductor materials. These interfaces are commonly known as leaky graphs, curves, or surfaces in the literature, as outlined in [52].

In this section, we examine rank-one modifications (perturbations) to H_0 following the principles described in [23] and the formal expression for the Hamiltonian is presented as

$$H_0 - \alpha|\Gamma\rangle\langle\Gamma| \ , \tag{2.3.3}$$

where $H_0 = -\frac{\hbar^2}{2m}\Delta + V$ and we have used Dirac notation to express inner products, and the Dirac delta function δ_Γ supported by the curve Γ with length L is defined by their action on test functions ψ as discussed in the reference [4]

$$\langle\delta_\Gamma|\psi\rangle = \langle\Gamma|\psi\rangle \quad := \quad \frac{1}{L(\Gamma)} \int_\Gamma \psi \ ds \ , \tag{2.3.4}$$

where ds is the integration element over the curve Γ and $|\Gamma\rangle\langle\Gamma|$ written in Dirac's bra-ket notation is $\langle\delta_\Gamma, \cdot\rangle\delta_\Gamma$.

In the field of theoretical physics, it is well known that the resolvent of free Hamiltonians, subject to modification by a δ interaction supported along a curve, can be explicitly expressed using formulas commonly known as Krein's formulas [22, 23, 52]. The resolvent formula remains unchanged even when a general Schrödinger operator is

used instead of the free Hamiltonian. Hence, we obtain

$$R(E) = R_0(E) + \frac{1}{\Phi(E)} R_0(E)|\Gamma\rangle\langle\Gamma|R_0(E) \ , \tag{2.3.5}$$

where $\Phi(E) = \frac{1}{\alpha} - G_0(\Gamma,\Gamma|E)$ and $G_0(\Gamma,\Gamma|E) = \frac{1}{L^2}\iint_{\Gamma\times\Gamma} G_0(\gamma(s),\gamma(s'))ds\ ds'$. This can be expressed in terms of the Green's functions as

$$G(x,y|E) = G_0(x,y|E) + \frac{1}{\Phi(E)} G_0(x,\Gamma|E)G_0(\Gamma,y|E) \ . \tag{2.3.6}$$

Here $G_0(x,\Gamma|E) = \frac{1}{L}\int_\Gamma G_0(x,\gamma(s))ds$. The work presented in [53] includes the study of such δ interactions that generalize to curves embedded in manifolds.

Let us define $g(x,y|E) = \sum_{n\neq k}\phi_n(x)\phi_n(y)(E-E_n)^{-1}$ as well as projections onto the curve as $\langle x|g(E)|\Gamma\rangle = \sum_{n\neq k}\phi_n(x)\langle\Gamma|\phi_k\rangle(E-E_n)^{-1}$. To ensure clarity, we specifically focus on a discrete spectrum, because it is simple to generalize to a continuous spectrum. These functions are holomorphic with respect to E in a sufficiently small neighborhood of E_k. Repeating the process as previously outlined and using the Green's function expansion, we obtain the following formula, as shown below

$$\begin{aligned} G(x,y|E) = g(x,y|E) &+ \frac{\phi_k(x)\phi_k(y)}{E-E_k} + \frac{\frac{\phi_k(x)\langle\phi_k|\Gamma\rangle}{E-E_k}\frac{\langle\Gamma|\phi_k\rangle\phi_k(y)}{E-E_k}}{\frac{1}{\alpha} - \langle\Gamma|g(E)|\Gamma\rangle - |\langle\Gamma|\phi_k\rangle|^2(E-E_k)^{-1}} \\ &+ \frac{\langle x|g(E)|\Gamma\rangle\frac{\langle\Gamma|\phi_k\rangle\phi_k(y)}{E-E_k}}{\frac{1}{\alpha} - \langle\Gamma|g(E)|\Gamma\rangle - |\langle\Gamma|\phi_k\rangle|^2(E-E_k)^{-1}} + \frac{\frac{\phi_k(x)\langle\phi_k|\Gamma\rangle}{E-E_k}\langle\Gamma|g(E)|y\rangle}{\frac{1}{\alpha} - \langle\Gamma|g(E)|\Gamma\rangle - |\langle\Gamma|\phi_k\rangle|^2(E-E_k)^{-1}} \\ &+ \frac{\langle x|g(E)|\Gamma\rangle\langle\Gamma|g(E)|y\rangle}{\frac{1}{\alpha} - \langle\Gamma|g(E)|\Gamma\rangle - |\langle\Gamma|\phi_k\rangle|^2(E-E_k)^{-1}} \ . \end{aligned} \tag{2.3.7}$$

Here we have assumed that there is a continuous representative for each eigenvector, so that the expression $\langle\Gamma|\phi_k\rangle = \frac{1}{L}\int_\Gamma \phi_k(\gamma(s))ds$ is well defined, this holds true even when considering the generalized eigenvectors of a Laplacian that has been modified by a potential that satisfies some conditions, as discussed in [6]. Specifically, for the free Hamiltonian, it is noteworthy that the domain of H_0 is defined within the Sobolev space. Consequently, these expressions for arbitrary vectors within this domain are always well-defined, a fact stated by the Sobolev embedding theorem [54]). When we multiply both the numerators and denominators by $(E-E_k)$ and expand them around E_k, we observe the cancellation of the pole at E_k, under the condition that $\langle\Gamma|\phi_k\rangle \neq 0$.

In this case the new wave functions are expressed by

$$\psi_k(x) = \mathcal{N} G_0(x, \Gamma | E_k^*) = \mathcal{N} \int_\Gamma G_0(x, \gamma(s) | E_k^*) ds \ . \tag{2.3.8}$$

Eigenvalues and eigenvectors are obtained for multiple curves and points by systematically applying the given set of parameters for each additional rank-one perturbation.

In all our discussions, It is important to focus on elliptic operators with some special properties, such as those subject to typically a summability condition on the potentials. This condition is crucial for the generalized eigenvectors with certain regularity properties, whether they are evaluated at a point or integrated over a curve.

2.3.3. A Particle in a Compact Manifold under the Influence of a $\delta-$Interaction

One additional possibility for H_0 could involve a system where a particle intrinsically moves within a compact and connected two or three-dimensional manifold M with a specified metric structure g:

$$(H_0\psi)(x) = -\frac{\hbar^2}{2m} \left(\frac{1}{\sqrt{\det g}} \sum_{i,j=1}^{d} \frac{\partial}{\partial x^i} \left(\sqrt{\det g} g^{ij} \frac{\partial \psi(x)}{\partial x^j} \right) \right) \ , \tag{2.3.9}$$

where $x = (x^1, \ldots, x^d)$ are the local coordinates, and g^{ij} are the components of inverse of the metric g. Then it is well known [55, 56] that there exists a complete orthonormal system of C^∞ eigenfunctions $\{\phi_n\}_{n=0}^\infty$ in $L^2(M)$ and the spectrum $\sigma(H_0) = \{E_n\} = \{0 = E_0 \leq E_1 \leq E_2 \leq \ldots\}$, with E_n tending to infinity as $n \to \infty$ and each eigenvalue has finite multiplicity: $H_0\phi_n = E_n\phi_n$. Some eigenvalues can occur with repeated instances based on their respective multiplicities. The multiplicity of the first eigenvalue, denoted as $E_0 = 0$, is one and the associated eigenfunction is constant.

By introducing a point like δ interaction on such Schrödinger operator H_0, physically, we are modeling a system where a particle is intrinsically moving in a two-dimensional compact manifold $\mathcal{M}$ without boundary and interacts with a δ source located at some point a in $\mathcal{M}$. Renormalization is necessary due to the short-distance

singular behavior of the free Green's function on a manifold. This singularity is evident in the asymptotic behavior of the heat kernel, where $K_t(a,a) \sim 1/t$ as $t \to 0^+$ and the formula (2.2.1) for Riemannian manifolds, as presented in the work by [57]. We know this fact very well that the diagonal free Green's function has the same singular structure and it is clear to see that the reason behind this singular structure lies in the short-term behavior of the heat kernel and the nature of the manifold $\mathcal{M}$. We assume that this manifold locally exhibits a flat space around the certain point where the δ interaction is located. This issue has been discussed in our earlier publications [58–61] in the context of a finite number of δ centers. Subsequently, the Green's function can be equivalently formulated as follows:

$$G(x,y|E) = G_0(x,y|E) + \frac{G_0(x,a|E)G_0(a,y|E)}{\frac{1}{\alpha_R} - \sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)}} \ , \tag{2.3.10}$$

for any points x, y and a in $\mathcal{M}$. Please be aware that this expression is structurally identical to our previous formula for a two-dimensional problem, without the requirement for a continuous spectrum. Then, all the results we reached in solving previous problems effortlessly extend to this case as well. Consequently, We avoid repeating our arguments; instead, in the following section, we focus on a slightly different model situated on a compact manifold, where we offer some more details. The convergence of the series $\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)}$ will be shown.

Now that we have come to the end of this topic, we can start proving the convergence of the series $\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2(E+\mu^2)}{(E_n-E)(E_n+\mu^2)}$

We aim to demonstrate that the Green's function is finite apart from the obvious poles that we've mentioned,

$$\lim_{N\to\infty} \sum_{n=0}^{N} \frac{|\phi_n(a)|^2}{(E_n-E)(E_n+\mu^2)} < \infty \ . \tag{2.3.11}$$

On a compact manifold, we know that the Laplace-Beltrami operator $-\nabla_g^2$ has a discrete spectrum $0 \le E_0 \le E_1 \le E_2 ... \le E_n \to \infty$, and with finite multiplicity. Let's start by considering that $E \in \mathbb{R}^+$ for simplicity. Next, we'll choose a finite value for M

that is large enough to satisfy the condition where $E_M > 2\left(E + \frac{\mu^2}{2}\right)$, and note that $E_n \geq E_M$ for $n > M$. Then, it is evident that for $n \geq M$, with the clear condition that $N > M$ as $N \to \infty$ eventually, we can obtain the following inequality

$$\frac{|\phi_n(a)|^2}{(E_n - E)(E_n + \mu^2)} < 2\frac{|\phi_n(a)|^2}{(E_n + \mu^2)^2} \ . \tag{2.3.12}$$

This implies that

$$\sum_{n\geq M}^{N} \frac{|\phi_n(a)|^2}{(E_n - E)(E_n + \mu^2)} < 2\sum_{n=0}^{N} \frac{|\phi_n(a)|^2}{(E_n + \mu^2)^2} \ . \tag{2.3.13}$$

One can express the right hand side of the above inequality as follows:

$$\sum_{n=0}^{N} \frac{|\phi_n(a)|^2}{(E_n + \mu^2)^2} = \sum_{n=0}^{N} \int_0^\infty dt\ t\ |\phi_n(a)|^2 e^{-(E_n+\mu^2)t} \ , \tag{2.3.14}$$

and using the eigenfunction expansion of the heat kernel (2.3.36) as we let $N \to \infty$ we obtain

$$\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{(E_n + \mu^2)^2} = \int_0^\infty dt\ t\ K_t(a,a) e^{-\mu^2 t} \ . \tag{2.3.15}$$

The upper bound for the diagonal part of the heat kernel on compact manifolds is provided in (see [43])

$$K_t(a,a) < \left(\frac{1}{V(\mathcal{M})} + \frac{C}{t}\right) \ , \tag{2.3.16}$$

where $V(\mathcal{M})$ is the volume of $\mathcal{M}$ and C is a constant depending only on the geometric properties of $\mathcal{M}$. This upper bound demonstrates the convergence of the sum $\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{(E_n - E)(E_n+\mu^2)}$. The convergence of the same sum can also be demonstrated for Schrödinger operators with locally integrable potentials using the upper bound formula for the heat kernel $K_t(a,a) \leq \frac{1}{4\pi t}$, given in example 2.1.9 in [66]. We can easily show that the convergence as follows;

$$\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{(E_n + \mu^2)^2} = \int_0^\infty dt\ t\ K_t(a,a) e^{-\mu^2 t} \leq \frac{1}{4\pi} \int_0^\infty dt e^{-\mu^2 t} \leq \frac{1}{4\pi\mu^2}. \tag{2.3.17}$$

One can see that this series is convergent.

For the complex values of $E = E_R + iE_I$ with the condition where $E_I \neq 0$, , it can be demonstrated that the above series converges absolutely.

$$\sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{|(E_n - E_R - iE_I)|(E_n + \mu^2)} = \sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{\sqrt{(E_n - E_R)^2 + E_I^2}(E_n + \mu^2)}$$
$$\leq \sqrt{2} \sum_{n=0}^{\infty} \frac{|\phi_n(a)|^2}{(|E_n - E_R| + |E_I|)(E_n + \mu^2)}$$
$$\leq \sum_{n>M}^{\infty} \frac{\sqrt{2}|\phi_n(a)|^2}{(E_n + \mu^2)(|E_n - E_R| + |E_I|)} + \frac{\sqrt{2}}{|E_I|} \sum_{n \leq M} \frac{|\phi_n(a)|^2}{(E_n + \mu^2)} < \infty \tag{2.3.18}$$

Choosing an M such that for $n > M$, we observe $E_n > 2|E_R|$, we notice that all the terms become finite. As a result, in all possible cases, we end up with finite expressions.

2.3.4. A Semi-relativistic Model on a 2-Dimensional Compact Manifold

In our earlier study [62], we presented a possible relativistic model describing δ interactions within the context of a two-dimensional compact Riemannian manifold $(\mathcal{M}, g)$. Expanding upon this concept using second quantization, we expressed the model Hamiltonian in the following equation

$$H = \frac{1}{2} \int_{\mathcal{M}} d_g^2 x : \phi^\dagger(-\nabla_g^2 + m^2)\phi + \pi^2 : \, - \alpha \, \phi^{(-)}(a)\phi^{(+)}(a) \, , \tag{2.3.19}$$

where $d_g^2 x = \sqrt{\det g} \, dx_1 \, dx_2$ and (x_1, x_2) is the local coordinates. The positive and the negative frequency part of the bosonic field ϕ is denoted by $\phi^{(-)}$ and $\phi^{(+)}$, respectively. The expansion can be represented in terms of creation and annihilation operators, with indices denoted by n,

$$\phi^{(+)}(x) = \sum_{n=0}^{\infty} \frac{f_n(x)}{\sqrt{2\omega_n}} a_n, \tag{2.3.20}$$

$$\phi^{(-)}(x) = \sum_{n=0}^{\infty} \frac{\overline{f_n(x)}}{\sqrt{2\omega_n}} a_n^\dagger \tag{2.3.21}$$

where $f_n(x)$ are the eigenfunctions of $\nabla_g^2 = \frac{1}{\sqrt{\det g}} \sum_{i,j=1}^{2} \frac{\partial}{\partial x^i} \left(g^{ij} \sqrt{\det g} \frac{\partial}{\partial x^j} \right)$, the Laplace-Beltrami operator:

$$-\nabla_g^2 f_n(x) = e_n^2 f_n(x) \, , \tag{2.3.22}$$

and $\omega_n = \sqrt{e_n^2 + m^2}$, note that to follow the expressions more easily we use units where $\hbar = 1$ and $c = 1$. In this way, ω_n and energy are included in the same units. We notice that the index n plays the same role as the momentum k in flat space, even though there is no direct correlation with a possible translation symmetry in general. This analogy becomes more evident when we limit our model to a single-particle sector.

$$|\psi\rangle = \sum_{n=0}^{\infty} \psi_n \frac{a_n^\dagger}{\sqrt{2\omega_n}}|0\rangle, \tag{2.3.23}$$

and in accordance with the same procedures described in [62], we proceed to compute the Green's function specifically within the one-particle sector. To achieve this, we must solve the eigenvalue problem within the basis of the eigenfunction.

$$(H - E)|\psi\rangle = |\chi\rangle \ , \tag{2.3.24}$$

for a given state $|\chi\rangle$. Consequently, the Green's function for the single-particle sector can be obtained by solving the following equation.

$$\left(\sqrt{e_n^2 + m^2} - E\right)\psi_n - \alpha \sum_{l=0}^{\infty} \frac{\overline{f_n(a)}}{\sqrt{\omega_l}} \frac{f_l(a)}{\sqrt{\omega_l}} \psi_l = \chi_n \ . \tag{2.3.25}$$

The solution ψ_n of this equation is given by

$$\psi_n = \frac{1}{(\omega_n - E)}\chi_n + \frac{1}{(\omega_n - E)}\overline{f_n(a)}\left[\frac{1}{\alpha} - \sum_{l=0}^{\infty} \frac{|f_l(a)|^2}{\omega_l(\omega_l - E)}\right]^{-1} \sum_{r=0}^{\infty} \frac{f_r(a)}{\omega_r} \frac{1}{(\omega_r - E)}\chi_r \ . \tag{2.3.26}$$

To read the Green's function, notice that

$$\begin{aligned} \sum_{n=0}^{\infty} f_n(x)\frac{\psi_n}{\sqrt{\omega_n}} = \psi(x) = \sum_{n=0}^{\infty} \int_{\mathcal{M}} d_g^2 y \ \frac{f_n(x)\overline{f_n(y)}}{(\omega_n - E)}\chi(y) \\ + \sum_{n=0}^{\infty} \frac{f_n(x)}{(\omega_n - E)} \frac{\overline{f_n(a)}}{\sqrt{\omega_n}} \left[\frac{1}{\alpha} - \sum_{l} \frac{|f_l(a)|^2}{\omega_l(\omega_l - E)}\right]^{-1} \sum_{r} \int_{\mathcal{M}} d_g^2 y \ \frac{f_r(a)}{\sqrt{\omega_r}} \frac{\overline{f_r(y)}}{(\omega_r - E)}\chi(y) \ , \end{aligned} \tag{2.3.27}$$

where we have used $\chi_n = \sqrt{\omega_n}\int_{\mathcal{M}} d_g^2 x \ \chi(x)\overline{f_n(x)}$ and orthogonality of eigenfunctions f_n. This can be expressed as an equation,

$$\psi(x) = \int_{\mathcal{M}} d_g^2 y \ G_0(x, y|E)\chi(y) + \tilde{G}_0(x, a|E)\Phi(E)^{-1} \int dy \ \tilde{G}_0(a, y|E)\chi(y) \ , \tag{2.3.28}$$

where

$$G_0(x,y|E) = \sum_{n=0}^{\infty} \frac{f_n(x)\overline{f_n(y)}}{(\omega_n - E)} \tag{2.3.29}$$

$$\tilde{G}_0(x,y|E) = \sum_{n=0}^{\infty} \frac{f_n(x)}{(\omega_n - E)} \frac{\overline{f_n(y)}}{\sqrt{\omega_n}} \tag{2.3.30}$$

$$\Phi(E) = \frac{1}{\alpha} - \sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n - E)} \, . \tag{2.3.31}$$

Subsequently, we can arrive at the following formula of the green's function

$$G(x,y|E) = G_0(x,y) + \tilde{G}_0(x,a|E)\Phi^{-1}(E)\tilde{G}_0(a,y|E). \tag{2.3.32}$$

To illustrate the cancellation of the original poles, it is necessary to carefully examine the analytical structure of $G(x,y)$.

$$G(x,y) = \sum_{n=0}^{\infty} \frac{f_n(x)\overline{f_n(y)}}{(\omega_n - E)} + \sum_{n=0}^{\infty} \frac{f_n(x)}{(\omega_n - E)} \frac{\overline{f_n(a)}}{\sqrt{\omega_n}} \Phi^{-1}(E) \sum_{r=0}^{\infty} \frac{f_r(a)}{\sqrt{\omega_r}} \frac{\overline{f_r(y)}}{(\omega_r - E)} \tag{2.3.33}$$

Certainly, we can see that the sum in the definition of Φ is divergent.This divergence becomes evident when following the same line of reasoning discussed in [62]. To provide a comprehensive perspective, let's restate the expression $\frac{1}{\omega_n(\omega_n - E)}$ in a different way as follows

$$\frac{1}{\omega_n(\omega_n - E)} = -\frac{1}{E}\left(\frac{1}{\omega_n} - \frac{1}{\omega_n - E}\right) = -\frac{1}{E}\int_0^{\infty} e^{-s\omega_n}(1 - e^{sE})\, ds \, , \tag{2.3.34}$$

where we assume that $\mathrm{Re}\,(\omega_n - E) > 0$.Subsequent expressions for the solvent in terms of heat kernels are often assumed to be analytic continuity onto the complex plane. This continuity is typically achieved with the use of the subordination identity

$$e^{-sA} = \frac{s}{2\sqrt{\pi}} \int_0^{\infty} e^{-s^2/(4u) - uA^2} \, \frac{du}{u^{3/2}} \, , \tag{2.3.35}$$

and expressing the eigenfunction expansion for the heat kernel related to the Laplace-Beltrami operator on Riemannian manifolds suing the formula in [55]

$$K_u(x,y) = \sum_{n=0}^{\infty} e^{-ue_n^2} f_n(x)\overline{f_n(y)} \, , \tag{2.3.36}$$

we obtain

$$\sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n - E)} = -\frac{1}{E}\int_0^\infty \left(\int_0^\infty K_u(a,a) e^{-um^2 + s^2/(4u)} \, \frac{du}{u^{3/2}} \right) \frac{(1-e^{sE})s}{2\sqrt{\pi}} \, ds \, . \tag{2.3.37}$$

Using integration by parts and scaling the integration variable, we arrive at the following result

$$\sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n - E)} = \frac{1}{\sqrt{\pi}}\int_0^\infty \left(\int_0^\infty K_u(a,a) e^{-um^2 + sE\sqrt{u}} \, du \right) e^{-s^2/4} \, ds \tag{2.3.38}$$

The diagonal heat kernel $K_u(a,a)$ on two-dimensional Riemannian manifolds exhibits a divergent behavior, as shown in this equation $K_u(a,a) \sim \frac{1}{u}$ in the short time asymptotic limit. As a result, it can bee seen that the integral over u is divergent. To deal with this problem, we apply the concept of renormalization and include a short "time" cut off ϵ in the lower limit of u integral. We sum over n up to a cut off N. Following this, we determine the coupling constant in terms of this cut off in such a way that

$$\frac{1}{\alpha(N)} = \frac{1}{\alpha_R} + \sum_{n=0}^{N} \frac{|f_n(a)|^2}{\omega_n(\omega_n + \mu^2)} \, , \tag{2.3.39}$$

$-\mu^2$ can be associated with the experimentally determined bound state energy of the particle, which is below the lowest eigenvalue ω_0 in the presence of a single Dirac δ center, as we will demonstrate. In order to achieve this, we eliminate the cutoff by taking the limit $N \to \infty$ in Φ and obtain the renormalized Φ

$$\begin{aligned} \Phi_R &= \frac{1}{\alpha_R} + \sum_{n=0}^{\infty} \left[\frac{|f_n(a)|^2}{\omega_n(\omega_n + \mu^2)} - \frac{|f_n(a)|^2}{\omega_n(\omega_n - E)} \right] \\ &= \frac{1}{\alpha_R} + \sum_{n=0}^{\infty} |f_n(a)|^2 \frac{(-E - \mu^2)}{\omega_n(\omega_n + \mu^2)(\omega_n - E)} \\ &= \frac{1}{\alpha_R} - (E + \mu^2) \sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n + \mu^2)(\omega_n - E)} \, . \end{aligned} \tag{2.3.40}$$

In the case where the real part of $\omega_0 - E$ is positive, one can demonstrate the finiteness of the expression using heat kernel estimates, as detailed in [62]). Additionally, it can be shown that as long as $E \neq \omega_n$, this expression retains its well-defined and analytic properties. By considering E around E_k, we isolate this particular pole in our

formulations.

$$\sum_{n\neq k}\frac{f_n(x)\overline{f_n(y)}}{(\omega_n-E)}+\frac{f_k(x)\overline{f_k(y)}}{(\omega_k-E)}+\Big(\sum_{n\neq k}\frac{f_n(x)}{(\omega_n-E)}\frac{\overline{f_n(a)}}{\sqrt{\omega_n}}+\frac{f_k(x)}{(\omega_k-E)}\frac{\overline{f_k(a)}}{\sqrt{\omega_k}}\Big)$$
$$\times\frac{1}{\frac{1}{\alpha_R}-(E+\mu^2)\Big[\sum_{r\neq k}\frac{|f_r(a)|^2}{\omega_r(\omega_r+\mu^2)(\omega_r-E)}+\frac{|f_k(a)|^2}{\omega_k(\omega_k+\mu^2)(\omega_k-E)}\Big]}$$
$$\times\Big(\sum_{l\neq k}\frac{f_l(a)}{\sqrt{\omega_l}}\frac{\overline{f_l(y)}}{(\omega_l-E)}+\frac{f_k(a)}{\sqrt{\omega_k}}\frac{\overline{f_k(y)}}{(\omega_k-E)}\Big)\,. \tag{2.3.41}$$

Note that here the singular part comes from,

$$\frac{f_k(x)\overline{f_k(y)}}{(\omega_k-E)}-\frac{|f_k(a)|^2f_k(x)\overline{f_k(y)}}{\omega_k(\omega_k-E)^2\big[(E+\mu^2)\frac{|f_k(a)|^2}{\omega_k(\omega_k-E)(\omega_k+\mu^2)}+\text{regular terms}\big]}+\text{regular terms}\,. \tag{2.3.42}$$

We now use $E+\mu^2=E-\omega_k+\omega_k+\mu^2$ in the numerator and reduce this to

$$\frac{f_k(x)\overline{f_k(y)}}{(\omega_k-E)}-\frac{|f_k(a)|^2f_k(x)\overline{f_k(y)}}{\omega_k(\omega_k-E)^2\big(\frac{|f_k(a)|^2}{\omega_k(\omega_k-E)}+\text{regular terms}\big)}+\text{regular terms}\,. \tag{2.3.43}$$

Now based on our prior discussions, it appears that the pole at ω_k has been effectively cancelled. As a consequence, it becomes evident that the interaction we suggest exhibits a similar characteristic as outlined in the Sturm-Liouville interlacing theorem. The illustration we have for the two-dimensional non-relativistic problem is equally valid in this scenario. At the end of this part, we prove that there always exists a bound state below ω_0 for any given α_R, However, it is essential to exercise caution and avoid driving the bound state below $-m$ to ensure internal consistency within the model.

Now we will try to prove the accuracy of some of the expressions we use when talking about this subject. Let us look at the behavior of the sum $\sum_{n=0}^{\infty}\frac{(E+\mu^2)|\phi_n(a)|^2}{(E_n-E)(E_n+\mu^2)}$ as $E\to-\infty$. In order to show

$$\sum_{n=0}^{\infty}\frac{(E+\mu^2)|\phi_n(a)|^2}{(E_n-E)(E_n+\mu^2)}\to-\infty\ \text{as}\ \ E\to-\infty. \tag{2.3.44}$$

When considering a compact manifold, we turn to a well-known inequality for the heat kernel, as formulated by Cheeger and Yau [63]

$$K_t(x,y)\geq K_t^{\kappa}(d_g(x,y))\,. \tag{2.3.45}$$

Supposing that the Ricci curvature, expressed as a 2-form, is bounded from below by $-\kappa g(.,.)$, a condition commonly considered reasonable. The symbol K_t^κ represents the heat kernel of a simply connected, complete, two-dimensional manifold with constant sectional curvature. Additionally, $d_g(x,y)$ denotes the geodesic distance between points x and y on the manifold.We have the option to select $K_t^\kappa(x,y)$ as the heat kernel for the two-dimensional hyperbolic manifold. This choice is influenced by the contributions of Davies and Mandouvalos [64], there exists a lower bound for the diagonal heat kernel on the hyperbolic two dimensional manifold , $C_{DM}\frac{e^{-\kappa t/4}}{t(1+\kappa t)^{1/2}}$ where C_{DM} is a constant, depending on dimension. This bound can even be simplified to see [65]

$$K_t(a,a) \geq C_{DM}\frac{e^{-3\kappa t/4}}{t} \ . \tag{2.3.46}$$

Applying the Feynman parametrization to this term $1/(E_n - E)(E_n + \mu^2)$

$$\frac{1}{AB} = \int_0^1 \frac{du}{(Au + (1-u)B)^2} \ , \tag{2.3.47}$$

and writing the denominator by using exponential integral form

$$\frac{1}{(Au + (1-u)B)^2} = \int_0^\infty e^{-t(Au+(1-u)B)}\ t\ dt \tag{2.3.48}$$

and after applying the eigenfunction expansion of the heat kernel as presented in Equation (2.3.36), we can determine an upper bound for the summation as follows.

$$\begin{aligned}
\sum_{n=0}^{\infty} \frac{(|E| - \mu^2)|\phi_n(a)|^2}{(E_n + |E|)(E_n + \mu^2)} &= \sum_{n=0}^{\infty}(|E| - \mu^2)\int_0^1 \frac{|\phi_n(a)|^2 du}{[E_n + u|E| + (1-u)\mu^2]^2} \\
&= (|E| - \mu^2)\int_0^1 du \int_0^\infty dt\ t\ K_t(a,a)e^{-(t(1-u)\mu^2 + u|E|)} \\
&\geq C_{DM}(|E| - \mu^2)\int_0^1 \frac{du}{3\kappa/4 + (1-u)\mu^2 + u|E|} \\
&= C_{DM}\ln\Big(\frac{|E| + 3\kappa/4}{\mu^2 + 3\kappa/4}\Big),
\end{aligned} \tag{2.3.49}$$

the above result illustrates that the limit goes to ∞, a solution always exists for $1/\alpha_R < 0$. Other bounds with less restrictive conditions exist, but the result remains unchanged. Similarly, we can make use of lower bounds for the heat kernel corresponding to uniformly elliptic Schrödinger operators on $\mathbb{R}^2$ (see, e.g., Theorem 3.3.4 in [66]). We consider a potential function V that is non-singular and belongs to the Kato class,

ensuring the self-adjointness of the corresponding Schrödinger operator, , there is a natural lower limit for the diagonal heat kernel, expressed as C/t. Consequently, we obtain the same result.

In the our semi-relativistic model, we can once again demonstrate that the function $\Phi(E)$ has a root within the range of $-\mu^2$ to ω_0 when we consider cases where $E < \omega_0$ and assume positive values for α_R. We aim for internal consistency by restricting our model from generating values below $-m$. Nevertheless, it is essential to demonstrate that solutions exist in cases where $\alpha_R < 0$. To verify this, we need to confirm that the function $\Phi(E)$ is a monotonically increasing function from the range $-\infty$ to ∞ as we change E from $-\infty$ to ω_0^-. It is clear that $\Phi(E)$ increases monotonically with E, as discussed earlier, within the interval between the poles. however, demonstrating that it goes to $-\infty$ as $E \to -\infty$. requires a more detailed analysis. For this purpose, we estimate the sum from below assuming $E < 0$,

$$\sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n+\mu^2)(\omega_n+|E|)} > \sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{(\omega_n+\mu^2)^2(\omega_n+|E|)} \, . \tag{2.3.50}$$

Using the Feynman parametrization formula

$$\frac{1}{(\omega_n+\mu^2)^2(\omega_n+|E|)} = 2\int_0^1 \frac{u}{\left[\omega_n+u\mu^2+(1-u)|E|\right]^3} \, du \, , \tag{2.3.51}$$

and exponentiating the denominator

$$\frac{1}{\left[\omega_n+u\mu^2+(1-u)|E|\right]^3} = \int_0^\infty s^2 \, e^{-s\left[\omega_n+u\mu^2+(1-u)|E|\right]} \, ds, \tag{2.3.52}$$

and then using the subordination identity (2.3.35), the sum can be expressed in terms of the heat kernel thanks to the eigenfunction expansion of the heat kernel (2.3.36). consequently, when we again use the Cheeger-Yau bound for the heat kernel with the condition $R(.,.) > -\kappa g(.,.)$, we finally obtain a lower limit for the summation.

$$\sum_{n=0}^{\infty} e^{-\omega_n^2 t}|f_n(a)|^2 = e^{-m^2 t}K_t(a,a) > C_{DM}\frac{e^{-(m^2+3\kappa/4)t}}{t}. \tag{2.3.53}$$

Substituting these results back into the original expressions, we obtain.

$$\sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n+\mu^2)(\omega_n+|E|)} > \frac{1}{\sqrt{\pi}} \int_0^1 u \left[\int_0^\infty s^3 \left(\int_0^\infty \frac{e^{-(m^2+3\kappa/4)t - s^2/4t}}{t^{5/2}}\, dt \right) e^{-s\left(u\mu^2+(1-u)|E|\right)}\, ds \right] du\,. \tag{2.3.54}$$

We acknowledge that the integral with respect to t corresponds to the integral representation of the modified Bessel function [67]

$$K_{3/2}(z) = \frac{1}{2}\left(\frac{z}{2}\right)^{3/2} \int_0^\infty \frac{e^{-t-z^2/4t}}{t^{3/2+1}}\, dt\,, \tag{2.3.55}$$

and for simplicity, he modified Bessel function of half-integer order can be expressed in a different way as follows:

$$K_{3/2}(z) = \sqrt{\frac{2}{\pi z}} e^{-z} + \sqrt{\frac{2}{\pi}} \frac{e^{-z}}{z^{3/2}}\,. \tag{2.3.56}$$

It would be sufficient for us to focus on the second term in the Equation (2.3.56). for our purpose. Here $z = s\sqrt{m^2 + \frac{3\kappa}{4}}$. This term after the integration with respect to s in (2.3.54) becomes

$$\begin{aligned}
&(|E|-\mu^2) \sum_{n=0}^{\infty} \frac{|f_n(a)|^2}{\omega_n(\omega_n+\mu^2)(\omega_n+|E|)} \\
&> \text{Cst}\ (|E|-\mu^2) \int_0^1 \frac{u}{((m^2+3\kappa/4)^{1/2} + u\mu^2 + (1-u)|E|)}\, du \\
&> \text{Cst}\ (|E|-\mu^2) \int_0^1 \frac{u}{((m^2+3\kappa/4)^{1/2} + \mu^2 + (1-u)|E|)}\, du \\
&= \text{Cst}\ (|E|-\mu^2) \int_0^1 \frac{(1-u)}{((m^2+3\kappa/4)^{1/2} + \mu^2 + u|E|)}\, du \\
&= \text{Cst} \frac{|E|-\mu^2}{|E|} \left(\frac{|E| + (m^2+3\kappa/4)^{1/2} + \mu^2}{|E|} \ln \frac{|E| + [m^2+3\kappa/4]^{1/2} + \mu^2}{\mu^2 + [m^2+3\kappa/4]^{1/2}} - 1 \right),
\end{aligned} \tag{2.3.57}$$

Hence, this once again demonstrates that the sum goes to ∞ as $|E| \to \infty$. Here it's worth emphasizing that the first term in Equation (2.3.56) makes a positive and regular contribution to the sum, which do not change our conclusion.

2.4. Degenerate Case

We're considering the possibility of degeneracy within the eigenstates. To clarify our explanation, we're concentrating on the case of a two-dimensional compact manifold. The same idea can be applied to more general cases as well. In this specific situation, let's consider an eigenvalue E_k that exhibits a d-fold degeneracy within a manifold, where it is confirmed to be finite for each state. As we extend this concept to other instances, it is consistently assumed to maintain finite degeneracy. We then select a set of orthonormal vectors, denoted as ϕ_k^α, to serve as a basis for this space. In the Green's function formula, when considering the energy E around E_k, it is possible to explicitly express the leading terms with E_k poles;

$$G(x,y|E) = g(x,y|E) + \sum_{\alpha=1}^{d} \frac{\phi_k^\alpha(x)\overline{\phi_k^\alpha(y)}}{E_k - E} + \left[g(x,a|E) + \sum_{\alpha=1}^{d} \frac{\phi_k^\alpha(x)\overline{\phi_k^\alpha(a)}}{(E_k - E)} \right] \times \frac{1}{\frac{1}{\alpha_R} - k(a,a|E) - \sum_{\alpha=1}^{d} \frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}(E+\mu)}{(E_k-E)(E_k+\mu)}} \left[g(a,y|E) + \sum_{\beta=1}^{d} \frac{\phi_k^\beta(a)\overline{\phi_k^\beta(y)}}{E_k - E} \right], \tag{2.4.1}$$

here α_R refers to the renormalized coupling constant and

$$\begin{aligned} g(x,y|E) &:= \sum_{n\neq k}^{\infty} \frac{\phi_n(x)\overline{\phi_n(y)}}{E_n - E} \\ k(x,y|E) &:= \sum_{n\neq k}^{\infty} \frac{\phi_n(x)\overline{\phi_n(y)}(E+\mu)}{(E_n - E)(E_n + \mu)} \,. \end{aligned} \tag{2.4.2}$$

We'll proceed to rework the term related to the pole within the denominator.

$$\frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}(E+\mu)}{(E_k-E)(E_k+\mu)} = \frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}(E+\mu-E_k+E_k)}{(E_k-E)(E_k+\mu)} = \frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}}{(E_k-E)} - \frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}}{(E_k+\mu)}, \tag{2.4.3}$$

In the expression, the critical section involves isolating the pole term while keeping the part regular. We focus on the product of the two pole terms, then manipulate one of the $E_k - E$ terms into the denominator to obtain a leading order term plus a series

expansion in terms of $E_k - E$.

$$G(x,y|E) = f(x,y|E) + \sum_{\alpha=1}^{d} \frac{\phi_k^\alpha(x)\overline{\phi_k^\alpha(y)}}{E_k - E} + \frac{1}{E_k - E}\sum_{\alpha=1}^{d}\phi_k^\alpha(x)\overline{\phi_k^\alpha(a)}\frac{1}{-\sum_\gamma \phi_k^\gamma(a)\overline{\phi_k^\gamma(a)} + (E-E_k)h(a,a|E)}\sum_{\beta=1}^{d}\phi_k^\beta(a)\overline{\phi_k^\beta(y)}\,, \tag{2.4.4}$$

where

$$\begin{aligned} f(x,y|E) = g(x,y|E) &+ \frac{g(x,a|E)g(a,y|E)}{\frac{1}{\alpha_R} - k(a,a|E) - \sum_{\alpha=1}^{d}\frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}(E+\mu)}{(E_k-E)(E_k+\mu)}} \\ &+ \frac{g(x,a|E)}{(E_k-E)\left(\frac{1}{\alpha_R} - k(a,a|E)\right) - \sum_{\alpha=1}^{d}\frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}(E+\mu)}{(E_k+\mu)}}\sum_{\beta=1}^{d}\phi_k^\beta(a)\overline{\phi_k^\beta(y)} \\ &+ \frac{g(a,y|E)}{(E_k-E)\left(\frac{1}{\alpha_R} - k(a,a|E)\right) - \sum_{\alpha=1}^{d}\frac{\phi_k^\alpha(a)\overline{\phi_k^\alpha(a)}(E+\mu)}{(E_k+\mu)}}\sum_{\beta=1}^{d}\phi_k^\beta(x)\overline{\phi_k^\beta(a)}\,, \end{aligned} \tag{2.4.5}$$

and

$$h(a,a|E) = k(a,a|E) - \frac{1}{\alpha_R} - \sum_{\alpha=1}^{d}\frac{|\phi_k^\alpha(a)|^2}{E_k + \mu^2}\,. \tag{2.4.6}$$

In this case, $f(x,y|E)$ exhibits regular behavior around E_k. Within the denominator, there exists an initial finite term followed by a function that maintains regularity, multiplied by $(E - E_k)$, which can be made sufficiently small. Let's assume that at least one of the wave functions, denoted as $\phi_k^\alpha(a)$, is non-zero. Consequently, we can perform an expansion of this combination in the denominator and combine them with the regular function f, defining a new regular function, denoted as l. By doing so, we arrive at a following formulation.

$$\begin{aligned} G(x,y|E) = l(x,y|E) &+ \sum_{\alpha=1}^{d}\frac{\phi_k^\alpha(x)\overline{\phi_k^\alpha(y)}}{E_k - E} \\ &- \frac{1}{E_k - E}\sum_{\alpha=1}^{d}\phi_k^\alpha(x)\overline{\phi_k^\alpha(a)}\frac{1}{\sum_{\gamma=1}^{d}\phi_k^\gamma(a)\overline{\phi_k^\gamma(a)}}\sum_{\beta=1}^{d}\phi_k^\beta(a)\overline{\phi_k^\beta(y)}\,. \end{aligned} \tag{2.4.7}$$

Let us define $A_{\alpha\beta} = \overline{\phi_k^\alpha(a)}\phi_k^\beta(a)$, which is a manifestly Hermitian matrix, with trace $\mathrm{Tr}A = \sum_{\alpha=1}^{d}\overline{\phi_k^\alpha(a)}\phi_k^\alpha(a) = \sum_{\alpha=1}^{d}|\phi_k^\alpha(a)|^2$ Moreover, if we consider $\phi_k^\alpha(a)$ as compo-

nents of a vector in a d-dimensional space, matrix A has only one non-zero eigenvalue, specifically $\mathrm{Tr}A$, associated with the eigenvector $\phi_k^\gamma(a)$. As $A_{\alpha\beta}v_\beta = 0$ for all vectors v orthogonal to the single vector $\phi_k^\beta(a)$, this implies the existence of $d-1$ zero eigenvalues.

Given that $A_{\alpha\beta}$ is a Hermitian matrix, it can be diagonalized through an alternate representation using a unitary matrix $U_{\alpha\beta}$.

$$U^\dagger A U = \mathrm{diag}(0, 0, \cdots, \mathrm{Tr}(A)) \ . \tag{2.4.8}$$

When considering the sum $\sum_{\beta=1}^{d} U_{\alpha\beta}\phi_k^\beta(x) = \psi_k^\alpha(x)$, where U represents a unitary transformation within the d-dimensional subspace, it yields orthogonal vectors once more within within the subspace E_k. It's worth noting that the combined structure involving the pole transitions accordingly.

$$\sum_{\alpha=1}^{d} \frac{\phi_k^\alpha(x)\overline{\phi_k^\alpha(y)}}{E_k - E} = \sum_{\alpha=1}^{d} \frac{\psi_k^\alpha(x)\overline{\psi_k^\alpha(y)}}{E_k - E} \ . \tag{2.4.9}$$

The other part instead

$$\begin{aligned}
&- \frac{1}{E_k - E} \sum_{\alpha=1}^{d} \phi_k^\alpha(x)\overline{\phi_k^\alpha(a)} \frac{1}{\sum_{\gamma=1}^{d} \phi_k^\gamma(a)\overline{\phi_k^\gamma(a)}} \sum_{\beta=1}^{d} \phi_k^\beta(a)\overline{\phi_k^\beta(y)} \\
&= -\frac{1}{E_k - E} \frac{1}{\mathrm{Tr}(A)} \sum_{\alpha=1}^{d} \phi_k^\alpha(x) A_{\alpha\beta}\overline{\phi_k^\beta(y)} \\
&= -\frac{1}{E_k - E} \frac{1}{\mathrm{Tr}(A)} \Big[\psi_k^1(x)\cdot 0 \cdot \overline{\psi_k^1(y)} + ... + \psi_k^{d-1}(x)\cdot 0 \cdot \overline{\psi_k^{d-1}(y)} + \psi_k^d(x)\mathrm{Tr}(A)\overline{\psi_k^d(y)}\Big] \\
&= -\frac{1}{E_k - E}\psi_k^d(x)\overline{\psi_k^d(y)} \ .
\end{aligned} \tag{2.4.10}$$

Therefore, we observe a single cancellation of the wave function corresponding to $\mathrm{Tr}A$, where the terms $\psi_k^d(x)$ cancel each other out. and we end up with a $d-1$ dimensional subspace with a pole E_k. Degeneracy is lifted by removing one of the properly chosen eigenstates. Note that the essential point of the argument is coming from this process of diagonalization, and it extends equally well to all other cases involving degeneracy.

3. BORN-OPPENHEIMER APPROXIMATION APPLIED TO KINK MODEL IN ONE DIMENSION

3.1. A Brief Summary About the One-Dimensional Kink Model

Kink systems are a well-known topic in field theory and many studies have been done on it and are still being done. In one dimension, especially in theoretical physics, kinks often appear as structures in field theories as topological defects. Kinks are defined as topological structures that arise from sudden changes in the values of a field. For instance, consider a scalar-based field theory. In different regions of this field, there might be different minimum points. In the transitional areas between these different minimum points, the values of the field can suddenly change. These regions of change are referred to as kinks. Kinks in one-dimensional space are generally expressed as solutions to specific differential equations. Mathematically, in one dimension, kink structures are regions where the field transitions from one minimum state to another in a changing manner across space. These structures are particularly studied in field theories, cosmology, or areas like condensed matter physics in material science. "Kinks are particularly significant in modeling and comprehending the behaviors of fields and particles. Field theories and such topological structures are employed to understand the interactions and aggregations of fundamental particles. Additionally, research on kinks is conducted in condensed matter physics and material science to comprehend the formation and properties of specific structures.

There is more than one potential used for the kink model, but we will only focus on the potential in structure of $\lambda\phi^4$ in our model. Now let's first try to find the equation of motion by defining the lagrangian density in the kink system in one dimension.

$$L = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi), \tag{3.1.1}$$

the potential of the model

$$V(\phi) = -\frac{1}{4}m^2\phi^2 + \frac{\lambda}{4}\phi^4 + \frac{\lambda}{4}v^4 = \frac{\lambda}{4}(\phi^2 - v^2)^2, \tag{3.1.2}$$

where

$$m = \sqrt{2\lambda v^2}. \tag{3.1.3}$$

It's important to note that the Lagrangian is invariant under the change of the sign of the field $\phi \to -\phi$ but the symmetry is spontaneously broken due to the potential having two degenerate minima at $\phi = \pm v$. Upon quantization of the theory, these two minima correspond to two vacua that are physically equivalent. This theory can be considered as a system with a single scalar particle of mass m. Now let's look at the equation of motion of the kink

$$\frac{d^2\phi}{dt^2} - \frac{d^2\phi}{dx^2} = -\lambda\phi(\phi^2 - v^2). \tag{3.1.4}$$

To simplify the model we will use the static solutions, which satisfy

$$\frac{d^2\phi}{dx^2} - \lambda\phi(\phi^2 - v^2) = 0. \tag{3.1.5}$$

İf we define $\phi = vf$ and $u = \frac{m}{\sqrt{2}}x$ the energy of this static solution takes the following form

$$E = \frac{1}{2\sqrt{2}}\frac{m^3}{\lambda}\int du\left(\frac{1}{2}\left(\frac{df}{du}\right)^2 + \frac{1}{4}(f^2 - 1)^2\right) \tag{3.1.6}$$

It is obvious that $f(u)$ depends neither on m nor λ and the solution has an energy of order $\frac{m^3}{\lambda}$, which is much greater than the mass m of the elementary scalar. If the coupling is weak there is a divergence in the limit $\lambda \to 0$. This distinct property of solitons in field theory clarifies why they are not encountered in standard perturbative approaches to quantum field theory. We can easily solve the field equation by multiplying the equation of motion we wrote above for the static situation by $\frac{d\phi}{dx}$.

$$\frac{d\phi}{dx}\left(\frac{d^2\phi}{dx^2} - \lambda\phi(\phi^2 - v^2)\right) = \frac{d}{dx}\left(\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 - \frac{\lambda}{4}(\phi^2 - v^2)^2\right) = 0. \tag{3.1.7}$$

The term in parentheses is a constant, and if we solve the field equation by choosing

this constant as zero, we get the following result.

$$\phi(x) = v \tanh\left(\frac{m}{2}x\right). \tag{3.1.8}$$

This is the kink solution,

$$\phi(x) = -v \tanh\left(\frac{m}{2}x\right) \tag{3.1.9}$$

and this result gives us the anti kink solution. The localization of energy indicates that the kink can be seen as a particle and its mass derived from the total energy of the static solution

$$M_{cl} = \frac{m^3}{3\lambda}\ . \tag{3.1.10}$$

Procedures for kink system quantization are explained in great detail in this book [68]. Therefore, to give more insight into the subject and make it easier to understand, we will briefly show some things here. We start by identifying the classical vacuum solution, which corresponds to the minimum point of the potential. In cases where there are multiple degenerate minima, we select one, let's say $\phi = v$, as our initial reference. If we denote ϕ_{vac} as v, we can express this as

$$\phi(x,t) = \phi_{vac} + \eta(x,t)\ . \tag{3.1.11}$$

Using this we can arrive at the following normal mode equation

$$\left(-\frac{d^2}{dx^2} + V''(\phi_{vac})\right) f_j(x) = \omega_j^2 f_j(x), \tag{3.1.12}$$

where

$$\eta(x,t) = f_j(x) e^{i\omega_j t}. \tag{3.1.13}$$

Let's define the second derivative of the potential in terms of ϕ_{vac}

$$V''(\phi_{vac}) = -\frac{m^2}{2} + 3\lambda v^2 \tanh^2\left(\frac{m}{2}x\right) = m^2\left(1 - \frac{3}{2}\frac{1}{\cosh^2\left(\frac{m}{2}x\right)}\right). \tag{3.1.14}$$

These types of potentials are called reflectionless potentials. and its solutions are given in terms of some kind of hypergeometric functions. As a result, normal mode

frequencies can be found by solving the following equation

$$\left(-\frac{d^2}{dx^2} + m^2\left(1 - \frac{3}{2}\frac{1}{\cosh^2\left(\frac{m}{2}x\right)}\right)\right) f_j(x) = \omega_j^2 f_j(x). \tag{3.1.15}$$

This differential equation has two bound state solutions and the other solutions are scattering state solutions. We can express these solutions as follows:

$$\begin{aligned}
f_0(x) &= \sqrt{\frac{3m}{8}}\frac{1}{\cosh^2\left(\frac{m}{2}x\right)} \qquad \text{and} \qquad \omega_0^2 = 0, \\
f_1(x) &= \sqrt{\frac{3m}{4}}\frac{\sinh\left(\frac{m}{2}x\right)}{\cosh^2\left(\frac{m}{2}x\right)} \qquad \text{and} \qquad \omega_1^2 = \frac{3}{4}\mathrm{m}^2, \\
f_k^+(x) &= C_k\Bigg[\left(4k^2 + m^2 - 3m^2\tanh^2\left(\frac{m}{2}x\right)\right)\cos(kx) \\
&\qquad -6km\tanh\left(\frac{m}{2}x\right)\sin(kx)\Bigg] \qquad \text{and} \qquad \omega^2(\mathrm{k}) = \mathrm{k}^2 + \mathrm{m}^2, \\
f_k^-(x) &= C_k\Bigg[\left(4k^2 + m^2 - 3m^2\tanh^2\left(\frac{m}{2}x\right)\right)\sin(kx) \\
&\qquad +6km\tanh\left(\frac{m}{2}x\right)\cos(kx)\Bigg] \qquad \text{and} \qquad \omega^2(\mathrm{k}) = \mathrm{k}^2 + \mathrm{m}^2.
\end{aligned} \tag{3.1.16}$$

We can find the normalization constant C_k in the region $\frac{m}{2}x \gg 1$

$$C_k = \frac{1}{\sqrt{\pi(4k^2 + m^2)(4k^2 + 4m^2)}}\ . \tag{3.1.17}$$

Since it is difficult to see the phase shift from here, we can calculate the phase of the system by combining the scattering state wave functions as follows,

$$f_k(x) = f_k^4(x) + if_k^-(x) = C_k\left(4k^2 + m^2 - 3m^2\tanh^2\left(\frac{m}{2}x\right) + 6ikm\right)e^{ikx}, \tag{3.1.18}$$

and $x \to \infty$ the phase shift becomes

$$\delta(k) = -2\arctan\left(\frac{3mk}{m^2 - 2k^2}\right). \tag{3.1.19}$$

Now if we define kink mass

$$\begin{aligned} M_{kink} &= E_{kink} - E_{vac} \\ &= \Delta E_{cl} + \Delta E_{zp} + \Delta E_{ct} + O(\lambda), \end{aligned} \tag{3.1.20}$$

where

$$\Delta E_{cl} = E_{cl}(\phi_{kink}) - E_{cl}(\phi_{vac}) = M_{cl} \ . \tag{3.1.21}$$

M_{cl} here is the classical kink mass and

$$\Delta E_{zp} = \frac{1}{2}\sum_j \omega_j^{kink} - \frac{1}{2}\sum_j \omega_j^{vac} \tag{3.1.22}$$

is the sum of the shifts of the oscillator zero-point energies, and

$$\Delta E_{ct} = E_{ct}(\phi_{kink}) - E_{ct}(\phi_{vac}) \tag{3.1.23}$$

is the contribution from the counterterms. This term has various divergent terms but how these divergent terms were eliminated is also explained in this book [68]. The formula for the kink energy involves divergent integrals of the zero-point energies of the continuous modes around the kink and the vacuum states. To resolve this, we introduce a finite one-dimensional space of length a and impose periodic boundary conditions on $\eta(x)$, under the assumption that $a \to \infty$ at the end of the calculations. Although this transformation converts the integrals into sums by discretizing the spectra, these sums remain divergent. To ensure finiteness, let's consider space as being made up of $2N$ points, leading to a total of $2N$ normal modes. Eventually, we'll extend this notion as $N \to \infty$. The vacuum modes are currently identified by separate wavenumbers

$$k_n^{vac} a = 2\pi n, \qquad n = \pm 1, \pm 2, ..., \pm N \ . \tag{3.1.24}$$

The continuum modes about the kink satisfy

$$k_n^{kink} a + \delta(k_n^{kink}) = 2\pi n, \qquad n = \pm 1, \pm 2, ..., \pm N. \tag{3.1.25}$$

These imply that $k_n^{kink} = -k_{-n}^{kink}$ and $k_{n+1}^{kink} \approx k_n^{vac}$ for $0 < n \ll ma$, while for $n \gg ma$

$$(k_n^{kink} - k_n^{vac})a = -\delta(k_n^{vac}) + O(a^{-1}) \tag{3.1.26}$$

tends to zero. The absence of kink continuum modes with $n = \pm 1$ compensates for the two localized modes, with $\omega_0^{kink} = 0$ and $\omega_1^{kink} = \sqrt{\frac{3}{4}}m$, that have no counterparts in the vacuum sector. If we rewrite the zero point energy using this information we get:

$$\Delta E_{zp} = \frac{1}{2}(\omega_0^{kink} - \omega_{-1}^{vac}) + \frac{1}{2}(\omega_1^{kink} - \omega_1^{vac}) + \sum_{n=2}^{N}(\omega_n^{kink} - \omega_n^{vac}) \ . \tag{3.1.27}$$

While the first two terms come from bound state frequencies, the next terms will be calculated using continuum state solutions

$$\Delta E_{zp} = \frac{1}{2}(0 - m) + \frac{1}{2}\left(\sqrt{\frac{3}{4}}m - m\right) + \sum_{n=2}^{N}(\omega_n^{kink} - \omega_n^{vac}) \ . \tag{3.1.28}$$

The final term in the above equation corresponds to the contribution arising from the kink continuum modes and the remaining vacuum modes. The $\frac{1}{2}$ prefactor cancellation is compensated by a factor of 2 because the summation involves only positive n values. To compute this contribution from the continuum, we employ Equation (3.1.26) and express it as follows:

$$\begin{aligned}
\sum_{n=2}^{N}(\omega_n^{kink} - \omega_n^{vac}) &= \sum_{n=2}^{N}\left[\sqrt{(k_n^{kink})^2 + m^2} - \sqrt{(k_n^{vac})^2 + m^2}\right] \\
&= \sum_{n=2}^{N}\left[\sqrt{(k_n^{vac})^2 - 2k_n^{vac}\delta(k_n^{vac}) + m^2} - \sqrt{(k_n^{vac})^2 + m^2}\right] \\
&= -\sum_{n=2}^{N}\sqrt{(k_n^{vac})^2 + m^2}\left[\frac{k^{vac}\delta(k^{vac})}{((k_n^{vac})^2 + m^2)a} + O(a^{-2})\right].
\end{aligned} \tag{3.1.29}$$

If we now take the limits $N \to \infty$ and $a \to \infty$, this sum is converted to an integral, with

$$\frac{1}{a}\sum_{n=2}^{N} \to \frac{1}{2pi}\int_0^\infty dk. \tag{3.1.30}$$

When we examine the equation provided in terms of phase shifts above,

$$-\frac{1}{2\pi}\int_0^\infty dk\frac{k\delta(k)}{\sqrt{k^2+m^2}} = -\frac{1}{2\pi}\delta(k)\sqrt{k^2+m^2}|_0^\infty + \frac{1}{2\pi}\int_0^\infty dk\sqrt{k^2+m^2}\frac{d\delta(k)}{dk} \tag{3.1.31}$$

The integral on the right-hand side of this equation is

$$\begin{aligned}\frac{1}{2\pi}\int_0^\infty dk\sqrt{k^2+m^2}\frac{d\delta(k)}{dk} &= -\frac{3}{2\pi}m\int_0^\infty \frac{dk}{\sqrt{k^2+m^2}} - \frac{3}{4\pi}m\int_0^\infty \frac{m^2dk}{\sqrt{k^2+m^2}\left(2k^2+\frac{m^2}{2}\right)} \\ &= -\frac{3}{2\pi}m\int_0^\infty \frac{dk}{\sqrt{k^2+m^2}} - \frac{\sqrt{3}}{6}m \end{aligned} \tag{3.1.32}$$

while the surface term gives

$$-\frac{1}{2\pi}\delta(k)\sqrt{k^2+m^2}|_0^\infty = -\frac{3}{2\pi}m + m\ . \tag{3.1.33}$$

If we add the contribution of the continuum state, the zero point energy is as follows

$$\Delta E_{zp} = \left(\frac{\sqrt{3}}{12} - \frac{3}{2\pi}\right)m - \frac{3}{2\pi}m\int_0^\infty \frac{dk}{\sqrt{k^2+m^2}}\ . \tag{3.1.34}$$

We're still dealing with divergence. However, we haven't accounted for the contributions originating from the counterterm Lagrangian yet.

$$\Delta E_{ct} = -\frac{1}{2}\delta m^2\int dx(\phi_{kink}^2(x)-\phi_{vac}^2(x)) = -\frac{1}{2}\left[\frac{3\lambda}{2\pi}\int_0^\infty \frac{dk}{\sqrt{k^2+m^2}}\right]\left(-\frac{2}{\lambda}m\right) \tag{3.1.35}$$

The quantity is of order unity due to the cancellation of the λ factor in δm^2 by the $\frac{1}{\lambda}$ originating from the ϕ_{kink}^2, perfectly offsetting the divergence arising from the zero-point energies. Combining our findings, we arrive at this solution of the kink mass M_{kink} as

$$M_{kink} = \frac{m^3}{3\lambda} + \left(\frac{\sqrt{3}}{12} - \frac{3}{2\pi}\right)m + O\left(\frac{\lambda}{m}\right) \tag{3.1.36}$$

for the energy of the ground state in the kink sector.

3.2. Quantum Corrections to the Kink Solution in the Presence of a Heavy Non-relativistic Scalar Particle

We study the following model consisting of one real scalar field ϕ interacting with an another real scalar field Ψ in $(1+1)$ dimension, described by the Hamiltonian

$$H = \int_{-\infty}^{\infty} dx \Big[\frac{1}{2} : \pi(x)\pi(x) : + \frac{1}{2} : \partial_x\phi(x)\partial_x\phi(x) : + \frac{\lambda}{4} : \left(\phi^2(x) - v^2\right)^2 : \\ - \frac{1}{2M}\Psi^\dagger(x)\partial_x^2\Psi(x) + \mu^2\Psi^\dagger(x)\Psi(x) : \phi^2(x) : \Big] ,$$

where $v = \frac{m}{\sqrt{2\lambda}}$ (Evslin choice). The field ϕ and its conjugate momenta π in the Schrödinger picture can formally be expanded in terms of its normal modes, given by

$$\phi(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{1}{\sqrt{2\omega_p}} \left(a_{-p} + a_p^\dagger\right) e^{-ipx} , \tag{3.2.1}$$

$$\pi(x) = -i \int_{-\infty}^{\infty} \frac{dp}{2\pi} \sqrt{\frac{\omega_p}{2}} \left(a_{-p} - a_p^\dagger\right) e^{-ipx} , \tag{3.2.2}$$

where $\omega_p = \sqrt{p^2 + m^2}$ and :: is the normal ordering operation with respect to the creation $a_p^\dagger$ and annihilation operator a_p, more precisely, this is the naive vacuum, of the non-interacting theory around the zero of the field ϕ. In our model, we assume that the mass of the quantum particle associated with the excitation of Ψ field is heavy, therefore can be treated non-relativistically. For this to make sense in a coupled theory, we typically need,

$$\frac{1}{2M}\langle \partial_x\Psi^\dagger\partial_x\Psi\rangle << \text{Energy scale of } \phi . \tag{3.2.3}$$

The parameter μ^2 is the coupling constant and M is the mass of the Ψ particle. We choose units such that $\hbar = 1$ and $c = 1$ in this work (as common practice in high energy physics). In natural units, then, λ has dimensions of m^2, v is dimensionless, μ^2 has also mass dimensions (energy). We first treat the ϕ fields classically in the presence of quantum particle Ψ. In the one-particle sector for the Ψ fields, we assume

$$\langle \Psi^\dagger(x)\Psi(x)\rangle = \langle 0| \int_{-\infty}^{\infty} dz\ \psi^*(z)\Psi(z)\Psi^\dagger(x)\Psi(x) \int_{-\infty}^{\infty} dy\ \psi(y)\Psi^\dagger(y)|0\rangle = |\psi(x)|^2 \approx \delta(x) \tag{3.2.4}$$

where $|0\rangle$ is the vacuum. This assumption implies that the wave function for the Ψ particle is sharply localized around the light particle due to the interaction term $\mu^2\Psi^\dagger\Psi\phi_{cl}^2$ in the classical background field ϕ_{cl}. We show the *consistency* of this approximation, by explicitly calculating the spread of the resulting wave function below.

Classically, this model has two degenerate minima at $\phi = \pm v$ in the absence of the Ψ field. Under the above assumptions, the classical equation of motions for the ϕ field is given by

$$\frac{\partial^2\phi_{cl}}{\partial t^2} - \frac{\partial^2\phi_{cl}}{\partial x^2} = -\lambda(\phi_{cl}^2 - v^2)\phi_{cl} - 2\mu^2\delta(x)\phi_{cl}(0) \ . \tag{3.2.5}$$

This non-linear wave equation admits static solutions $\phi = \pm v$ corresponding to degenerate vacua in the limit as $\mu \to 0$. We also know that there are kink solutions that interpolates between these two vacuum configurations [69]

$$\phi_{cl}^{kink}(x) = v \tanh\left(\frac{m(x - x_0)}{2}\right) \ , \tag{3.2.6}$$

where x_0 is the location of the kink, when there is no δ-function. If the sign in front of tanh is negative, then solution is called anti-kink. We shall consider only kink solutions in this work (as there is really no difference in the other case). If we assume that the heavy particle does not move and fixed at $x = 0$, as if it is a classical background, and the light particle moves in this background potential (this corresponds to the Born-Oppenheimer approximation in this setting), the only admissible classical solution for the ϕ-field is $x_0 = 0$. To take into account quantum corrections, one can look at fluctuations around the kink solution as being done in the usual approach when the particle with mass M is not there. Here we do have a unique solution $\phi_{cl}^{kink}(x)$ to our $\delta(x)$-modified classical Equation (3.2.5) thanks to the fact that $\phi_{cl}^{kink}(0) = 0$. It is important to notice that translational symmetry is broken as the heavy particle is localized at $x = 0$. Therefore, the solution has a finite energy (mass)

$$M_{cl} = \int_{-\infty}^{\infty} dx \left(\frac{1}{2}\left(\frac{\partial\phi_{cl}^{kink}}{\partial x}\right)^2 + \frac{\lambda}{4}\left((\phi_{cl}^{kink}(x))^2 - v^2\right)^2 + \mu^2\delta(x)\phi_{cl}^{kink}(0)\right) dx = \frac{m^3}{3\lambda} \ , \tag{3.2.7}$$

which is exactly the same as the energy of the usual kink as $\phi_{cl}^{kink}(0) = 0$.

We are interested in quantum fluctuations around the kink solution and its effect/correction to the energy (mass) of this kink configuration.

Note that if we take the above kink solution for ϕ -field, to leading order the heavy system is subject to a "potential". If we consider the one-particle sector for the Ψ under this classical background kink solution for ϕ, we get the following Schrödinger equation

$$-\frac{1}{2M}\partial_x^2\psi(x) + \frac{\mu^2 m^2}{2\lambda}\tanh^2\left(\frac{mx}{2}\right)\psi(x) = E\psi(x)\ , \tag{3.2.8}$$

where $\psi(x)$ is the single particle wave function for the heavy particle. Rescaling x by $\sqrt{2M}$, and expanding the function tanh into Taylor series for large values of M, to leading order, we obtain

$$-\frac{1}{2M}\partial_x^2\psi(x) + \frac{\mu^2 m^4}{8\lambda}x^2\psi(x) = E\psi(x)\ . \tag{3.2.9}$$

This is the well-known quantum harmonic oscillator, where the ground state wave function is

$$\psi_{gr}(x) = \left(\frac{\mu m^2}{2\pi}\sqrt{\frac{M}{\lambda}}\right)^{1/4} e^{-\frac{\mu m^2}{4}\sqrt{\frac{M}{\lambda}}x^2}\ , \tag{3.2.10}$$

and the ground state energy is given by $E_{gr} = \frac{\mu m^2}{4\sqrt{M\lambda}}$. One can see that $\psi_{gr}^2(x) \to \delta(x)$ as $M \to \infty$ since $\frac{n}{\sqrt{\pi}}e^{-n^2x^2}$ is a delta sequence. This result is consistent with our approximation above. For large mass $M >> m$, we do get a highly peaked wave function around the location of the kink.

If we keep as an approximation $\delta(x)$ for the wave function $\psi_{gr}^2(x)$, the fluctuations around the kink $\phi = \phi_{cl}^{kink} + \eta$ with $\eta = f_s(x)e^{-\omega_s t}$ would satisfy

$$-\frac{d^2 f_s(x)}{dx^2} + m^2\left(1 - \frac{3/2}{\cosh^2\left(\frac{mx}{2}\right)}\right)f_s(x) + 2\mu^2\delta(x)f_s(x) = \omega_s^2 f_s(x)\ , \tag{3.2.11}$$

where f_s are the orthonormal normal modes of the fluctuations. Let us concentrate on

the Hamiltonian,

$$\tilde{H}_0 := -\frac{d^2}{dx^2} - \frac{3m^2}{2\cosh^2\left(\frac{mx}{2}\right)} \ . \tag{3.2.12}$$

The spectrum of this operator as well as associated (generalized) states are exactly known.

Consider the Schrödinger operator associated with the reflectionless interaction V given by

$$(\tilde{H}_0\psi)(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - \frac{\hbar^2}{2m}\kappa^2\frac{N(N+1)}{\cosh^2(\kappa x)}\psi(x) \ , \tag{3.2.13}$$

where $N \in \mathbb{N}$. In this case, the discrete spectrum is given by the set of eigenvalues $E_n = -\frac{\hbar^2\kappa^2}{2m}(N-n)^2$, where $n = 0, 1, 2, \ldots N-1$. The number of bound states is finite and equal to N, corresponding eigenfunctions are given by

$$\phi_n^{(N)}(x) = \sqrt{\kappa}\left((N-n)\frac{(2N+1-n)!}{n!}\right)^{1/2} P_N^{n-N}(\tanh(\kappa x)) \ , \tag{3.2.14}$$

where $P_\mu^\nu(x)$ is Legendre function, defined by $P_\nu^\mu(x) = \frac{1}{\Gamma(1-\mu)}\left(\frac{1+x}{1-x}\right)^{1/2} {}_2F_1(-\nu, \nu+1; 1-\mu; \frac{1-x}{2})$ in terms of hypergeometric functions ${}_2F_1$. In this example, the continuous spectrum is the positive real axis, i.e, $\sigma_c(H_0) = [0, \infty)$ and the generalized eigenfunctions are given by $\chi_k^{(N)}(x) = \left(\frac{k}{2\sinh(\pi k/\kappa)}\right)^{1/2} P_N^{ik/\kappa}(\tanh(\kappa x))$ with the generalized eigenvalues $E_k = \frac{\hbar^2 k^2}{2m}$, with $k \in \mathbb{R}$.

A comparison with our problem shows that, we must choose $N = 2$. Here, eigenvalues ω_k^2 are *energy squared*, for continuous states we can parametrize the energy-mass difference, $\omega^2 - m^2$ by momentum square k^2. In that case one can write down the discrete states as well as the continuum states, If we use the solutions in J. Evslin (manifestly finite derivation), we have even and odd solutions for our Hamiltonian H_0,

$$f_0^+(x) = \sqrt{\frac{3m}{8}}\frac{1}{\cosh^2(mx/2)} \quad \text{with} \quad \omega_0 = 0 \tag{3.2.15}$$

$$f_1^-(x) = \sqrt{\frac{3m}{4}}\frac{\sinh(mx/2)}{\cosh^2(mx/2)} \quad \text{with} \quad \omega_1 = \sqrt{\frac{3}{4}}m. \tag{3.2.16}$$

for the continuum states,

$$f_k^+(x) = \quad C_k\Big[(\frac{4k^2}{m^2} - 2 + 3\mathrm{sech}^2(\frac{mx}{2}))\cos(kx) - 6k/m\tanh(\frac{mx}{2})\sin(kx)\Big] \quad (3.2.17)$$

$$f_k^-(x) = \quad C_k\Big[(\frac{4k^2}{m^2} - 2 + 3\mathrm{sech}^2(\frac{mx}{2}))\sin(kx) + 6k/m\tanh(\frac{mx}{2})\cos(kx)\Big], \quad (3.2.18)$$

where $C_k = \frac{1}{\sqrt{\pi(4k^2/m^2+1)(4k^2/m^2+4)}}$ to get orthonormalization in a generalized sense.

Our problem is to study the modification of this spectrum due to a delta-interaction. We recently studied this problem in [71] for the discrete states, here we have (generalized) eigenstates for the continuum, strictly speaking this is a more general problem. However, parity invariance is preserved for the modified problem, that means we can separate states into $\pm$-parity eigenstates, thanks to one-dimensional nature of the problem, this allows us to find the exact continuum states for this case as explained in Appendix A. The result establishes that the odd bound state does not change, but the even one shifts as a result of the perturbation. Incidentally, for the delta-function modification one needs the exact greens function of the original Hamiltonian as well, fortunately, according to a paper by Grosche we have [We need to convert the answer into the form we use, he has an $h^2/2m$ in front and no scaling of x with m] the result. We remark that the Greens function is for the operator H_0, which has dimension *energy squared*, so the Greens function has dimensions *inverse length times inverse energy square*. We use ω^2 for the complex energy E here to remind ourselves this difference. Note that Grosche looks at negative part and calls it s, so s refers to $E < 0$, for $E > 0$, he uses $\sqrt{s} = -i\sqrt{E}$. For us this transsformation must occur at $\omega > m$, to convert the formulae, it is more natural to think of $\omega^2 - m^2$ as s

$$G(x, y|\omega) = \sum_{n=0}^{1} \frac{\psi_n(x)\overline{\psi_n(y)}}{\omega_n^2 - \omega^2} + \int_0^\infty dk \frac{\psi_k^\pm(x)\overline{\psi_k^\pm(y)}}{k^2 + m^2 - \omega^2}, \quad (3.2.19)$$

as a result (by modifying the formula in Grosche accordingly note he is missing an

inverse length κ, so one must put it back and use $\kappa \to m$ in our case),

$$\begin{aligned} G(x,y|\omega) &= \frac{1}{\sqrt{m^2-\omega^2}} \exp\Big(-|x-y|\sqrt{m^2-\omega^2}\Big) \\ &+ \frac{3m}{16}\frac{1}{\cosh^2(mx/2)\cosh^2(my)(\omega^2)}\Bigg[1-\Big(1-\frac{m}{\sqrt{m^2-\omega^2}}\Big) \\ &\times \cosh\Big(m|x-y|\Big[1+\frac{\sqrt{m^2-\omega^2}}{m}\Big]\Big)\Bigg] \\ &- \frac{3m}{8}\frac{\sinh(mx/2)\sinh(my/2)}{\cosh^2(mx/2)\cosh^2(my/2)[3m^2/4-\omega^2]}\Bigg[1-\Big(1-\frac{1}{2}\frac{m}{\sqrt{m^2-\omega^2}}\Big) \\ &\times \cosh\Big(m|x-y|\Big[\frac{1}{2}+\frac{\sqrt{m^2-\omega^2}}{m}\Big]\Big)\Bigg]. \end{aligned}$$

The even eigenstate, corresponding to $\omega_0 = 0$ now shifts to a higher value, $(\omega_0^*)^2$, given by the solution of

$$\frac{1}{2\mu^2} = \frac{1}{\sqrt{m^2-\omega^2}} + \frac{3}{16}\frac{m^2}{\omega^2}\frac{1}{\sqrt{m^2-\omega^2}}, \tag{3.2.20}$$

and the eigenfunction is also modified to

$$\hat{f}_0^+(x) = -\frac{G(0,x|\omega_*^2)}{dG(0,0|\omega^2)/d\omega^2|_{\omega_*^2}}. \tag{3.2.21}$$

In a similar spirit, we get the modified *even* continuum eigenstates with $\omega_k^2 = k^2 + m^2$,

$$\hat{f}_k^+(x) = f_k^+(x) + \frac{G(x,0|\omega^2+i0)f_k^+(0)}{\Phi(\omega^2+i0)}, \tag{3.2.22}$$

while the odd ones $f_k^-(x)$ remain unaltered. To verify normalization of these functions is a bit of a challenge[I believe our discontiunity computation actually gives it correctly, but a distributional verification would be nice]. This is required to obtain the correct basis functions. (here we mean by $F(\omega^2+i0)$ the limit $\lim_{\epsilon\to 0^+} F(\omega^2+i\epsilon)$). These new eigenstates can now be used to quantize the fluctuations, that we represent as η-fields (to linear order). Recall that we have then the (modified) completeness relation:

$$\hat{f}_0^+(x)\overline{\hat{f}_0^+(y)} + f_1^-(x)\overline{f_1^-(y)} + \int_0^\infty dk \hat{f}_k^+(x)\overline{\hat{f}_k^+(y)} + \int_0^\infty dk f_k^-(x)\overline{f_k^-(y)} = \delta(x-y). \tag{3.2.23}$$

As a result if we expand the field operator η via this basis (by the way, this basis is not the usual plane wave basis asymptotically, so the wave functions are actually

real, more conventional basis would be to pick combinations of $if^-(x)$ and $\hat{f}^+(x)$ and multiply them with an exponential. this is peculiar to one dimensions, we have waves with 4-wave vector (k,ω) as well as $(-k,\omega)$ superposed. This will be a non-equivalent quantization, the vacuum will be different, maybe we should switch to the usual plane-wave type one as Evslin does.)

$$\begin{aligned}\eta(x,t) &= \hat{f}_0^+(x)\frac{b_0 e^{-i\omega_0^* t}}{\sqrt{2\omega_0^*}} + \overline{\hat{f}_0^+(x)}\frac{b_0^\dagger e^{i\omega_0^* t}}{\sqrt{2\omega_0^*}} + f_1^-(x)\frac{b_1 e^{-i\omega_1 t}}{\sqrt{2\omega_1}} + \overline{f_1^-(x)}\frac{b_1^\dagger e^{i\omega_1 t}}{\sqrt{2\omega_1}} \\ &\quad + \int_0^\infty dk\Big[\frac{\hat{f}_k^+(x)}{\sqrt{2\omega_k}}\Big(c_k e^{-i\omega_k t} + c_k^\dagger e^{i\omega_k t}\Big) + \frac{f_k^-(x)}{\sqrt{2\omega_k}}\Big(d_k e^{-i\omega_k t} + d_k^\dagger e^{i\omega_k t}\Big)\Big],\end{aligned} \tag{3.2.24}$$

as well as

$$\Pi(x) = \partial_t \eta(x) \tag{3.2.25}$$

with the usual commutation relations among $b_0, b_0^\dagger$, $b_1, b_1^\dagger$, $c_k, c_k^\dagger$ and $d_k, d_k^\dagger$, and assuming distinct families do commute among each others, we get the canonical commutation for the field operators,

$$[\eta(x,t), \Pi(y,t)] = i\delta(x-y). \tag{3.2.26}$$

We showed with our calculations that when we add a heavy particle to the standard kink model, this heavy particle creates a repulsive delta potential in the system. We will try to calculate how much this resulting delta potential will change the kink mass. In order to calculate the change in kink mass, we first need to find the new phase shift, coming from the new wave function. First, let's start by defining the new wave function of the system by applying the formula (3.2.19) that we found in our previous article on how the delta function will change the wave function.

$$\hat{f}_k^+(x) = f_k^+(x) + \frac{G(x,0|\omega^2+i0)}{\frac{1}{2\mu^2} - G(0,0|\omega^2+i0)} f_k^+(0) \tag{3.2.27}$$

Let's specify the expressions we will use below.

$$f_k^+(0) = C_k\left(\frac{4k^2}{m^2}+1\right), \qquad G(0,0|\omega^2+i0) = \frac{1}{\sqrt{m^2-(\omega^2+i0)}}\left(1+\frac{3}{16}\frac{m^2}{(\omega^2+i0)}\right)$$

Since we will find a phase shift in the scattering state, it is necessary to analyze the

behavior of the wave function as $x \to \infty$.

$$\lim_{x\to\infty} f_k^+(x) = C_k\left[\left(\frac{2k^2}{m^2} - 1 + 3i\frac{k}{m}\right)e^{ikx} + \left(\frac{2k^2}{m^2} - 1 - 3i\frac{k}{m}\right)e^{-ikx}\right], \tag{3.2.28}$$

and

$$\begin{aligned}\lim_{x\to\infty} G(x,0|k^2) &= \frac{i}{k}e^{ikx} - \frac{3m}{4}\frac{e^{-mx}}{(k^2+m^2)}\left(1 - i\frac{m}{k}\right)\cosh(x(m-ik)) \\ &= \frac{i}{k}e^{ikx} - \frac{3}{8}\frac{m}{(k^2+m^2)}\left(1 - i\frac{m}{k}\right)\left(\cos(kx) - i\sin(kx)\right) \\ &= \frac{i}{k}e^{ikx} - \frac{3}{8}\frac{m}{(k^2+m^2)}\left(1 - i\frac{m}{k}\right)e^{-ikx}\end{aligned} \tag{3.2.29}$$

where

$$\omega_k^2 = k^2 + m^2 \tag{3.2.30}$$

kink's new wave function becomes as follows as x goes to infinity

$$\begin{aligned}\lim_{x\to\infty} \hat{f}_k^+(x) &= C_k\Bigg[\left(\frac{2k^2}{m^2} - 1 + 3i\frac{k}{m}\right)e^{ikx} + \left(\frac{2k^2}{m^2} - 1 - 3i\frac{k}{m}\right)e^{-ikx} \\ &+ \frac{\left(\frac{i}{k}e^{ikx} - \frac{3}{8}\frac{m}{(k^2+m^2)}\left(1 - i\frac{m}{k}\right)e^{-ikx}\right)}{\frac{1}{2\mu^2} - \frac{i}{k}\left(-1 + \frac{3}{16}\frac{m^2}{(k^2+m^2)}\right)}\left(\frac{4k^2}{m^2} + 1\right)\Bigg] \\ &= C_k\Bigg[\left(\frac{2k^2}{m^2} - 1 - 3i\frac{k}{m} - \frac{\left(\frac{3}{8}\frac{m}{(k^2+m^2)}\left(1 - i\frac{m}{k}\right)\right)}{\frac{1}{2\mu^2} - \frac{i}{k}\left(-1 + \frac{3}{16}\frac{m^2}{(k^2+m^2)}\right)}\left(\frac{4k^2}{m^2} + 1\right)\right)e^{-ikx} \\ &+ \left(\frac{2k^2}{m^2} - 1 + 3i\frac{k}{m} + \frac{\frac{i}{k}}{\frac{1}{2\mu^2} - \frac{i}{k}\left(-1 + \frac{3}{16}\frac{m^2}{(k^2+m^2)}\right)}\left(\frac{4k^2}{m^2} + 1\right)\right)e^{ikx}\Bigg].\end{aligned} \tag{3.2.31}$$

The above term is quite complex computationally, but we know that μ^2 is a very weak coupling constant, so the other terms in the denominator are quite small compared to $\frac{1}{\mu^2}$ and can be neglected or by using the same logic we can find the change in the wave function and the new phase difference with a simpler approach by using the Lippman Schwinger equation

$$\left(\frac{d^2}{dx^2} + k^2 + \frac{3}{2}\frac{m^2}{\cosh^2\left(\frac{m}{2}x\right)}\right)\tilde{f}_k(x) = 2\mu^2\tilde{f}_k(x) \tag{3.2.32}$$

where

$$\tilde{f}_k(x) = f_k(x) + 2\mu^2 G(x,0|E) f_k(0) \ . \tag{3.2.33}$$

The new wave function is below

$$\begin{aligned}\lim_{x\to\infty} \hat{f}_k^+(x) &= C_k \Bigg[\left(\frac{2k^2}{m^2} - 1 + 3i\frac{k}{m}\right) e^{ikx} + \left(\frac{2k^2}{m^2} - 1 - 3i\frac{k}{m}\right) e^{-ikx} \\ &+ 2\mu^2 \Bigg(\left(\frac{i}{k} e^{ikx} - \frac{3}{8} \frac{m}{(k^2+m^2)} \left(1 - i\frac{m}{k}\right) e^{-ikx} \right) \Bigg) \left(\frac{4k^2}{m^2} + 1\right) \Bigg],\end{aligned} \tag{3.2.34}$$

and the new phase shift is

$$\delta(k) = -2 \arctan \left(\frac{3mk + \frac{2\mu^2}{k}(4k^2 + m^2)}{m^2 - 2k^2} \right) \ . \tag{3.2.35}$$

We need to find the derivative of the new phase shift as we will require it to determine the change in the kink mass indicated in equation (3.1.31) at the beginning of the topic.

$$\frac{d\delta(k)}{dk} = -\left(\frac{k^4(12m + 32\mu^2) + k^2(6m^3 + 40\mu^2 m^2) - 4\mu^2 m^4}{4k^6 + k^4(5m^2 + 48\mu^2 m + 64\mu^4) + k^2(m^4 + 12\mu^2 m^3 + 32\mu^4 m^2) + 4\mu^4 m^4} \right) \tag{3.2.36}$$

$$-\frac{1}{2\pi} \int_0^\infty dk \frac{k\delta(k)}{\sqrt{k^2+m^2}} = \frac{1}{2\pi} \int_0^\infty dk \sqrt{k^2+m^2} \frac{d\delta(k)}{dk} - \frac{1}{2\pi} \sqrt{k^2+m^2} \delta(k)|_0^\infty \tag{3.2.37}$$

The first term on the right side of the integral above is divergent. Therefore, to eliminate the divergence, we need to choose a method as follows:

$$\frac{1}{2\pi} \int_0^\infty dk \left(\sqrt{k^2+m^2} \frac{d\delta(k)}{dk} + \frac{\beta}{\sqrt{k^2+m^2}} \right) = \frac{1}{2\pi} \int_0^\infty \frac{dk}{\sqrt{k^2+m^2}} \left((k^2+m^2) \frac{d\delta(k)}{dk} + \beta \right). \tag{3.2.38}$$

Now let's focus on this term $(k^2+m^2)\frac{d\delta(k)}{dk}$

$$= -\left(\frac{k^6(12m + 32\mu^2) + k^4(18m^3 + 72\mu^2 m^2) + k^2(6m^5 + 36\mu^2 m^4) - 4\mu^2 m^6}{4k^6 + k^4(5m^2 + 48\mu^2 m + 64\mu^4) + k^2(m^4 + 12\mu^2 m^3 + 32\mu^4 m^2) + 4\mu^4 m^4} \right) \tag{3.2.39}$$

and we can eliminate the divergent part and then calculate the correction

$$\begin{aligned}&-k^6(12m+32\mu^2)-k^4(18m^3+72\mu^2m^2)-k^2(6m^5+36\mu^2m^4)+4\mu^2m^6\\&+\beta\big(4k^6+k^4(5m^2+48\mu^2m+64\mu^4)+k^2(m^4+12\mu^2m^3+32\mu^4m^2)+4\mu^4m^4\big)\ .\end{aligned}\tag{3.2.40}$$

The k^6 term is responsible for the divergence occurring here. Setting β to eliminate this term appropriately could help us overcome this problem.

$$\beta = 3m + 8\mu^2 \tag{3.2.41}$$

and the other terms

$$\begin{aligned}&-k^4(18m^3+72\mu^2m^2)-k^2(6m^5+36\mu^2m^4)+4\mu^2m^6\\+\ &(3m+8\mu^2)\big(k^4(5m^2+48\mu^2m+64\mu^4)+k^2(m^4+12\mu^2m^3+32\mu^4m^2)+4\mu^4m^4\big)\\=\ &k^4(-18m^3-72\mu^2m^2+15m^3+144\mu^2m^2+192\mu^4m+40\mu^2m^2+384\mu^4m+512\mu^6)\\+\ &k^2(-6m^5-36\mu^2m^4+3m^5+36\mu^2m^4+96\mu^4m^3+8\mu^2m^4+96\mu^4m^3+256\mu^6m^2)\\+\ &4\mu^2m^6+12\mu^4m^5+32\mu^6m^4\\=\ &k^4(-3m^3+112\mu^2m^2+576\mu^4m+512\mu^6)\\+\ &k^2(-3m^5+8\mu^2m^4+192\mu^4m^3+256\mu^6m^2)\\+\ &4\mu^2m^6+12\mu^4m^5+32\mu^6m^4\ .\end{aligned}\tag{3.2.42}$$

Now we can start doing the integral carefully

$$\begin{aligned}&\int_0^\infty\frac{dk}{\sqrt{k^2+m^2}}\left(\frac{k^4(-3m^3+112\mu^2m^2)+k^2(-3m^5+8\mu^2m^4)+4\mu^2m^6}{4k^6+k^4(5m^2+48\mu^2m)+k^2(m^4+12\mu^2m^3)+4\mu^4m^4}\right)\\=\ &-3m^3\int_0^\infty\frac{dk}{\sqrt{k^2+m^2}(4k^2+m^2)}\\+\ &4\mu^2m^2\int_0^\infty\frac{dk}{\sqrt{k^2+m^2}}\frac{(k^2+m^2)^2}{(4k^6+5m^2k^4+m^4k^2+4\mu^4m^4)}\\+\ &108\mu^2m^2\int_0^\infty\frac{dk}{\sqrt{k^2+m^2}}\frac{k^2}{(k^2+m^2)(4k^2+m^2)}\\=\ &-\frac{\pi}{\sqrt{3}}m+36\mu^2(1-\frac{\pi}{3\sqrt{3}})\\+\ &4\mu^2\int_0^\infty\frac{dx}{\sqrt{x^2+1}}\frac{(x^2+1)^2}{(4x^6+5x^4+x^2+4\frac{\mu^4}{m^2})}\ .\end{aligned}\tag{3.2.43}$$

The final result coming from the above integral is,

$$\frac{1}{2\pi}\int_0^\infty \frac{dk}{\sqrt{k^2+m^2}}\left(\frac{k^4(-3m^3+112\mu^2m^2)+k^2(-3m^5+8\mu^2m^4)+4\mu^2m^6}{4k^6+k^4(5m^2+48\mu^2m)+k^2(m^4+12\mu^2m^3)+4\mu^4m^4}\right)$$
$$=-\frac{\sqrt{3}}{6}m+\frac{18}{\pi}\mu^2(1-\frac{\pi}{3\sqrt{3}})+\frac{2\mu^2}{\pi}\int_0^\infty \frac{dx}{\sqrt{x^2+1}}\frac{(x^2+1)^2}{(4x^6+5x^4+x^2+4\frac{\mu^4}{m^2})}\ . \quad (3.2.44)$$

The right hand side integral can be solved as follows;

$$\int_0^\infty \frac{dx}{\sqrt{x^2+1}}\frac{(x^2+1)^2}{(4x^6+5x^4+x^2+4\frac{\mu^4}{m^2})}=\int_0^{\frac{\mu^2}{m}} dx\frac{(x^2+1)^{\frac{3}{2}}}{x^2+4\frac{\mu^4}{m^2}}+\int_{\frac{\mu^2}{m}}^\infty \frac{dx}{x^2}\frac{\sqrt{x^2+1}}{4x^2+1}\ . \quad (3.2.45)$$

We see that all correction terms are very small proportional to the coupling constant μ^2. And the surface term becomes,

$$-\frac{1}{2\pi}\left[\lim_{k\to\infty}\delta(k)\sqrt{k^2+m^2}-\lim_{k\to 0}\delta(k)\sqrt{k^2+m^2}\right]=-\frac{(3m+8\mu^2)}{2\pi}+\frac{5m}{4}. \quad (3.2.46)$$

Alternatively, we can find the kink mass correction by using perturbation theory. When we put the effect of the heavy particle on the kink into the normal mode equation we found for the kink, we see that it is not easy to solve both the $\delta(x)$ and $\frac{1}{\cosh^2}$ potentials together. therefore, since the effect of the heavy particle will be small, we need to add it to the system as perturbation. As we mentioned above, there are two bound states in the kink normal mode equation and they are discrete, so it will be sufficient to calculate the first order perturbation to find the corrections that will come in the first two modes. Let's rewrite the two bound state solutions

$$f_0(x)=\sqrt{\frac{3m}{8}}\frac{1}{\cosh^2\left(\frac{m}{2}x\right)}$$
$$f_1(x)=\sqrt{\frac{3m}{4}}\frac{\sinh\left(\frac{m}{2}x\right)}{\cosh^2\left(\frac{m}{2}x\right)}\ , \quad (3.2.47)$$

$$\delta\omega_0^2 = <f_0|2\mu^2\delta(x)|f_0>=\frac{3}{4}\mu^2m\int dx\frac{\delta(x)}{\cosh^4\left(\frac{m}{2}x\right)}=\frac{3}{4}\mu^2m$$
$$\delta\omega_1^2 = <f_1|2\mu^2\delta(x)|f_1>=\frac{3}{2}\mu^2m\int dx\delta(x)\frac{\sinh\left(\frac{m}{2}x\right)}{\cosh^2\left(\frac{m}{2}x\right)}=0\ . \quad (3.2.48)$$

If we write shifted normal modes for discrete states

$$\tilde{\omega}_0^2 = \frac{3}{4}\mu^2 m, \qquad \tilde{\omega}_1^2 = \frac{3}{4}m^2 \ , \tag{3.2.49}$$

let's rewrite the zero-point energy using shifted normal modes

$$\begin{aligned} \Delta E_{zp} &= \frac{1}{2}(\tilde{\omega}_0^{kink} - \omega_{-1}^{vac}) + \frac{1}{2}(\tilde{\omega}_1^{kink} - \omega_1^{vac}) + \sum_{n=2}^{\infty}(\tilde{\omega}_n^{kink} - \omega_n^{vac}) \\ &= \frac{1}{2}(\sqrt{\frac{3}{4}}\mu\sqrt{m} - m) + \frac{1}{2}(\sqrt{\frac{3}{4}}m - m) + \sum_{n=2}^{\infty}(\tilde{\omega}_n^{kink} - \omega_n^{vac}) \ . \end{aligned} \tag{3.2.50}$$

Now let's go back to the heavy particle equation and see how much fluctuations around the kink field affect the heavy particle system

$$\begin{aligned} -\frac{1}{2M}\nabla_x^2\psi(x) + \mu^2(\phi_{kink}(x) + \eta(x))^2\psi(x) &= (E + \delta E)\psi(x) \\ -\frac{1}{2M}\nabla_x^2\psi(x) + \mu^2\phi_{kink}^2(x) + 2\mu^2\phi_{kink}(x)\eta(x)\psi(x) + \mu^2\eta^2(x)\psi(x) &= (E + \delta E)\psi(x) \ . \end{aligned} \tag{3.2.51}$$

We can find the energy shift using the perturbation calculation

$$\begin{aligned} \delta E &= \mu^2 \int dx dx' \psi^\dagger(x) < f| \Big(2\phi_{kink}(x)\eta(x') + \eta^2(x') \Big) \psi(x) |f> \\ &= \mu^2 \int dx dx' \psi^\dagger(x) \Bigg(\phi_{kink}(x) \sqrt{\frac{2}{\omega}} < f|(a + a^\dagger)|f> \\ &+ \frac{1}{2\omega} < f| \Big((a^\dagger)^2 + aa^\dagger + a^\dagger a + a^2 \Big) |f> \Bigg) \psi(x) \\ &= \frac{\mu^2}{2\omega_1} \int dx |\psi(x)|^2 |f_1(x)|^2 \\ &= \frac{3m}{4} \frac{\mu^2}{2\omega_1} \sqrt{\frac{\mu m^2}{2\pi}} \sqrt{\frac{M}{\lambda}} \int dx e^{-\frac{\mu m^2}{2}\sqrt{\frac{M}{\lambda}}x^2} \frac{\sinh^2\left(\frac{m}{2}x\right)}{\cosh^4\left(\frac{m}{2}x\right)} \ , \end{aligned} \tag{3.2.52}$$

where

$$\omega_1 = \sqrt{\frac{3}{4}}m \ .$$

As we know from the Born Oppenheimer approximation, since the movement of the heavy particle is very slow, we can consider it very close to the origin, which means

that the wave function of the light particle will be evaluated at small x values.

Now we need to find the series expansion of the light particle's wave function for small x values

$$\frac{\sinh^2\left(\frac{m}{2}x\right)}{\cosh^4\left(\frac{m}{2}x\right)} = \frac{2}{3m}\frac{d}{dx}\tanh^3\left(\frac{m}{2}x\right) = \frac{m^2}{4}x^2 - \frac{5}{48}m^4x^4 + \frac{77}{2880}m^6x^6 + O(x^8) \quad (3.2.53)$$

After expanding the light particle's wave function as above, we can easily find the contribution to the heavy particle's energy

$$\begin{aligned}
\delta E &= \sqrt{\frac{3}{16}}\mu^2\sqrt{\frac{\mu m^2}{2\pi}\sqrt{\frac{M}{\lambda}}}\int dx e^{-\frac{\mu m^2}{2}\sqrt{\frac{M}{\lambda}}x^2}\left(\frac{m^2}{4}x^2 - \frac{5}{48}m^4x^4 + \frac{77}{2880}m^6x^6 + ...\right) \\
&= \sqrt{\frac{3}{16}}\mu^2\left[\frac{m^2}{4}\frac{1}{\mu m^2}\sqrt{\frac{\lambda}{M}} - \frac{15m^4}{48}\frac{1}{\mu^2m^4}\frac{\lambda}{M} + ...\right] \\
&= \frac{\sqrt{3}}{4}\frac{\lambda}{m^2}E_g - \frac{5}{4}\sqrt{3}\frac{\lambda}{M} + ... \\
&= \frac{1}{4\sqrt{3}}\frac{m}{M_{cl}}E_g - \frac{5}{12\sqrt{3}}\frac{m^2}{\mu^2}\frac{E_g^2}{M_{cl}^2} + ... \ . \qquad (3.2.54)
\end{aligned}$$

As we can see, the effect of a small fluctuation in the field on the heavy particle system is at the rate of $\frac{m}{M_{cl}}Eg$, which means that since the energy created by the fluctuation is very small, its effect on the system is negligible.

4. BORN OPPENHEIMER APPROXIMATION FOR A SIMPLE SYSTEM WHICH IS RENORMALIZABLE

4.1. Two heavy particles interacting with a light one

We consider two heavy particles interacting with a single light particle via a contact interaction in two dimensions. We write down the Schrödinger equation for this simple model;

$$\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2-\frac{\hbar^2}{2m}\nabla_x^2-\lambda\delta(x-x_1)-\lambda\delta(x-x_2)]\Big]\Psi(x;x_1,x_2)=E\Psi(x;x_1,x_2). \quad (4.1.1)$$

Here x_1, x_2 refer to the heavy particles coordinates and x refers to the light one (for simplicity ∇_{x_i} is written as ∇_i). The choices of the masses also reflect this difference. Let us pretend that the Born-Oppenheimer approximation can be applied to this system, thus we use a decomposition of the wave function into fast and slow degrees of freedom:

$$\Psi(x;x_1,x_2)=\phi(x|x_1,x_2)\psi(x_1,x_2). \quad (4.1.2)$$

We assume that this decomposition respects the translational invariance of the system, moreover we assume for the time being that the delta-functions are actually regularized since we know that there is a divergence hidden in this problem. We substitute the proposed solution into the Schrödinger equation,

$$\begin{aligned}&\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2\psi(x_1,x_2)\Big]\phi(x|x_1,x_2)+\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2\phi(x|x_1,x_2)\Big]\psi(x_1,x_2)\\&-\frac{\hbar^2}{2M}\sum_i 2\frac{\partial\phi}{\partial x_i}\frac{\partial\psi}{\partial x_i}+\Big[\big(-\frac{\hbar^2}{2m}\nabla_x^2-\lambda\delta(x-x_1)-\lambda\delta(x-x_2)\big)\phi(x|x_1,x_2)\Big]\psi(x_1,x_2)\\&\quad=E\phi(x|x_1,x_2)\psi(x_1,x_2). \quad (4.1.3)\end{aligned}$$

In general, we should assume an expansion, in terms of a complete set of solutions to the system relative to the light particle. Here the separation between the light binding energy for the gorund state configuration and the other levels is very large, we expect

negligible overlap with other solutions so we ignore them. Ordinarily we would assume that we could find the solution to the equation below,

$$-\frac{\hbar^2}{2m}\nabla_x^2\phi(x|x_1,x_2)-\lambda[\delta(x-x_1)+\delta(x-x_2)]\phi(x|x_1,x_2)=E(x_1,x_2)\phi(x|x_1,x_2). \quad (4.1.4)$$

That would mean that the heavy particles would act like fixed centers and the light particle would move in this background. Then we would find,

$$\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2\psi(x_1,x_2)+E(x_1,x_2)\psi(x_1,x_2)\Big]\phi(x|x_1,x_2)-\frac{\hbar^2}{M}\sum_i \nabla_i\phi\cdot\nabla_i\psi$$
$$+\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2\phi(x|x_1,x_2)\Big]\psi(x_1,x_2)=E\phi(x|x_1,x_2)\psi(x_1,x_2), \quad (4.1.5)$$

and if we could neglect the last two terms on the left hand side, we would end up with the Born-Oppenheimer result,

$$\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2+E(x_1,x_2)\Big]\psi(x_1,x_2)=E\psi(x_1,x_2). \quad (4.1.6)$$

Nevertheless we will see that this would be wrong, and we would end up with a divergent result. The expression

$$\Big[-\frac{\hbar^2}{2M}\sum_i {\nabla_i}^2\phi(x|x_1,x_2)\Big] \quad (4.1.7)$$

contains a term that we can convert into

$$\Big[-\frac{\hbar^2}{2M}{\nabla_x}^2\phi(x|x_1,x_2)\Big] \quad (4.1.8)$$

hence should be incorporated into the term (4), resulting into

$$-\Big(\frac{\hbar^2}{2m}+\frac{\hbar^2}{2M}\Big)\nabla_x^2\phi(x|x_1,x_2)-\lambda[\delta(x-x_1)+\delta(x-x_2)]\phi(x|x_1,x_2)$$
$$=E(x_1,x_2)\phi(x|x_1,x_2), \quad (4.1.9)$$

to be renormalized all together in this two-dimensional case. Note that because of the divergence, the usual rule of ignoring m/M terms at this order does not work here. Moreover, the effective potential generated from the derivative terms contain a $\frac{1}{z^2}$ term, where z is the relative coordinate for the two heavy particles. This term cannot be added as a perturbation since it changes the character of the wave function at the origin,

hence should be used in the leading order Born-Oppenheimer type approximation.

To set up the formalism, we will introduce an ansatz for the solution of the light degrees of freedom, assuming for the time being that the delta functions are properly regularized–one possibility is to use the heat kernel itself, this will preserve the translational invariance of the whole system, for the time being we will proceed formally:

$$\phi(x|x_1,x_2) = A(x_1,x_2)\Big(\eta_+(x|x_1,x_2) + \eta_-(x|x_1,x_2)\Big). \tag{4.1.10}$$

Later, we use as coordinates, the center of mass of the heavy particles and the relative position,

$$X = \frac{x_1+x_2}{2} \quad \text{and} \quad z = x_1 - x_2,$$

we will see that these are the natural coordinates for our system. Let us search for the solution in the following form,

$$\phi(x|x_1,x_2) = N\left[\int_0^\infty \frac{dt}{\hbar} K_t(x,x_1)e^{-\frac{\nu^2}{\hbar}t} + \int_0^\infty \frac{dt}{\hbar} K_t(x,x_2)e^{-\frac{\nu^2}{\hbar}t}\right],$$

where

$$-\frac{\hbar^2}{2m_*}\nabla_x^2 K_t(x,y) + \hbar\frac{\partial K_t(x,y)}{\partial t} = 0, \tag{4.1.11}$$

is the usual heat equation in two-dimensions corresponding to a mass,

$$\frac{1}{m_*} = \frac{1}{m} + \frac{1}{M}, \tag{4.1.12}$$

the solution of which is the well-known Gaussian when we demand that it goes to a delta-function as "time" variable t goes to zero. Here, with the mentioned divergence in mind, we choose a corrected mass m_* for the heat kernel. Consequently, to get a solution (assuming the cut-off being removed), we need to satisfy the equation,

$$\frac{1}{\lambda} - \frac{1}{\hbar}\int_0^\infty dt K_t(x_1,x_1)e^{-\frac{\nu^2}{\hbar}t} = \frac{1}{\hbar}\int_0^\infty dt K_t(x_1,x_2)e^{-\frac{\nu^2}{\hbar}t}.$$

As a result to cure the divergence we need to choose the coupling constant as

$$\frac{1}{\lambda} = \frac{1}{\hbar}\int_0^\infty dt K_t(x_1, x_1) e^{-\frac{\epsilon^2}{\hbar}t},$$

in which an arbitrary bound state energy ϵ^2 appears for the system. This is the binding energy between a heavy particle and a light particle interacting with a contact interaction. Instead of the coupling constant this is what we need to choose, or we think of this as the measured quantity. The energy of the system when the two heavy particles interacting with a light particle is to be determined from this input. Here the dimensionless coupling constant is to be traded off with this binding energy, for this particular choice there is no need to introduce a finite part to the coupling constant. Thus we find a well-defined expression,

$$\frac{2m_*}{4\pi\hbar^2}\int_0^\infty \frac{dt}{t}(e^{-\frac{\epsilon^2}{\hbar}t} - e^{-\frac{\nu^2}{\hbar}t}) = \frac{2m_*}{4\pi\hbar^2}\int_0^\infty \frac{dt}{t} e^{-\frac{\nu^2}{\hbar}t - \frac{2m_* z^2}{4\hbar t}}.$$

Consequently we find the equation to be satisfied for the binding energy of the total system, in this approximation,

$$\ln\left(\frac{\nu^2}{\epsilon^2}\right) = 2K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu|z|\right),$$

where K_0 denotes the well-known modified Bessel function. Let us keep this expression in mind and calculate the resulting normalized wave functions, this requires evaluating

$$1 = \frac{N^2}{\hbar^2}\Bigg[\int_0^\infty dt_1 dt_2 [K_{t_1+t_2}(x_1, x_1) + K_{t_1+t_2}(x_2, x_2)] e^{-\frac{\nu^2}{\hbar}(t_1+t_2)} + 2\int_0^\infty dt_1 dt_2 K_{t_1+t_2}(x_1, x_2) e^{-\frac{\nu^2}{\hbar}(t_1+t_2)}\Bigg],$$

where we use the reproducing property of the Gaussian expression for the heat kernels. The integrals can be done easily by transforming to the variables,

$$t = t_1 + t_2, s = t_1 - t_2$$

$$1 = \frac{N^2}{\hbar^2}\left[\int_0^\infty dt\, t e^{-\frac{\nu^2}{\hbar}t}\left[K_t(x_1, x_1) + K_t(x_2, x_2)\right] + 2\int_0^\infty dt t K_t(x_1, x_2) e^{-\frac{\nu^2}{\hbar}t}\right],$$

or equivalently,

$$1 = 2\frac{N^2}{\hbar^2}\left(\frac{2m_*}{4\pi\hbar}\right)\left[\int_0^\infty dt e^{-\frac{\nu^2}{\hbar}t} + \int_0^\infty dt e^{-\frac{\nu^2}{\hbar}t - \frac{2m_* z^2}{4\hbar t}}\right].$$

This gives us,

$$N = \frac{1}{\sqrt{2}}\sqrt{\hbar}\nu\sqrt{\frac{4\pi\hbar}{2m_*}}\frac{1}{\sqrt{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu|z|K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu|z|\right)\right]}},$$

where $K_1(.)$ refers to the modified Bessel function. Consequently, we have the normalized wave function,

$$\phi(x|x_1,x_2) = \frac{1}{\sqrt{2\pi}}\frac{\frac{\sqrt{2m_*}}{\hbar}\nu}{\sqrt{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu|z|K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu|z|\right)\right]}}\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu|x-x_1|\right)\right.$$
$$\left. + K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu|x-x_2|\right)\right]$$

where $K_0(.)$ again is the zeroth order modified Bessel function. Using the more natural variables, $X = \frac{x_1+x_2}{2}$ and $z = x_1 - x_2$, we can rewrite

$$\begin{aligned}\phi(x|X,z) &= \frac{\frac{1}{\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu}{\sqrt{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu|z|K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu|z|\right)\right]}}\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu|x-X+\frac{z}{2}|\right)\right.\\ &\left. + K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu|x-X-\frac{z}{2}|\right)\right]\\ &= A(z)\Big[\eta_+(\nu(z),x-X+z/2)+\eta_-(\nu(z),x-X-z/2)\Big].\end{aligned}$$

Here we use,

$$A(z) = \frac{1}{\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\frac{1}{\sqrt{1+\frac{\sqrt{2m_*}}{\hbar}\nu|z|K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu|z|\right)}},$$
$$\eta_\pm(\nu,x-X\pm z/2) = K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu\left|x-X\pm\frac{z}{2}\right|\right).$$

Let us emphasize again that here $\nu = \nu(|z|)$, so it also depends on the distance $|z|$ between the two heavy centers and this will be crucial in our computations. As we will see, heavy particle limit implies that $|z|$ can be considered as small relative to the light particle length scale to be made precise below (in a subtle way).

We now take a step back and write equation (3) in the new coordinates with the proposed wave functions in mind,

$$\begin{aligned}
&\Big[-\frac{\hbar^2}{4M}\nabla_X^2-\frac{\hbar^2}{M}\nabla_z^2\Big]\psi(X,z)\phi(x|X,z)\\
+&\Big[\big(-\frac{\hbar^2}{2m}\nabla_x^2-\lambda\delta(x-x_1)-\lambda\delta(x-x_2)\big)\phi(x|X,z)\Big]\psi(X,z)\\
&=E\phi(x|X,z)\psi(X,z). \qquad (4.1.13)
\end{aligned}$$

We can write this as,

$$\begin{aligned}
&\Big(\Big[-\frac{\hbar^2}{4M}\nabla_X^2-\frac{\hbar^2}{M}\nabla_z^2\Big]\psi(X,z)\Big)\phi(x|X,z)+\Big(\Big[-\frac{\hbar^2}{4M}\nabla_X^2-\frac{\hbar^2}{M}\nabla_z^2\Big]\phi(x|X,z)\Big)\psi(X,z)\\
&\quad-\frac{\hbar^2}{4M}\nabla_X\psi(X,z)\cdot\nabla_X\phi(x|X,z)-\frac{\hbar^2}{M}\nabla_z\psi(X,z)\cdot\nabla_z\phi(x|X,z)\\
&\quad+\Big[\big(-\frac{\hbar^2}{2m}\nabla_x^2-\lambda\delta(x-x_1)-\lambda\delta(x-x_2)\big)\phi(x|X,z)\Big]\psi(X,z)\\
&\quad=E\phi(x|X,z)\psi(X,z)\ . \qquad (4.1.14)
\end{aligned}$$

Let us consider the second term and using the decomposition of the wave function we see that the first Laplacian becomes

$$\begin{aligned}
&(-\frac{\hbar^2}{4M}\nabla_X^2)\phi(x|X,z)\\
&\quad=A(z)(-\frac{\hbar^2}{4M}\nabla_X^2)[\eta_+(\nu(z),x-X+z/2)+\eta_-(\nu(z),x-X-z/2)]\\
&\quad=A(z)(-\frac{\hbar^2}{4M}\nabla_x^2)[\eta_+(\nu(z),x-X+z/2)+\eta_-(\nu(z),x-X-z/2)]\\
&\quad=(-\frac{\hbar^2}{4M}\nabla_x^2)\phi(x|X,z)\ . \qquad (4.1.15)
\end{aligned}$$

This term is actually *singular and should be renormalized with the light particle solution.* The other term, $\nabla_z^2\phi$, requires more care, let us note that the functions $\eta_\pm$ depend on z in two ways, one is through the difference $x-X\pm z/2$ the other is through the term $\nu(z)$. It is the first dependence that we should pay more attention to, let us divide the z derivatives acting on these functions as follows,

$$\nabla_z=\nabla_z|_\nu+(\nabla_z\nu)\frac{\partial}{\partial\nu}\ . \qquad (4.1.16)$$

Therefore, we have $\nabla_z^2=\nabla_z^2|_\nu+(\nabla_z^2\nu)\frac{\partial}{\partial\nu}+(\nabla_z\nu)^2\frac{\partial^2}{\partial\nu^2}+2(\nabla_z\nu)\frac{\partial}{\partial\nu}\nabla_z|_\nu$. Again, the

important term here is the first one, acting on the $\eta_\pm$ part of the wave function,

$$\nabla_z^2|_\nu(\eta_+ + \eta_-) = \frac{1}{4}(\nabla_x^2\eta_+ + \nabla_x^2\eta_-), \tag{4.1.17}$$

because, $\nabla_z\eta_\pm = \pm\frac{1}{2}\nabla_x\eta_\pm$. Hence, we have this part, named as the singular part, to be separated from the heavy system as claimed,

$$\Big[-\frac{\hbar^2}{M}\nabla_z^2\phi(x|X,z)\Big]_{\text{sing}} = -\frac{\hbar^2}{4M}\nabla_x^2\phi(x|X,z). \tag{4.1.18}$$

As a result, adding the terms (2.1.14) and (2.1.16) into the light particle solution, we have

$$\begin{aligned}
&\left(\Big[-\frac{\hbar^2}{4M}\nabla_X^2 - \frac{\hbar^2}{M}\nabla_z^2\Big]\psi(X,z)\right)\phi(x|X,z) + \left(\Big[-\frac{\hbar^2}{M}\nabla_z^2\Big]_{\text{reg}}\phi(x|X,z)\right)\psi(X,z)\\
&-\frac{\hbar^2}{4M}\nabla_X\psi(X,z)\cdot\nabla_X\phi(x|X,z) - \frac{\hbar^2}{M}\nabla_z\psi(X,z)\cdot\nabla_z\phi(x|X,z)\\
&+\left(\Big[-\frac{\hbar^2}{2M}\nabla_x^2 - \frac{\hbar^2}{2m}\nabla_x^2 - \lambda\delta(x-x_1) - \lambda\delta(x-x_2)\Big]\phi(x|X,z)\right)\psi(X,z)\\
&= E\phi(x|X,z)\psi(X,z).
\end{aligned} \tag{4.1.19}$$

Here, we named the remaining piece as the regular part. To simplify the computations we may assume $\psi(X,z) = e^{iQX}\Psi(z)$, that would essentially remove all the center of mass terms of the heavy particles from this expression, and we take the expectation value with the light degrees of freedom (note that we are projecting to *the ground state of the light system for fixed centers*, this is so much below from the other levels that we expect errors to be very small):

$$\begin{aligned}
&\int dx\phi(x|X,z)\left[\Big(-\frac{\hbar^2}{M}\nabla_z^2\Psi(z)\Big)\phi(x|X,z) + \left(\Big[-\frac{\hbar^2}{M}\nabla_z^2\Big]_{\text{reg}}\phi(x|X,z)\right)\Psi(z)\right.\\
&\left.-\frac{\hbar^2}{4M}\Psi(z)Q\cdot\nabla_X\phi(x|X,z) - \frac{\hbar^2}{M}\nabla_z\Psi(z)\cdot\nabla_z\phi(x|X,z)\right]\\
&+\underbrace{\int dx\left(\phi(x|X,z)\Big[-\frac{\hbar^2}{2M}\nabla_x^2 - \frac{\hbar^2}{2m}\nabla_x^2 - \lambda\delta(x-x_1) - \lambda\delta(x-x_2)\Big]\phi(x|X,z)\right)}_{-\nu^2(|z|)\quad\text{after renormalization}}\Psi(z)\\
&=\Big[E - \frac{\hbar^2Q^2}{4M}\Big]\Psi(z) = \delta E\Psi(z).
\end{aligned} \tag{4.1.20}$$

Thus we should work out all the individual terms here, we will see that the effective potential does not only come from the expansion of the binding energy $-\nu^2(|z|)$, the cross terms will also matter, especially the repulsive $\frac{1}{|z|^2}$ generated by these terms will make the wave function to vanish mildly at the origin. As a result,

$$\begin{aligned}
&-\frac{\hbar^2}{M}\nabla_z^2\Psi(z) - \nu^2(|z|)\Psi(z) - \frac{\hbar^2}{M}\int dx\phi(x-X|z)\nabla_z\phi(x-X|z)\cdot\nabla_z\Psi(z)\\
&+\Bigg(\int dx\phi(x-X|z)\Big[-\frac{\hbar^2}{M}\nabla_z^2\Big]_{\text{reg}}\phi(x-X|z)\\
&-\frac{\hbar^2}{4M}\int dx\phi(x-X|z)Q\cdot\nabla_X\phi(x-X|z)\Bigg)\Psi(z)\\
&=\delta E\Psi(z). \qquad (4.1.21)
\end{aligned}$$

Note that we deliberately wrote $\phi(x|X,z)=\phi(x-X|z)$ to emphasize this translational invariance of x, as a result $\nabla_X\phi(x-X|z) = -\nabla_x\phi(x-X|z)$, furthermore, we can redefine $x \to x-X$, hence the apparent dependence on X dissappears, we end up with,

$$\begin{aligned}
&-\frac{\hbar^2}{M}\nabla_z^2\Psi(z) - \nu^2(|z|)\Psi(z) - \frac{\hbar^2}{M}\int d^2x\phi(x|z)\nabla_z\phi(x|z)\cdot\nabla_z\Psi(z)\\
&+\Bigg(\int d^2x\phi(x|z)\Big[-\frac{\hbar^2}{M}\nabla_z^2\Big]_{\text{reg}}\phi(x|z) + \frac{\hbar^2}{4M}Q\cdot\underbrace{\int d^2x\phi(x|z)\nabla_x\phi(x|z)}_{\text{being an exact differential=0}}\Bigg)\Psi(z)\\
&=\delta E\Psi(z). \qquad (4.1.22)
\end{aligned}$$

In the subsequent pages we will complete this delicate calculation and obtain the effective potential. Let us reiterate that the seemingly negligible character of these terms are misleading, the resulting potential being rather singular and repulsive, this influences the behaviour of the wave function significantly around the origin. As we will see, *δE is not small*, it contains the energy of the light as well as the heavy system as it is written, it is the length scale associated to the heavy particle pair which is small compared to the light particle's spread of the wave function when the light particle is bound to an *isolated heavy particle*. The reader who is interested in the resulting potential can skip the calculations presented in the next section; they are essentially of a technical nature.

4.2. Effective Potential for the Heavy Degrees of Freedom

In this section, we provide some of the calculational details for the effective potential acting between the two heavy particles. Let us start with the regular expression

$$\int dx\phi(x|z)\Big[-\frac{\hbar^2}{M}\nabla_z^2\Big]_{\rm reg}\phi(x|z), \tag{4.2.1}$$

we recall that

$$\phi(x|z)=A(z)\Big(\eta_+(x+z/2)+\eta_-(x+z/2)\Big). \tag{4.2.2}$$

Let us explicitly write this expectation value as

$$\begin{aligned}
&-\frac{\hbar^2}{M}\int dxA(z)(\eta_++\eta_-)\Big[\nabla_z^2\Big(A(z)(\eta_++\eta_-)\Big)\Big]_{\rm reg}\\
&=-\frac{\hbar^2}{M}\int d^2xA(z)(\eta_++\eta_-)\Bigg[\underbrace{A(z)\Big[\nabla_z^2(\eta_++\eta_-)\Big]_{\rm reg}}_{(1)}\\
&+\underbrace{(\eta_++\eta_-)\nabla_z^2A(z)}_{(2)}+\underbrace{2\nabla_zA(z)\cdot\nabla_z(\eta_++\eta_-)}_{(3)}\Bigg]
\end{aligned} \tag{4.2.3}$$

so after the integration the numbered terms produce the following results:

$$\begin{aligned}
(1)&=-\frac{\hbar^2}{M}A^2\int d^2x(\eta_++\eta_-)\Big[\nabla_z^2(\eta_++\eta_-)\Big]_{\rm reg}\\
(2)&=-\frac{\hbar^2}{M}\left(\frac{1}{A}\nabla_z^2A\right)\\
(3)&=-\frac{\hbar^2}{M/2}A\int d^2x(\eta_++\eta_-)\nabla_zA\cdot\nabla_z(\eta_++\eta_-)
\end{aligned} \tag{4.2.4}$$

Let us recall that acting on $\eta_\pm$ the regular part of the z derivatives are given by

$$[\nabla_z^2]_{\rm reg}\eta_\pm=\Big[(\nabla_z^2\nu)\frac{\partial}{\partial\nu}+(\nabla_z\nu)^2\frac{\partial^2}{\partial\nu^2}+2(\nabla_z\nu)\cdot\frac{\partial}{\partial\nu}\nabla_z|_\nu\Big]\eta_\pm, \tag{4.2.5}$$

here in *cylindrical coordinates* z,θ, $\nabla_z^2=\frac{\partial^2}{\partial z^2}+\frac{1}{z}\frac{\partial}{\partial z}$, note that not to complicate the notation we use the same letter z for the radial coordinate. This will not lead to any confusion, since pure z derivatives only appear in ∇_z, and usually converted into radial derivatives for the particular solution. Note that this expression can be equivalently

written as:

$$[\nabla_z^2]_{\rm reg}\eta_\pm = \left[(\nabla_z^2\nu)\frac{\partial}{\partial\nu} + (\frac{\partial\nu}{\partial z})^2\frac{\partial^2}{\partial\nu^2} + 2\frac{\partial\nu}{\partial z}\frac{\partial}{\partial\nu}\hat{z}\cdot\nabla_z|_\nu\right]\eta_\pm. \tag{4.2.6}$$

This is the form that we will be using. For some of the calculations to follow, we remind the equation satisfied by ν below,

$$\ln\left(\frac{\nu^2}{\epsilon^2}\right) = 2K_0\left(\frac{\sqrt{2m}}{\hbar}\nu z\right)\ . \tag{4.2.7}$$

As a crucial step in our Born-Oppenheimer type approximation, we *assume* that $\frac{\sqrt{2m_*}}{\hbar}\epsilon z \ll 1$, the validity of which is to be justified later. We note that z is small compared to the distance scale defined by the wave function of the light particle, $\sqrt{2m_*}\epsilon/\hbar$, however we have a stronger result, thanks to the form of the eigenvalue expression, indeed $\sqrt{2m}\nu z/\hbar$ is small. If we assume $\frac{\nu}{\epsilon}$ to be large, we need a logartihmic increase on the other side as well, which turns out to be a consistent assumption. Then we expand the equation giving the bound state energy ν as a function of z, using the well-known short distance behaviour of $K_0(x) \approx -\ln(xe^\gamma/2) + ...$,

$$\ln\left(\frac{\nu^2}{\epsilon^2}\right) = -2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z e^\gamma\right) - 2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z e^{\gamma-1}\right)\frac{2m_*}{4\hbar^2}\nu^2z^2 + ..., \tag{4.2.8}$$

Then we collect the similar terms together,

$$\begin{aligned} &2\ln\left(\frac{\nu^2}{\epsilon^2}\right)\left[1 + \frac{1}{8}\frac{2m_*}{\hbar^2}\nu^2z^2 + ...\right] \\ &= -2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right) - 2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma-1}\right)\frac{2m_*}{4\hbar^2}\nu^2z^2 + ..., \end{aligned} \tag{4.2.9}$$

note that in the second logarithm term the factor $e^{\gamma-1}$ can be replaced with e^γ since this constant factor being multiplied with z^2 is of lower order, as long as we keep up to the second order expansion, so to simplify the expression we change this term to e^γ. Hence we can rewrite all of it as:

$$\ln\left(\frac{\nu^2}{\epsilon^2}\right) = -\left[\frac{1 + \frac{2m_*}{4\hbar^2}\nu^2z^2 + ...}{1 + \frac{2m_*}{8\hbar^2}\nu^2z^2 + ...}\right]\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right). \tag{4.2.10}$$

By expanding again the denominator,

$$\ln\left(\frac{\nu^2}{\epsilon^2}\right) = -\left[1 + \frac{2m_*}{8\hbar^2}\nu^2z^2...\right]\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right). \tag{4.2.11}$$

Let us reorganize this expression, to this purpose we define

$$\xi = \left(\frac{\nu^2}{\epsilon^2}\right)\frac{\sqrt{2m_*}}{\hbar}\epsilon z, \tag{4.2.12}$$

then,

$$\ln\left(\xi\frac{e^\gamma}{2}\right) = -\frac{1}{4}\xi e^{-\gamma}x\ln x + ..., \tag{4.2.13}$$

here we introduced $x = \frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma$. This equation can be solved order by order by iteration, since $x\ln(x) \ll 1$, we see that $\xi \approx 2e^{-\gamma}$, to a first approximation, which defines our zeroth order expression. We shall content ourselves with computing the correct first order result, namely

$$\nu^2 \approx \frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{ze^\gamma}e^{-\frac{e^{-2\gamma}}{2}x\ln x} = \frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{ze^\gamma}\left(1 - \frac{e^{-\gamma}}{4}\frac{\sqrt{2m_*}}{\hbar}\epsilon z\ln\left[\frac{\sqrt{2m_*}}{\hbar}\epsilon z\right] + ...\right), \tag{4.2.14}$$

where we dropped the precise constant in the logarithmic term. Notice that we have the emergence of the characteristic length scale $\zeta_0 = \frac{\hbar}{\sqrt{2m_*\epsilon}}$, which describes the spread of the light particle-heavy particle bound state wave function in our calculations. Then we see immediately that indeed

$$\frac{\sqrt{2m}}{\hbar}\nu(z)z \ll 1, \tag{4.2.15}$$

is true, hence we have the desired consistency for all our expansions below.

Knowing the exact relation for ν, one can immediately find the resulting derivative of ν with respect to the variable z:

$$\frac{\partial\nu}{\partial z} = -\frac{\frac{\sqrt{2m_*}}{\hbar}\nu^2 K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1 + \frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]}. \tag{4.2.16}$$

We remind for the convenience of the reader the small argument expansion of Bessel function $K_1(x)$,

$$K_1(x) \approx \frac{1}{2}\frac{1}{(x/2)} + \frac{1}{2}x\ln(\frac{x}{2}) + ... \quad \text{as } x \to 0^+. \tag{4.2.17}$$

The following next order term is of order x which we neglect, however this leads to an

ambiguity in the logarithmic part, any multiplicative constant can be admitted in the argument since it only affects the result at the neglected next order. At small distance, using the above approximation, we find

$$\frac{\partial\nu}{\partial z} \approx -\frac{1}{2}\frac{\nu}{z} - \frac{1}{8}\Big(\frac{\sqrt{2m_*}}{\hbar}\Big)^2\nu^3 z\ln\left[\frac{\sqrt{2m_*}}{2\hbar}\nu z\right], \tag{4.2.18}$$

which should be further simplified by using the expansion of $\nu(z)$ to first order. For the time being we only need the zeroth order expressions, so we will keep it as it is given. We also need the expression for the second derivative, which we can find exactly and present in Appendix B, we write here the leading order expansion, using the *radial variable* z, as follows

$$\frac{\partial^2\nu}{\partial z^2} \approx \frac{3}{4}\frac{\nu}{z^2} + \dots . \tag{4.2.19}$$

Note that here we should expand ν to first order again to find a consistent expansion. We remark that *for simplicity we kept m_* as it is*, it can be replaced with m at various places, but we may do this at the end.

Let us go back and work out each term separately, as we numbered them, the first piece becomes the following;

$$\begin{aligned}(1) = &-\frac{\hbar^2}{M}A^2\int d^2x(\eta_+ + \eta_-)\left(2\nabla_z\nu\cdot\nabla_z|_\nu\partial_\nu + \Big[\frac{1}{z}\frac{\partial\nu}{\partial z} + \frac{\partial^2\nu}{\partial z^2}\Big]\partial_\nu + \left(\frac{\partial\nu}{\partial z}\right)^2\partial_\nu^2\right)\\
&\times(\eta_+ + \eta_-) = -\frac{\hbar^2}{M}A^2\int d^2x\Bigg[\nabla_z\nu\cdot\eta_+\nabla_x\partial_\nu\eta_+ - \nabla_z\nu\cdot\eta_-\nabla_x\partial_\nu\eta_-\\
&+\underbrace{\nabla_z\nu\cdot\eta_-\nabla_x\partial_\nu\eta_+ - \nabla_z\nu\cdot\eta_+\nabla_x\partial_\nu\eta_-}_{(1_b)}\\
&+\underbrace{(\eta_+ + \eta_-)\Big[\frac{1}{z}\frac{\partial\nu}{\partial z} + \frac{\partial^2\nu}{\partial z^2}\Big]\partial_\nu(\eta_+ + \eta_-)}_{(1_c)} + \underbrace{(\eta_+ + \eta_-)\left(\frac{\partial\nu}{\partial z}\right)^2\partial_\nu^2(\eta_+ + \eta_-)}_{(1_d)}\Bigg],\end{aligned} \tag{4.2.20}$$

note that we used $\nabla_z|_\nu\eta_\pm = \pm\frac{1}{2}\nabla_x\eta_\pm$ in the first few terms. Shifting the integration variable by $\pm z/2$, one can check that

$$\int d^2x\left[\nabla_z\nu\cdot\eta_+\nabla_x\partial_\nu\eta_+ - \nabla_z\nu\cdot\eta_-\nabla_x\partial_\nu\eta_-\right] = 0. \tag{4.2.21}$$

Let us consider the other cross term, by an explicit computation of the derivative terms we find out that,

$$\begin{aligned}(1_b) &= -\frac{\hbar^2}{M}A^2\int d^2x\left[\eta_-\frac{\partial\nu}{\partial z}\hat{z}\cdot\nabla_x\partial_\nu\eta_+ - \eta_+\frac{\partial\nu}{\partial z}\hat{z}\cdot\nabla_x\partial_\nu\eta_-\right]\\ &= -\frac{\hbar^2}{M}A^2\frac{2m_*}{\hbar^2}\nu z\frac{\partial\nu}{\partial z}\int d^2x\eta_+\eta_-\\ &= -\frac{\hbar^2}{M}A^2\frac{2m_*}{\hbar^2}\nu z\frac{\partial\nu}{\partial z}\frac{\pi\hbar}{2m_*}\frac{\sqrt{2m_*}}{\nu}zK_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right).\end{aligned} \tag{4.2.22}$$

Up to this point we have an exact calculation. Let us now expand each term to leading order under the small z/ζ_0 assumption as before,

$$(1_b) \approx -\frac{2m_*}{M}A^2\frac{\partial\nu}{\partial z}\frac{z}{\nu}\frac{\pi\hbar^2}{2m_*} \approx \frac{1}{2}\frac{m_*}{M}\nu^2 \approx \frac{1}{2}\frac{m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{z} = \frac{1}{2}\frac{m_*}{M}\epsilon^2\frac{\zeta_0}{z}, \tag{4.2.23}$$

which shows that it is a small perturbation to the leading terms. We now calculate the next term,

$$\begin{aligned}(1_c) &= -\frac{\hbar^2}{M}A^2\Big[\frac{1}{z}\frac{\partial\nu}{\partial z}+\frac{\partial^2\nu}{\partial z^2}\Big]\int d^2x(\eta_+ + \eta_-)\partial_\nu(\eta_+ + \eta_-)\\ &= -\frac{\hbar^2}{2M}A^2\Big[\frac{1}{z}\frac{\partial\nu}{\partial z}+\frac{\partial^2\nu}{\partial z^2}\Big]\int d^2x\partial_\nu(\eta_+ + \eta_-)^2 = -\frac{\hbar^2}{2M}A^2\Big[\frac{1}{z}\frac{\partial\nu}{\partial z}+\frac{\partial^2\nu}{\partial z^2}\Big]\partial_\nu\frac{1}{A^2}\\ &= -\frac{\hbar^2}{2M}\Big[\frac{1}{z}\frac{\partial\nu}{\partial z}+\frac{\partial^2\nu}{\partial z^2}\Big](A^2\partial_\nu A^{-2}).\end{aligned} \tag{4.2.24}$$

Again this is an exact computation. Let us now find the leading contribution of this expression, we write below the expansion of $A^2\partial_\nu A^{-2}$ to leading order as $A^2\partial_\nu A^{-2} \approx -\frac{2}{\nu}+...$ The details of the calculation are given in Appendix B, using our leading order expansions for $\frac{\partial\nu}{\partial z}$ and $\frac{\partial^2\nu}{\partial z^2}$ given by (4.2.18) and (4.2.19) respectively, as well as the expansion above, we find

$$(1_c) \approx \frac{\hbar^2}{M}\frac{1}{4z^2}+... \ . \tag{4.2.25}$$

In a similar way, the last part (1_d) is computed,

$$
\begin{aligned}
&-\frac{\hbar^2}{M}A^2\left(\frac{\partial\nu}{\partial z}\right)^2\int d^2x(\eta_+ + \eta_-)\partial_\nu^2(\eta_+ + \eta_-)\\
&=-\frac{\hbar^2}{M}A^2\left(\frac{\partial\nu}{\partial z}\right)^2\int d^2x\left[\frac{1}{2}\partial_\nu^2(\eta_+ + \eta_-)^2-(\partial_\nu(\eta_+ + \eta_-))^2\right]\\
&=-\frac{\hbar^2}{M}A^2\left(\frac{\partial\nu}{\partial z}\right)^2\left[\frac{1}{2}\partial_\nu^2\frac{1}{A^2}-\int d^2x(\partial_\nu(\eta_+ + \eta_-))^2\right].
\end{aligned}
$$

Up to this point there is no approximation, we calculate the last part separately:

$$
\begin{aligned}
&\int d^2x(\partial_\nu(\eta_+ + \eta_-))^2\\
&=\frac{8\nu^2}{\hbar^2}\frac{\pi^2\hbar^2}{m^2}\int_0^\infty dt_1dt_2\,t_1t_2e^{-\frac{\nu^2}{\hbar}(t_1+t_2)}\left[K_{t_1+t_2}(0)+K_{t_1+t_2}(z/2,-z/2)\right]\\
&=\frac{\nu^2}{\hbar^2}\frac{\pi^2\hbar^2}{m_*^2}\int_{-t}^t ds(t^2-s^2)\int_0^\infty dte^{-\frac{\nu^2}{\hbar}t}\left[K_t(0)+K_t(z/2,-z/2)\right]\\
&=\frac{4\nu^2}{3\hbar^2}\frac{\pi^2\hbar^2}{m_*^2}\int_0^\infty dt\,t^3e^{-\frac{\nu^2}{\hbar}t}\left[K_t(0)+K_t(z/2,-z/2)\right]\\
&=\frac{4\nu^2}{3\hbar^2}\frac{\pi\hbar}{2m_*}\int_0^\infty dt\,t^2e^{-\frac{\nu^2}{\hbar}t}\left[1+e^{-\frac{2m_*z^2}{4\hbar t}}\right]\\
&=\frac{4\nu^2}{3\hbar^2}\frac{\pi\hbar}{2m_*}\left[\frac{2\hbar^3}{\nu^6}+\frac{\hbar^3}{4\nu^6}\Big(\frac{\sqrt{2m_*}\nu}{\hbar}z\Big)^3K_3\left(\frac{\sqrt{2m_*}\nu}{\hbar}z\right)\right].
\end{aligned}
\tag{4.2.26}
$$

Finally,

$$
(1_d)=-\frac{\hbar^2}{M}A^2\left(\frac{\partial\nu}{\partial z}\right)^2\left(\frac{1}{2}\partial_\nu^2\frac{1}{A^2}-\frac{4\nu^2}{3\hbar^2}\frac{\pi\hbar}{2m_*}\left[\frac{2\hbar^3}{\nu^6}+\frac{\hbar^3}{4\nu^6}\Big(\frac{\sqrt{2m_*}\nu}{\hbar}z\Big)^3K_3\left(\frac{\sqrt{2m_*}\nu}{\hbar}z\right)\right]\right).
\tag{4.2.27}
$$

As a result of a careful calculation, the details of which are given in Appendix B, we find the leading order of $A^2\partial_\nu^2A^{-2}$ term

$$
A^2\partial_\nu^2A^{-2}\approx\frac{6}{\nu^2}+\dots\,.
\tag{4.2.28}
$$

After an expansion of all these terms, again using the small argument behavior of

Bessel functions, to the leading order, we find that

$$(1_d) \approx \qquad \frac{\hbar^2}{M}\left[-\frac{3}{4z^2}+\frac{2}{3z^2}\right] \approx -\frac{\hbar^2}{M}\frac{1}{12z^2}+\dots\,. \tag{4.2.29}$$

As a result the leading term of the first part labeled as (1) above, is found as

$$(1) \approx \frac{\hbar^2}{M}\left[\frac{1}{4z^2}-\frac{1}{12z^2}\right]+\dots\,. \tag{4.2.30}$$

The next term here is labeled as (2),

$$-\frac{\hbar^2}{M}\frac{1}{A}\nabla_z^2 A = -\frac{\hbar^2}{M}\frac{1}{A}\left(\frac{\partial^2}{\partial z^2}+\frac{1}{z}\frac{\partial}{\partial z}\right)A\,. \tag{4.2.31}$$

Therefore, we need these derivatives, we collect the calculations in Appendix B, and we just state the result of these expansions. The first derivative term, to the leading order, is

$$\frac{1}{A}\left(\frac{1}{z}\partial_z A\right) \approx -\frac{1}{2z^2}+\dots\,. \tag{4.2.32}$$

The next derivative becomes, again to the leading order,

$$\frac{1}{A}\partial_z^2 A \approx \frac{3}{4z^2}+\dots\,. \tag{4.2.33}$$

As a consequence, the total derivative of normalization can be expanded at the leading order as

$$-\frac{\hbar^2}{M}\frac{1}{A}\nabla_z^2 A \approx -\frac{\hbar^2}{M}\frac{1}{4z^2}+\dots\,. \tag{4.2.34}$$

There is one more term, which corresponds to the expression number (3):

$$\begin{aligned}(3) &= -\frac{\hbar^2}{M}2A\partial_z A\int d^2x(\eta_+ +\eta_-)\left(\partial_z|_\nu(\eta_+ +\eta_-)+\frac{\partial\nu}{\partial z}\partial_\nu(\eta_+ +\eta_-)\right)\\ &= -\frac{\hbar^2}{M}2A\partial_z A\int d^2x\Big[\eta_+\partial_z|_\nu\eta_+ +\eta_-\partial_z|_\nu\eta_- +\eta_+\partial_z|_\nu\eta_- +\eta_-\partial_z|_\nu\eta_+\\ &\quad +\frac{\partial\nu}{\partial z}(\eta_+ +\eta_-)\partial_\nu(\eta_+ +\eta_-)\Big].\end{aligned} \tag{4.2.35}$$

To simplify our calculations, we make the following observation:

$$\partial_z|_\nu\int d^2x(\eta_+^2+\eta_-^2)=0. \tag{4.2.36}$$

As a result, equation (3) becomes

$$(3) = -\frac{\hbar^2}{M} 2A\partial_z A \int d^2x \left[\partial_z|_\nu \eta_+ \eta_- + \frac{1}{2}\frac{\partial \nu}{\partial z}\partial_\nu (\eta_+ + \eta_-)^2 \right]. \tag{4.2.37}$$

We divide the above term into two parts, the first of which can be easily found as

$$\begin{aligned}(3_a) &= -\frac{\hbar^2}{M} A\partial_z A \frac{\partial \nu}{\partial z}\partial_\nu \int d^2x (\eta_+ + \eta_-)^2 = -\frac{\hbar^2}{M} A\partial_z A \frac{\partial \nu}{\partial z}\partial_\nu \frac{1}{A^2} \\ &= -\frac{\hbar^2}{M}\frac{1}{A}\partial_z A \frac{\partial \nu}{\partial z} A^2 \partial_\nu \frac{1}{A^2} \approx \frac{\hbar^2}{M}\frac{1}{2z^2} + ...,\end{aligned} \tag{4.2.38}$$

where in the last line we present the short distance expansion of this part. In a similar way, we work out the second part,

$$(3_b) = -\frac{\hbar^2}{M} 2A\partial_z A \partial_z|_\nu \int d^2x \eta_+ \eta_- = -\frac{\hbar^2}{M} 2A\partial_z A \frac{\pi\hbar}{2m_*}\partial_z|_\nu \left[\frac{\sqrt{2m_*}}{\nu} z K_1 \left(\frac{\sqrt{2m_*}}{\hbar}\nu z \right) \right] \tag{4.2.39}$$

This expression is worked out in Appendix B, its expansion under the small z/ζ_0 approximation leads to

$$(3_b) \approx O\Big(\frac{m_*}{M}\nu^2\Big) + ..., \tag{4.2.40}$$

hence it is of lower order. Consequently the whole sum for (3) becomes in the leading approximation

$$(3) \approx \frac{\hbar^2}{M}\frac{1}{2z^2} + ... \tag{4.2.41}$$

We will now consider the cross term which contains first order derivative of the heavy particle wave functions in the averaged out Schrödinger equation given in Equation (4.1.22):

$$(*) := -\frac{\hbar^2}{M} \int d^2x \phi(x|z) \nabla_z \phi(x|z) \cdot \nabla_z \Psi(z). \tag{4.2.42}$$

We evaluate each term here,

$$
\begin{aligned}
(*) &= -\frac{\hbar^2}{M} 2\frac{\partial\Psi}{\partial z}\int d^2x A(\eta_+ + \eta_-)\left[(\eta_+ + \eta_-)\frac{\partial}{\partial z}A + A\frac{\partial}{\partial z}(\eta_+ + \eta_-)\right] \\
&= -\frac{\hbar^2}{M}\frac{\partial\Psi}{\partial z}\frac{2}{A}\partial_z A - \frac{\hbar^2}{M}\frac{\partial\Psi}{\partial z}2A^2\int d^2x(\eta_+ + \eta_-)\left(\partial_z|_\nu + \frac{\partial\nu}{\partial z}\partial_\nu\right)(\eta_+ + \eta_-) \\
&= -\frac{\hbar^2}{M}\frac{2}{A}\partial_z A\partial_z\Psi - \frac{\hbar^2}{M}\frac{\partial\Psi}{\partial z}2A^2\int d^2x\Bigg(\frac{1}{2}\partial_z|_\nu(\eta_+^2 + \eta_-^2) \\
&+ \partial_z|_\nu\eta_+\eta_- + \frac{1}{2}\frac{\partial\nu}{\partial z}\partial_\nu(\eta_+ + \eta_-)^2\Bigg) \\
&= -\frac{\hbar^2}{M}\frac{2}{A}\partial_z A\partial_z\Psi - \frac{\hbar^2}{M}\partial_z\Psi 2A^2\left(\frac{\pi\hbar}{2m_*}\frac{\partial}{\partial z}\Big|_\nu\frac{\sqrt{2m_*}}{\nu}|z|K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) + \frac{1}{2}\frac{\partial\nu}{\partial z}\partial_\nu\frac{1}{A^2}\right).
\end{aligned}
\tag{4.2.43}
$$

We now evaluate the derivative and use the Bessel function identity

$$
xK_{n-1}(x) - xK_{n+1}(x) = -2nK_n(x) \tag{4.2.44}
$$

for the resulting $K_2(\cdot)$, to arrive at

$$
\begin{aligned}
&-\frac{\hbar^2}{M}\partial_z\Psi\Bigg(\frac{2}{A}\partial_z A + A^2\frac{\pi\hbar}{2m_*}\Bigg[\frac{\sqrt{2m_*}}{\nu}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&-\frac{\sqrt{2m_*}}{\nu}z\frac{\sqrt{2m_*}\nu}{\hbar}\Big[\frac{\sqrt{2m_*}\nu}{\hbar}z\Big]^{-1}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&-\frac{\sqrt{2m_*}}{\nu}z\frac{\sqrt{2m_*}\nu}{\hbar}K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\Bigg] + \frac{\partial\nu}{\partial z}A^2\partial_\nu\frac{1}{A^2}\Bigg)
\end{aligned}
\tag{4.2.45}
$$

After cancelling K_1-terms, we expand this term to leading order, using the result for $A^2\partial_\nu A^{-2}$ that we found before, we find,

$$
(*) \approx C_1\frac{m_*}{M}\nu^2 z\partial_z\Psi\ln\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) + ..., \tag{4.2.46}
$$

where C_1 is a constant that we can explicitly compute. This is quite a remarkable result, we see that there is no $\frac{1}{z}$ term multiplying $\partial_z\Psi$ term. To get a well-defined operator we need to symmetrize this term, and the absence of $\frac{1}{z}$ implies that such a symmetrization will not lead to another $\frac{1}{z^2}$ correction to the potential term.

4.3. Energy Levels of the System

In the previous section we worked out all the leading terms for our system. We finally write down the leading order (effective) Schrödinger equation for the heavy degrees of freedom,

$$
\begin{aligned}
&-\frac{\hbar^2}{M}\nabla_z^2\Psi(z) - \nu^2(|z|)\Psi(z) - \frac{\hbar^2}{M}\int d^2x\phi(x|z)\nabla_z\phi(x|z)\cdot\nabla_z\Psi(z) \\
&+\left(\int d^2x\phi(x|z)\Big[-\frac{\hbar^2}{M}\nabla_z^2\Big]_{\text{reg}}\phi(x|z)\right)\Psi(z) \\
&\approx -\frac{\hbar^2}{M}\nabla_z^2\Psi(z) - \Big[\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{ze^\gamma}+...\Big]\Psi(z) + \Big[\frac{\hbar^2}{M}\frac{1}{12z^2}+...\Big]\Psi(z)+... = \delta E\Psi(z).
\end{aligned}
$$

This is a very interesting result, since the leading energy is not only given by the potential term that we have in the usual Born-Oppenheimer approximation but gets a non-perturbative contribution from the effective potential generated by the kinetic energy operator acting on the wave function of the light degrees of freedom.

The energy that one finds is by no means small, it grows with the mass ratio of the heavy one to the one of the light particle, namely M/m. Nevertheless, it has still an order by order expansion, the real expansion is being done with respect to the smallness of the average separation of the heavy particles relative to the spread of the light particle's true wave function for the given self-consistent configuration (which is again determined by z, albeit at a lower order).

The solution to the above equation is well-known in terms of the generalized Laguerre polynomials, being familiar from the hydrogenic atoms. In the ground state wave function we have no dependence on the angular coordinate therefore no angular momentum contribution. We write the resulting equation as

$$
-\frac{\hbar^2}{M}\left[\frac{\partial^2}{\partial z^2}+\frac{1}{z}\frac{\partial}{\partial z}-\frac{\beta^2}{z^2}\right]\Psi(z)-\frac{\alpha}{z}\Psi(z)=\delta E\Psi(z). \tag{4.3.1}
$$

By defining the following parameters and the new coordinate r

$$\delta E = -\frac{E_0}{K^2(n)} \qquad \text{where} \qquad E_0 = \frac{\alpha^2 M}{4\hbar^2} \qquad \text{also} \quad \beta^2 = 1/12$$
$$r = \frac{z}{z_0 K(n)} \qquad \text{where} \qquad z_0 = \frac{\hbar^2}{M\alpha} \qquad \text{and} \qquad \alpha = \frac{2\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma}, \tag{4.3.2}$$

we have a transformed equation:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{\beta^2}{r^2} + \frac{K}{r} - \frac{1}{4}\right] R_n = 0. \tag{4.3.3}$$

Considering the $r \to \infty$, one can see that we can write the solution in the form

$$R_n = C(n) e^{-\frac{r}{2}} \psi(r), \tag{4.3.4}$$

and putting this back into the equation, $\psi(r)$ must satisfy the equation

$$\frac{\partial^2 \psi}{\partial r^2} + \left(\frac{1}{r} - 1\right)\frac{\partial \psi}{\partial r} + \frac{1}{r}\left(K - \frac{1}{2}\right)\psi - \frac{\beta^2}{r^2}\psi = 0. \tag{4.3.5}$$

We investigate the small r behavior of the equation, and look for a solution by plugging r^δ into the most singular part of the equation (for $r \to 0^+$):

$$\delta(\delta - 1) r^{\delta - 2} + \frac{1}{r}\delta r^{\delta - 1} - (\beta^2) r^{\delta - 2} = 0.$$

We can easily see that

$$\delta^2 = \beta^2 \tag{4.3.6}$$

and we admit the regular solution, $\delta = \beta$, so that the wave function $\psi(r)$ should be of the form

$$\psi(r) = r^\beta g(r) \tag{4.3.7}$$

for a regular function $g(r)$. Let us plug this back into equation (56), to get

$$r\frac{\partial^2 g(r)}{\partial r^2} + (2\beta + 1 - r)\frac{\partial g(r)}{\partial r} + \left(K - \frac{1}{2} - \beta\right) g(r) = 0. \tag{4.3.8}$$

A general solution which is regular at $r = 0$ of this equation is

$$g(r) = L^{2\beta}_{K - \frac{1}{2} - \beta}(r). \tag{4.3.9}$$

where L_γ^α refers to the generalized Laguerre functions. In the absence of restrictions to the parameters the Laguerre functions grow exponentially at infinity; the normalizablity of the wave function imposes the restriction on the allowed values as

$$K(n) - \frac{1}{2} - \beta = n,$$

for any integer $n \geq 0$. Thus the resultant wave function becomes

$$R_n = C(n) r^\beta e^{-\frac{r}{2}} L_n^{2\beta}(r). \tag{4.3.10}$$

Consequently the energy becomes

$$E_n = -\frac{\alpha^2 M}{4\hbar^2} \frac{1}{\left(n + \frac{1}{2} + \beta\right)^2} = -\frac{2M}{m_*} \frac{\epsilon^2}{e^{2\gamma}\left(n + \frac{1}{2} + \beta\right)^2}.$$

When $n = 0$ this gives the true ground state

$$E_{gs} = -\frac{2M}{m} \frac{e^{-2\gamma}\epsilon^2}{(1+2\beta)^2},$$

where we replaced m_* with m to have the correct leading order expression. Moreover, we have the ground state wave function

$$R_0 = C r^\beta e^{-\frac{r}{2}} \qquad \text{and here} \qquad r = \frac{2z}{z_0(1+2\beta)}.$$

The properly normalized heavy particles wave function becomes

$$\Psi(z) = \sqrt{\frac{2}{\pi\Gamma(2\beta+2) z_0^2 (1+2\beta)^2}} \left(\frac{2z}{z_0(1+2\beta)}\right)^\beta e^{-\frac{z}{z_0(1+2\beta)}}. \tag{4.3.11}$$

These are finally our main results. It is essential to note that the energy goes with the M/m ratio. This is important because, as we let the heavy particle mass becomes infinite, the two heavy centers coalesce into a single center, renormalization that we perform does not allow this configuration, thus this limit leads to a divergence.

A crucial point to check for the consistency is the expectation value of the separation z within our approximation, that is with the solution we have found for the

heavy particle separation. Not surprisingly we find

$$< z > = \int_0^\infty \int_0^{2\pi} z dz d\theta |\Psi(z)|^2 z = \frac{e^\gamma}{4} \frac{\Gamma(2\beta+3)}{\Gamma(2\beta+2)} (1+2\beta) \frac{\hbar}{\sqrt{2m_*\epsilon}} \left(\frac{2m_*}{M}\right)$$
$$= \frac{e^\gamma}{2} \frac{\Gamma(2\beta+3)}{\Gamma(2\beta+2)} (1+2\beta) \left(\frac{m_*}{M}\right) \zeta_0, \tag{4.3.12}$$

where ζ_0 refers to the characteristic length scale of the light particle binding energy introduced in renormalization (it is the binding to a single heavy center). More properly we should compute the expectation value of the light particle binding energy. Which means we should find the leading order expectation value of

$$-\nu^2 = -\frac{\hbar}{\sqrt{2m_*}} \frac{2\epsilon}{e^\gamma z}. \tag{4.3.13}$$

As a result, the expectation value of the binding energy is:

$$\left\langle -\nu^2 \right\rangle = -4 \frac{M}{m_*} \frac{e^{-2\gamma}\epsilon^2}{(1+2\beta)^2} \approx -4 \frac{M}{m} \frac{e^{-2\gamma}\epsilon^2}{(1+2\beta)^2} = 2E_{gs}. \tag{4.3.14}$$

This shows that the binding is very large due to the light particle, the heavy centers are confined into a small region and thus they have very large kinetic energy due to extreme localization of the position, the sum comes out to be about half the value of this binding energy, as a result the system is strongly bound. If we think of this in terms of the time scales, our intuition is correct, the light particle is responding much more quickly than the heavy ones, even though they have comparable energies, thanks to the large mass difference. It remains as a challenge to corroborate this approach and gain a deeper understanding of the dynamics by means of a many body approach. We are not able to do it at the moment.

In Appendix C, we compute the next order corrections to the energy coming from the higher order expansions. These are not computed completely but some terms are found to illustrate the consistency of our approximations.

5. CONCLUSION

In this thesis, first part of our work focuses on analyzing the spectral characteristics of Schrödinger operators denoted as H_0, incorporating δ interactions. We consider H_0 under mild conditions commonly presumed in quantum systems. Diverging from conventional approaches, we investigate the pole structure of the Green function, G, and specifically demonstrate the elimination of poles from the original Green function, G_0. This removal occurs through eigenfunction expansions, contingent upon the non-vanishing nature of the original eigenfunction at the location of the delta function. Our findings shows that new bound state energies can be derived by solving the equation $\Phi(E) = 0$, where Φ is explicitly defined in terms of the diagonal Green's function. This discovery applies if the center of the delta function does not coincide with one of the nodes of the initial eigenfunction ϕ_k. Our investigations are confined to one-dimensional setups involving point-like delta interactions. We elucidate these concepts using the reflectionless potential for H_0 as a demonstrative case. Moreover, we introduce an alternative perturbative method for determining eigenvalues and eigenfunctions of the entire system, presented up to the second order in a heuristic manner. We extend these approaches to scenarios necessitating renormalization. In such cases, our results maintain consistency, although perturbative calculations differ at the second order of the delta interaction's coupling constant. Finally, we discuss potential avenues for extending our findings to encompass more generalized delta interactions such as supported on a curve and multi-center cases. Additionally, we consider scenarios involving particle motion on a compact two-dimensional manifold and explore semi-relativistic models on compact manifolds.

Secondly, upon introducing a heavy particle to a one-dimensional kink model, we employed the Born-Oppenheimer approach to resolve the system. The heavy particle created a repulsive δ potential. In the initial paper [71], we computed how the added delta potential changed the Green's function and wave function of the system. Utilizing this information, we calculated the new wave function of the kink and the associated

phase shift due to this modification. Subsequently, using this new phase shift, we computed the change in the kink mass. We observed that this change was of a small order, indicating the consistency of our calculations. Here, it's important to emphasize that the δ potential originating from the solution of the heavy particle equation of motion implies a modification in the kink model, where the original coupling constant becomes $\lambda \to \lambda + 8\mu^2$. Finally, we computed how the kink particle affected the energy of the heavy particle and showed that the perturbative correction is very small compared to the original one of order $\frac{m}{M_{cl}}$.

The final work of the thesis is related to three particle singular system in two dimension. In a singular system containing two heavy and one light particle, we employ the Born-Oppenheimer approximation assuming that the light particle's wave function spread significantly surpasses that of the heavy particles' relative coordinate wave function, represented by the variable z. In contrast to the conventional Born-Oppenheimer expansions, we observe that the heavy degrees of freedom remarkably contribute to the total energy of the system, approximately of the order $\frac{M}{m}$. Nonetheless, we still pursue an expansion of the total energy in terms of increasing powers of z and logarithms of z. Understanding this phenomenon from a many-body perspective, akin to our prior work on a one-dimensional version of this problem, holds considerable importance. Our imminent research plans involve a detailed investigation into this approach.

REFERENCES

1. Bohm, A., *The Rigged Hilbert Space and Quantum Mechanics*, Lecture Notes in Physics, Springer, 1978.

2. Bohm, A., Gadella, M., *Dirac Kets, Gamow Vectors and Gel'fand Triplets*, Lecture Notes in Physics, Springer, 1989.

3. Berezin, F. A., Shubin, M., *The Schrödinger Equation*, Springer, 2012.

4. Appel, W., *Mathematics for Physics and Physicists*, Princeton University Press, 2007.

5. Berezanskii, I. M., *Expansions in Eigenfunctions of Selfadjoint Operators*, American Mathematical Society, 1968.

6. Beliy, A. G., Kovalenko, V. F., Semenov, Y. A., "On the Continuity of Generalized Eigenfunctions of the Schrödinger Operator", *Reports on Mathematical Physics*, Vol. 12, No. 3, pp. 307-310, 1977.

7. Galindo, A., Pascual, P., *Quantum Mechanics I*, Springer, 2012.

8. Maurin, K., *General Eigenfunction Expansions and Unitary Representations of Topological Groups*, Polish Scientific Publishers, 1968.

9. Gadella, M., Gómez, F., "On the Mathematical Basis of the Dirac Formulation of Quantum Mechanics", *International Journal of Theoretical Physics*, Vol. 42, No. 10, pp. 2225-2254, 2003.

10. Weyl, H., "Über Gewöhnliche Differentialgleichungen Mit Singularitäten und die Zugehörigen Entwicklungen Willkürlicher Funktionen", *Mathematische Annalen*, Vol. 68, pp. 220-269, 1910.

11. Titchmarsh, E. C., *Eigenfunction Expansions Associated with Second-order Differential Equations, Part I*, Oxford, 1946.

12. Kodaira, K., "The Eigenvalue Problem for Ordinary Differential Equations of the Second Order and Heisenberg's Theory of S-Matrices", *American Journal of Mathematics*, Vol. 71, No. 4, pp. 921–945 1949.

13. Poerschke, T., Stolz, G., Weidmann, J., "Expansions in Generalized Eigenfunctions of Selfadjoint Operators", *Mathematische Zeitschrift*, Vol. 202, pp. 397-408, 1989.

14. Grosche, C., "Path Integrals for Potential Problems with δ-function Perturbation", *Journal of Physics A: Mathematical and General*, Vol. 23, No. 22, p. 5205, 1990.

15. Fassari, S., Inglese, G., "On the Spectrum of the Harmonic Oscillator with a Delta-type Perturbation" *Helv. Phys. Acta*, Vol. 67, No. 6, pp. 650-659, 1994.

16. Fassari, S., Inglese, G., "Spectroscopy of a Three Dimensional Isotropic Harmonic Oscillator with a δ Type Perturbation", *Helvetica Physica Acta*, Vol. 69, 1996.

17. Demiralp, E., "Bound States of n-dimensional Harmonic Oscillator Decorated with Dirac Delta Functions", *Journal of Physics A: Mathematical and General*, Vol. 38, p.4783, 2005.

18. Janke, W., Cheng, B. K., "Statistical Properties of a Harmonic Plus a Delta-Potential", *Physics Letters A*, Vol. 129, No. 3, pp. 140-144, 1988.

19. Uncu, H., Tarhan, D., Demiralp, E., Müstecaplıoğlu, Ö. E., "Bose-Einstein Condensate in a Harmonic Trap Decorated with Dirac δ Functions", *Physical Review A*, Vol. 76, No. 1, p. 013618, 2007.

20. Gadella,M., García-Ferrero, M. A., González-Martín, S., Maldonado-Villamizar, F. H., "The Infinite Square Well with a Point Interaction: A Discussion on the Different Parametrizations", *International Journal of Theoretical Physics*, Vol. 53,

No. 5, pp. 1614-1627, 2014.

21. Fassari, S., Gadella, M., Glasser, M. L., Nieto, L. M., "Spectroscopy of a One-Dimensional V-Shaped Quantum Well with a Point Impurity", *Annals of Physics*, Vol. 389, pp. 48-62, 2018.

22. Albeverio, S., Gesztesy, F., Hoegh-Krohn, R., Holden, H., *Solvable Models in Quantum Mechanics*, 2nd ed. American Mathematical Society, Chelsea, RI, with appendix by P. Exner, 2005.

23. Albeverio, S., Kurasov, P., *Singular Perturbation of Differential Operators*, Cambridge University Press, 2000.

24. Huang, K., *Quarks, Leptons and Gauge Fields*, World Scientific, Singapore, 1982.

25. Jackiw, R., *Delta-Function Potentials in Two- and Three-Dimensional Quantum Mechanics, M. A. B. Bég Memorial Volume*, World Scientific, Singapore, 1991.

26. Gosdzinsky, P., Tarrach, R., "Learning Quantum Field Theory from Elementary Quantum Mechanics", *American Journal of Physics*, Vol. 59, No. 70, 1991.

27. Mead, L. R., Godines, J. "An Analytical Example of Renormalization in Two-Dimensional Quantum Mechanics", *American Journal of Physics*, Vol. 59, No. 935, 1991.

28. Manuel, C., Tarrach, R., "Perturbative Renormalization in Quantum Mechanics", *Physics Letters B*, Vol. 328, No. 113, 1994.

29. Grosche, C., "Path integrals for Two- and Three-Dimensional δ-Function Perturbations", *Annalen der Physik*, Vol. 506, No. 4, 283-312 1994.

30. Albeverio, S., Fassari, S., Rinaldi, F., "Spectral Properties of a Symmetric Three-Dimensional Quantum Dot with a Pair of Identical Attractive δ Impurities Sym-

metrically Situated Around the Origin", *Nanosystems: Physics, Chemistry, Mathematics*, Vol. 7, No. 2, pp. 268-289, 2016.

31. Albeverio, S., Fassari, S., Rinaldi, F., "Spectral Properties of a Symmetric Three-Dimensional Quantum Dot with a Pair of Identical Attractive δ Impurities Symmetrically Situated Around the Origin II", *Nanosytems: Physics, Chemistry, Mathematics*, Vol. 5, No. 5, pp. 803–815, 2016.

32. Fassari, S., Gadella, M., Glasser,M. L., Nieto, L. M., Rinaldi, F., "Spectral Properties of the Two-Dimensional Schrödinger Hamiltonian with Various Solvable Confinements in the Presence of a Central Point Perturbation", *Physica Scripta*, Vol. 94, No. 5, p. 055202, 2019.

33. Landau, L. D., Lifshitz, E. M., *Quantum Mechanics: Non-Relativistic Theory*, 3rd ed., Butterworth-Heinemann, 1981.

34. Reed, M., Simon, B., *Methods of Modern Mathematical Physics III: Scattering Theory*, Academic Press, New York, 1979.

35. Gallone, M., Michelangeli, A., *Self-adjoint Extension Schemes and Modern Applications to Quantum Hamiltonians*, Springer International Publishing, 1st ed., 2023.

36. Dimock, J., Rajeev, S. G., "Multiparticle Schrödinger Operators with Point Interactions in the Plane", *Journal of Physics A: Mathematical and General*, Vol.37, No. 9157, 2004.

37. Reed, M., Simon, B., *Methods of Modern Mathematical Physics, Volume IV, Analysis of Operators*, Academic Press, New York, 1978.

38. Galindo, A., Pascual, P., *Quantum Mechanics II*, Springer, 2012.

39. Kato, T., *Perturbation Theory for Linear Operators*, Vol. 132, Springer, 2013.

40. Murdock, J. A., *Perturbations, Theory and Applications*, John Wiley and Sons, 1991.

41. Sólyom, J., *Fundamentals of the Physics of Solids: Volume II: Electronic Properties*, Appendix G, Springer, 2008.

42. Gilkey, P. B., *Invariance Theory, the Heat Equation, and the Atiyah-Singer Index Theorem*, 2nd edition, CRC Press, Boca Raton, 1995.

43. Erman, F., Turgut, O. T., "Point Interactions in Two and Three Dimensional Riemannian Manifolds", *Journal of Physics A: Mathematical and Theoretical*, Vol. 43, No. 33, 2010.

44. Besprosvany, J., "Recursive Analytical Formula for the Green's Function of a Hamiltonian Having a Sum of One-Dimensional Arbitrary Delta-Function Potentials" *Physics Review B*, Vol. 63, pp. 233108, 2001.

45. Erman, F., "Recursion Formula for the Green's Function of a Hamiltonian for Several Types of Dirac Delta-Function Potentials in Curved Spaces", *Turkish Journal of Physics*, Vol. 40, No. 3, pp. 316-323, 2016.

46. Brasche, J. F., Exner, P., Kuperin, Yu. A., Seba, P., "Schrödinger Operators with Singular Interactions", *Journal of Mathematical Analysis and Applications*, Vol. 184, No. 1, pp. 112-139, 1994.

47. Exner, P., Yoshitomi, K., "Asymptotics of Eigenvalues of the Schrödinger Operator with a Strong δ Interaction on a Loop", *Journal of Geometry and Physics*, Vol. 41, No. 4, pp. 344-358, 2002.

48. Kondej, S., "Spectral Asymptotics Induced by Approaching and Diverging Planar Circles", *Functional Analysis and Operator Theory for Quantum Physics: The Pavel Exner Anniversary Volume* edited by J. Dittrich, H. Kovarik, A. Laptev, European Mathematical Society, 2017.

49. Exner, P., Tater, M., "Spectra of Soft Ring Graphs", *Waves in Random Media*, Vol. 14, No. 1, p. 47, 2003.

50. Exner, P., Ichinose, T., "Geometrically Induced Spectrum in Curved Leaky Wires", *Journal of Physics A: Mathematical and General*, Vol. 34, No. 7, p. 1439, 2001.

51. Posilicano, A., "A Krein-like Formula for Singular Perturbations of Self-Adjoint Operators and Applications", *Journal of Functional Analysis*, Vol. 183, No. 1, pp. 109-147, 2001.

52. Exner, P. Kovarik, H., *Quantum Waveguides*, Springer, 2015.

53. Kaynak, B. T., Turgut, O. T., "Singular Interactions Supported by Embedded Curves", *Journal of Physics A: Mathematical and Theoretical*, Vol. 45, pp. 265-202, 2012.

54. Haroske, D., Triebel, H., *Distributions, Sobolev Spaces, Elliptic Equations*, European Mathematical Society, 2007.

55. Rosenberg, S., *The Laplacian on Riemannian Manifold*, Cambridge University Press, Cambridge, 1998.

56. Chavel, I., *Eigenvalues in Riemannian Geometry*, Pure and Applied Mathematics, Academic Press, Orlando, 1984.

57. Grigoryan, A., *Heat Kernel and Analysis on Manifolds*, AMS/IP Studies in Advanced Mathematics, ed. S.-T. Yau, American Mathematical Society, Rhode Island, 2009.

58. Altunkaynak, B. İ., Erman, F., Turgut, O. T., "Finitely Many Dirac-Delta Interactions on Riemannian Manifolds", *Journal of Mathematical Physics*, Vol. 47, No. 8, 2006.

59. Erman, F., Turgut, O. T., "Point Interactions in Two-and Three-Dimensional Riemannian Manifolds", *Journal of Physics A: Mathematical and Theoretical*, Vol. 43, No. 33, pp. 335204, 2010.

60. Erman, F., "On the Number of Bound States of Point Interactions on Hyperbolic Manifolds", *International Journal of Geometric Methods in Modern Physics*, Vol. 14, No. 1, pp. 1750011, 2017.

61. Doğan, Ç., Erman, F., Turgut, O. T., "Existence of Hamiltonians for Some Singular Interactions on Manifolds", *Journal of Mathematical Physics*, Vol. 53, No. 4, pp. 043511, 2012.

62. Doğan, Ç., Turgut, O. T., "Renormalized Interaction of Relativistic Bosons with Delta Function Potentials", *Journal of Mathematical Physics*, Vol. 51, pp. 082305, 2010.

63. Cheeger, J., Yau, S. T., "A Lower Bound for the Heat Kernel", *Communications on Pure and Applied Mathematics*, Vol. 34, No. 465, 1981.

64. Davies, E. B., Mandouvalos, N., "Heat Kernel Bounds for Complex Time and Schrödinger Kernel on Hyperbolic Spaces and Kleinian Groups", *Proceedings of the London Mathematical Society*, Vol. 3, No. 57, pp. 182–208, 1988.

65. Erman, F., Malkoç, B., Turgut, O. T., "Nondegeneracy of the Ground State for Nonrelativistic Lee Model", *Journal of Mathematical Physics*, Vol. 55, pp. 083522, 2014.

66. Davies, E. B., *Heat Kernels and Spectral Theory*, Cambridge University Press, 1989.

67. Gradshteyn, I. S., Ryzhik, I. M., *Table of Integrals, Series, and Products*, Academic press, 2014.

68. Weinbeg, E. J., *Classical Solutions in Quantum Field Theory, Solutons and Instantons in High Energy Physics*, Cambridge Universty Press, 2012.

69. Rajaraman, R., *Solitons and Instantons*, Elsevier, 1982.

70. Grosche, C., "Path Integrals for Potential Problems with δ-Function Perturbation", *Journal of Physics A: Mathematical and General*, Vol. 23, No. 22, p. 5205, 1990.

71. Akbas, K. G., Erman, F., Turgut, O. T., "On Schrödinger Operators Modified by δ Interactions", *Annals of Physics.*, Vol. 458, No. 2, pp. 169468, 2023.

72. Born, M., Oppenheimer, J. R., "Zur Quantentheorie der Molekeln" *Annalen der Physik*, Vol. 389, No. 20, 1927.

73. Landau, L. D., Lifshitz, E. M. *Quantum Mechanics: Nonrelativistic Theory*, Butterworth-Heinemann, 3rd edition, 1981.

74. Bethe, H., Jackiw, R., *Intermediate Quantum Mechanics*, W. A. Benjamin, Inc., 2nd edition, 1973.

75. Weinberg, S., *Lectures on Quantum Mechanics*, Cambridge University Press, 2nd edition, 2015.

76. Panati, G., Spohn, H., Teufel, S., "The Time-Dependent Born-Oppenheimer Approximation", *ESAIM: Mathematical Modelling and Numerical Analysis*, Vol. 41, pp. 297-314, 2007.

77. Hagedorn, G. A., Joye, T., *Mathematical Analysis of Born-Oppenheimer Approximations*, Spectral Theory and Mathematical Physics: A Festschrift in Honor of Barry Simon's 60th Birthday :Quantum Field Theory, Statistical Mechanics and Non-relativistic Quantum Systems, edited by F. Gesztesy et.al. , AMS publications, 2007.

78. Jecko, T., "On the Mathematical Treatment of the Born-Oppenheimer Approximation", *Journal of Mathematical Physics*, Vol. 55, pp. 053504, 2014.

79. Thorn, C., "Quark Confinement in the Infinite Momentum Frame", *Physics Review D*, Vol. 19, p. 639, 1979.

80. Beg, M. A. B., Furlong, R. C., "$\lambda\phi^4$ Theory in the Nonrelativistic Limit", *Physics Review D*, Vol. 31, p. 1370, 1985.

81. Jackiw, R., *Delta-function Potentials in Two and Three Dimensional Quantum mechanics*, M.A.B. Beg memorial volume, A. Ali and P. Hoodbhoy Editors, World Scientific Singapore, 1991.

82. Fernando Perez, J., Coutinho, F. A. B., "Schrödinger Equation in Two Dimensions for a Zero Range Potential and a Uniform Magnetic Field: An Exactly Solvable Model", *American Journal of Physics*, Vol. 59, p. 52, 1991.

83. Mead, L. R. and Godines, J., "An Analytical Example of Renormalization in Quantum Mechanics", *American Journal of Physics*, Vol. 59, p. 935, 1991.

84. Gosdzinsky, P., Tarrach, R., "Learning Quantum Field Theory from Elementary Quantum Mechanics", *American Journal of Physics*, Vol. 59, p. 70, 1991.

85. Albeverio, S., Gesztesy, F., Hoegh-Krohn, R., Holden, H., *Solvable Models in Quantum Mechanics*, 2nd Edition, AMS Chelsea Publishing, Providence, Rhode Island, 2004.

86. Mitra, I., Dasgupta, A., Dutta-Roy, B., *Regularization and Renormalization in Scattering from Dirac Delta Potentials*, *Amer. Jour. Phys.*, Vol. 66, p. 1101, 1998.

87. Seiler, R., "Does the Born-Oppenheimer Approximation Work?", *Helvetica Physica Acta*, Vol. 46, No. 230, 1973.

88. Combes, J. M., Duclos, P., Seiler, R., *The Born-Oppenheimer Approximation*, Plenum, New York, 1981.

89. Hunziker, W., *Distortion Analyticity and Molecular Resonance Curves*, *Ann. Inst. H. Poincare Sect. A.*, Vol. 45, 1986.

90. Hagedorn, G. A., *Classification and Normal Forms for Quantum Eigenvalue Crossings*, Asterisque, 1993.

91. Hagedorn, G. A., "Molecular Propagation Through Electron Energy Level Crossings", *Memoirs American Mathematical Soceity*, Vol. 111, No. 536, 1994.

92. Hagedorn, G. A., "Classification and Normal Forms for Avoided Crossings of Quantum Mechanical Energy Levels", *Journal of Physics A*, Vol. 31, 1998.

93. Hagedorn, G. A., "High Order Corrections to the Time-Independent Born-Oppenheimer Approximation I: Smooth Potentials", *Annales de l'Institut Henri Poincaré*, Vol. 47, 1987.

94. Hagedorn, G. A., "High Order Corrections to the Time-Independent Born-Oppenheimer Approximation II: Diatomic Coulomb Systems", *Communications in Mathematical Physics*, Vol. 116, 1988.

95. Klein, M., Martinez, A., Seiler, R., Wang, X., "On the Born-Oppenheimer Expansion for Polyatomic Molecules", *Communications in Mathematical Physics*, Vol. 143, pp. 607-639, 1992.

96. Weigert, S., Littlejohn, R. G., "Diagonalization of Multicomponent Wave Equations with a Born-Oppenheimer Example", *Physics Review A*, Vol. 45, p. 3506, 1993.

97. Gangopadhyay, G., Dutta-Roy, B., "The Born-Oppenheimer Approximation: the Toy Model", *American Journal of Physics*, Vol. 72, 2004.

98. Akbas, H., Turgut, O. T., "Born-Oppenheimer Approximation for a Singular System", *Arxiv-1602-02811, submitted for publication.*

99. Rosa, D. S., Bellotti, F. F., Jensen, A. S., Krein, G., Yamashita, M. T., "Bound States of a Light Atom and Two Heavy Dipoles in Two Dimensions", *Physics Review A*, Vol. 94, 2016.

100. Fonseca, A. C., Reddish, E. F., Shenley, P. E., "Effimov Effect in an Analytically Solvable Model", *Nuclear Physics A*, Vol. 320, 1979.

101. Bellotti, F. F., Frederico, T., Yamashita, M. T., Fedorov, D. V., Jensen, A. S., Zinner, N. T., "Mass Imbalanced Three Body Systems in 2-dimensions", *Journal of Physics B*, Vol. 46, 2013.

102. Rosa, R. D., Federico, T., Krein, G., Yamashita, M. T., "Effimov Effect in a D-dimensional Born-Oppenheimer Approach", *Journal of Physics B: Atomic, Molecular and Optical Physics*, Vol. 52, 2019.

103. Akbas, H.,Turgut, O. T., *Born-Oppenheimer Type Approximation for a Simple Renormalizable System*, Mathematical Challenges of Zero-Range Physics, Springer, 2021.

APPENDIX A: Some Properties of Green's Function

Here we give a general argument, based on generalized eigenfunction expansions, on how the modification by a delta-interaction affects the continuum. We recall the well-known expression for the (formal) projection onto the eigenspace E,

$$G_0(x,y|E+i0) - G_0(x,y|E-i0) = 2\pi i \int d\mu(\lambda)\delta(E(\lambda)-E)\chi_\lambda(x)\overline{\chi_\lambda(y)} \ , \quad \text{(A.0.1)}$$

here we use a spectral measure $d\mu(\lambda)$, which reflects the possible degeneracy of the continuum states. We restrict the parameter space to a constant energy surface via a delta function. Often, it is hard to compute these measures explicitly, we proceed formally as we really need the formula in one-dimension for our problem. In these problems, if the potential decays sufficiently fast at infinity, momentum can be used as a spectral parameter, then $E = k^2/2m$ and the delta function in spectral projection expression above selects k values for $\pm\sqrt{E}$. If we further invoke parity invariance we can reduce everything into a simpler expression. We claim that in our modified problem, the new generalized eigenfunctions $\eta_E^{\pm}(x)$ are given by

$$\begin{aligned} \eta_E^+(x) &= \chi_E^+(x) + \frac{G_0(x,0|E+i0)\chi_E^+(0)}{\Phi(E+i0)} \ . \\ \eta_E^-(x) &= \chi_E^-(x), \end{aligned} \quad \text{(A.0.2)}$$

where we define $\Phi(E) = \frac{1}{\alpha} - G_0(0,0|E)$. Indeed, this result can be justified formally by computing the action of the operator $H_0 - \alpha\delta(x) - E$ directly:

$$\begin{aligned} &(H_0 - E - \alpha\delta(x)) \left(\chi_E(x) + \frac{G_0(x,0|E+i0)\chi_E(0)}{\Phi(E+i0)} \right) \\ &\qquad = -\alpha\chi_E(0)\delta(x) + \frac{\chi_E(0)}{\Phi(E+i0)}\delta(x) - \alpha\frac{G_0(0,0|E+i0)\chi_E(0)}{\Phi(E+i0)}\delta(x) = 0 \ , \end{aligned} \quad \text{(A.0.3)}$$

where we have used $\Phi(E+i0) = \frac{1}{\alpha} - G_0(0,0|E+i0)$, as well as the fact that $G(x,0)$ is even (as can be verified by the expansion into generalized eigenfunctions). If we have an odd parity state, there is no effect, and for the even states, we get the indicated cancellation. Hence, the generalized eigenfunctions of H_0 modified by δ interactions

are given by the equation (A.0.2).

Let H_0 be the free Hamiltonian in $L^2(\mathbb{R})$. It is well-known that the generalized eigenfunctions are given by $\chi_E^+(x) = \frac{1}{2\pi}\cos(kx)$, and $\chi_E^- = \frac{1}{2\pi}\sin(kx)$ with (generalized) eigenvalues $E = \frac{\hbar^2 k^2}{2m}$. Then, using the explicit expression for the Green's function $G_0(x, y|E + i0) = \frac{im}{\hbar^2 k} e^{ik|x-y|}$, the above formula (A.0.2) yields

$$\eta_E^+(x) = \frac{1}{2\pi}\big[\cos(kx) + \frac{im}{\hbar^2 k}\frac{e^{ik|x|}}{\big(\frac{1}{\alpha} - \frac{im}{\hbar^2 k}\big)}\big] \ . \tag{A.0.4}$$

From this, one can easily find the well-known reflection and transmission coefficients by expressing (A.0.4) in terms of plane waves.

A more general, somewhat formal computation, using the expression for delta modified Green's functions can be given:

$$\begin{aligned} G(x, y|E + i0) - G(x, y|E - i0) &= G_0(x, y|E + i0) - G_0(x, y|E - i0) \\ &+ \frac{G_0(x, 0|E + i0)G_0(0, y|E + i0)}{\Phi(E + i0)} - \frac{G_0(x, 0|E - i0)G_0(0, y|E - i0)}{\Phi(E - i0)} \ . \end{aligned} \tag{A.0.5}$$

Adding and subtracting the terms $\frac{G_0(x,0|E+i0)G_0(0,y|E-i0)}{\Phi(E+i0)}$ and $\frac{G_0(x,0|E+i0)G_0(0,y|E-i0)}{\Phi(E-i0)}$, we obtain

$$\begin{aligned} G(x, y|E + i0) - G(x, y|E - i0) &= 2\pi i \int d\mu(\lambda)\delta(E(\lambda) - E)\chi_\lambda(x)\overline{\chi_\lambda(y)} \\ &+ \frac{G_0(x, 0|E + i0)G_0(0, y|E + i0)}{\Phi(E + i0)} - \frac{G_0(x, 0|E + i0)G_0(0, y|E - i0)}{\Phi(E + i0)} \\ &+ \frac{G_0(x, 0|E + i0)G_0(0, y|E - i0)}{\Phi(E + i0)} - \frac{G_0(x, 0|E - i0)G_0(0, y|E - i0)}{\Phi(E - i0)} \\ &+ \frac{G_0(x, 0|E + i0)G_0(0, y|E - i0)}{\Phi(E - i0)} - \frac{G_0(x, 0|E + i0)G_0(0, y|E - i0)}{\Phi(E - i0)} \ . \end{aligned} \tag{A.0.6}$$

The second and the third terms in the above equation can be combined as

$$\begin{aligned} &\frac{G_0(x, 0|E + i0)G_0(0, y|E + i0)}{\Phi(E + i0)} - \frac{G_0(x, 0|E + i0)G_0(0, y|E - i0)}{\Phi(E + i0)} \\ &\qquad = 2\pi i \frac{G_0(x, 0|E + i0)}{\Phi(E + i0)} \oint d\mu(\lambda)\overline{\chi_\lambda(y)}\chi_\lambda(0) \ , \end{aligned} \tag{A.0.7}$$

where we use a short hand $\oint d\mu(\lambda) := \int d\mu(\lambda)\delta(E(\lambda)-E)$. It follows from the explicit form of the function Φ that

$$\begin{aligned}\left(\frac{1}{\Phi(E+i0)}-\frac{1}{\Phi(E-i0)}\right) &= \frac{\Phi(E-i0)-\Phi(E+i0)}{\Phi(E+i0)\Phi(E-i0)} \\ &= \frac{G_0(0,0|E+i0)-G_0(0,0|E-i0)}{\Phi(E+i0)\Phi(E-i0)} \\ &= \frac{2\pi i}{\Phi(E+i0)\Phi(E-i0)}\oint d\mu(\lambda)\chi_\lambda(0)\overline{\chi_\lambda(0)} \quad \text{(A.0.8)}\end{aligned}$$

Hence, we obtain

$$\begin{aligned}&\frac{G_0(x,0|E+i0)G_0(0,y|E-i0)}{\Phi(E+i0)}-\frac{G_0(x,0|E+i0)G_0(0,y|E-i0)}{\Phi(E-i0)} \\ &\quad = 2\pi i\frac{G_0(x,0|E+i0)}{\Phi(E+i0)}\Big[\oint d\mu(\lambda)\chi_\lambda(0)\overline{\chi_\lambda(0)}\Big]\overline{\left(\frac{G_0(0,y|E-i0)}{\Phi(E-i0)}\right)}, \quad \text{(A.0.9)}\end{aligned}$$

where we have used the fact that $\overline{\Phi(E)}=\Phi(\overline{E})$ and $\overline{G(x,y|E)}=G(x,y|\overline{E})$. For the rest of the terms, we have

$$\begin{aligned}&\frac{G_0(x,0|E+i0)G_0(0,y|E-i0)}{\Phi(E-i0)}-\frac{G_0(x,0|E-i0)G_0(0,y|E-i0)}{\Phi(E-i0)} \\ &\quad = 2\pi i\oint d\mu(\lambda)\chi_\lambda(x)\overline{\chi_\lambda(0)}\overline{\left(\frac{G_0(0,y|E+i0)}{\Phi(E+i0)}\right)}, \quad \text{(A.0.10)}\end{aligned}$$

similar for the first combination. Putting all these results together, we finally obtain

$$\begin{aligned}G(x,y|E+i0)-G(x,y|E-i0) &= 2\pi i\oint d\mu(\lambda)\chi_\lambda(x)\overline{\chi_\lambda(y)} \\ &+ 2\pi i\frac{G_0(x,0|E+i0)}{\Phi(E+i0)}\oint d\mu(\lambda)\chi_\lambda(0)\overline{\chi_\lambda(y)} \\ &+ 2\pi i\oint d\mu(\lambda)\chi_\lambda(x)\overline{\chi_\lambda(0)}\overline{\left(\frac{G_0(0,y|E+i0)}{\Phi(E+i0)}\right)} \\ &+ 2\pi i\left(\frac{G_0(x,0|E+i0)}{\Phi(E+i0)}\right)\oint d\mu(\lambda)\chi_\lambda(0)\overline{\chi_\lambda(0)} \\ &\quad \times\overline{\left(\frac{G_0(0,y|E-i0)}{\Phi(E-i0)}\right)},\end{aligned}$$

Note that in general,

$$\oint d\mu(\lambda)\chi_\lambda(x)\overline{\chi_\lambda(y)} = \int d\mu(\lambda)\delta(E(\lambda)-E)\chi_\lambda(x)\overline{\chi_\lambda(y)} \neq \Psi(x)\overline{\Psi(y)}, \quad \text{(A.0.11)}$$

for some function Ψ, so the above expression cannot be further simplified as a product of two terms.

If we look at a one-dimensional problem with sufficiently fast decaying potential and preserving Parity invariance, the surface integrals simplify. We then get

$$\oint d\mu(\lambda)\chi_\lambda(x)\overline{\chi_\lambda(y)} = \chi_E^+(x)\overline{\chi_E^+(y)} + \chi_E^-(x)\overline{\chi_E^-(y)}. \tag{A.0.12}$$

Inserting this expression into the above general relation and noting $\chi_E^-(0) = 0$, we find

$$\begin{aligned}\frac{1}{2\pi i}[G(x,y|E+i0) - G(x,y|E-i0)] &= \left(\chi_E^+(x) + \frac{G_0(x,0|E+i0)\chi_E^+(0)}{\Phi(E+i0)}\right) \\ &\times\overline{\left(\chi_E^+(y) + \frac{G_0(y,0|E+i0)\chi_E^+(0)}{\Phi(E+i0)}\right)} \\ &+\chi_E^-(x)\overline{\chi_E^-(y)}\ ,\end{aligned}$$

confirming our previous assertion, by expressing the Greens function as a sum over even and odd generalized eigenprojections of fixed energy E.

APPENDIX B: Small Distance Expansions

Here, we provide the detailed computations of all the derivative terms and their expansions. Short distance expansions are used to find the leading order solution within this modified Born-Oppenheimer approximation. For all the approximations below we make use of the Bessel function expansion for $n \geq 2$,

$$K_n(x) \approx \frac{1}{2}(n-1)!\frac{1}{(x/2)^n} + ... \tag{B.0.1}$$

for small x and also the expansion of $K_0(x)$ that we mentioned in the text. Moreover in some cases $K_1(x)$'s next order term in the expansion may have importance and it is given by $K_1(x) \approx \frac{1}{2}\frac{1}{(x/2)} + \frac{1}{2}x\ln(\frac{x}{2}) + ...$ as $x \to 0^+$. In our calculations we need the second derivative of the square-root of the binding energy $\nu(z)$,

$$\begin{aligned}
\frac{\partial^2\nu}{\partial z^2} =& -2\frac{\frac{\sqrt{2m_*}}{\hbar}\nu\frac{\partial\nu}{\partial z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \\
&+ \frac{\frac{2m_*}{\hbar^2}\nu^2\left(z\frac{\partial\nu}{\partial z}+\nu\right)\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \\
&+ \frac{\frac{2m_*}{\hbar^2}\nu^2\left(z\frac{\partial\nu}{\partial z}+\nu\right)\left(K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^2}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]^2} - \frac{\frac{(2m_*)^{\frac{3}{2}}}{\hbar^3}\nu^3|z|\left(z\frac{\partial\nu}{\partial z}+\nu\right)K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]^2} \\
&\times\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right] \\
=& -2\frac{\frac{\sqrt{2m_*}}{\hbar}\nu\frac{\partial\nu}{\partial z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \\
&+ \frac{\frac{2m_*}{\hbar^2}\nu^2\left(z\frac{\partial\nu}{\partial z}+\nu\right)\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \\
&- \frac{\frac{(2m_*)^{\frac{3}{2}}}{\hbar^3}\nu^3 z\left(z\frac{\partial\nu}{\partial z}+\nu\right)K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]^2}K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)
\end{aligned}$$

$$
\begin{aligned}
&= -\frac{\frac{\sqrt{2m_*}}{\hbar}\nu\frac{\partial\nu}{\partial z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} - \frac{1}{z}\frac{\partial\nu}{\partial z} \\
&+ \frac{\frac{2m_*}{\hbar^2}\nu^2\left(z\frac{\partial\nu}{\partial z}+\nu\right)K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]}\left[1-\frac{\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]}\right] \\
&= -\frac{1}{2}\frac{\sqrt{2m_*}}{\hbar}\nu\left[-\frac{\nu}{2z}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3 z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right] \\
&\times\left[\frac{\hbar}{\sqrt{2m_*}\nu z}+\frac{1}{4}\frac{\sqrt{2m_*}}{\hbar}\nu z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]+\frac{\nu}{2z^2}+\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right) \\
&+\frac{1}{2}\frac{2m_*}{\hbar^2}\nu^2\left[\frac{\nu}{2}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\left[1-\frac{1}{4}\frac{2m_*}{\hbar^2}\nu^2 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right] \\
&\times\left[-\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)-\gamma\right]\left[\frac{1}{2}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^2 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right] \\
&= \frac{3}{4}\frac{\nu}{z^2}+a_1\frac{2m_*}{\hbar^2}\nu^3+a_2\frac{2m_*}{\hbar^2}\nu^3\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+...
\end{aligned}
$$

As a result we see that

$$
\frac{1}{\nu}\frac{\partial^2\nu}{\partial z^2} = \frac{3}{4z^2}+O\left(\frac{2m_*}{\hbar^2}\nu^2\right)+O\left(\frac{2m_*}{\hbar^2}\nu^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu|z|\right)\right), \tag{B.0.2}
$$

where a_1, a_2 are constants that we can find explicitly, moreover we did not further simplify the ν terms to see the pattern more explicitly, otherwise they should also be expanded.

In our computations we also need various derivatives of the normalization constant A. We will now start with the derivative of the inverse with respect to ν only keeping z constant,

$$
\begin{aligned}
\partial_\nu A^{-2} &= 2\pi\frac{\hbar^2}{2m_*}\Bigg[-\frac{2}{\nu^3}\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]+\frac{1}{\nu^2}\frac{\sqrt{2m_*}}{\hbar}z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&\quad -\frac{1}{\nu}\frac{2m_*}{\hbar^2}z^2\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]\Bigg] \\
&= 2\pi\frac{\hbar^2}{2m_*}\left[-\frac{2}{\nu^3}\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]-\frac{1}{\nu}\frac{2m_*}{\hbar^2}z^2 K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right].
\end{aligned}
$$

Let us now write the expression we need, and then expand for small z;

$$\begin{aligned} A^2\partial_\nu A^{-2} &= -\frac{2}{\nu} - \nu z^2 \frac{2m_*}{\hbar^2} \frac{K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu|z|\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)} \\ &\approx -\frac{2}{\nu} - \frac{1}{2}\nu z^2 \frac{2m_*}{\hbar^2}\left[-\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right) - \gamma\right] \\ &\quad \times \left[1 - \frac{1}{4}\frac{2m_*}{\hbar^2}\nu^2 z^2 \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right) + ...\right] \\ &\approx -\frac{2}{\nu} + b_1 \frac{2m_*}{\hbar^2}\nu z^2 + b_2 \frac{2m_*}{\hbar^2}\nu z^2 \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right) + ..., \end{aligned} \tag{B.0.3}$$

where b_1, b_2 again are some constants we can determine. Furthermore, we did not expand the ν terms: in principle they should also be expanded, however this form is better since in our computations some combinations of ν's will then cancel to give us a simpler result.

Let us now consider the following second ν derivative of A^{-2} that we need in our calculations:

$$\begin{aligned} \partial_\nu^2 A^{-2} = 2\pi \frac{\hbar^2}{2m_*}\Bigg[&\frac{6}{\nu^4}\left[1 + \frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right] - \frac{2}{\nu^3}\frac{\sqrt{2m_*}}{\hbar} z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\ &+ \frac{2}{\nu^2}\frac{2m_*}{\hbar^2} z^2 \left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) + \frac{\hbar}{\sqrt{2m_*}\nu z} K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right] \\ &+ \frac{1}{\nu^2}\frac{2m_*}{\hbar^2} z^2 K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) + \frac{1}{\nu}\frac{(2m_*)^{\frac{3}{2}}}{\hbar^3} z^3 K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\Bigg]. \end{aligned} \tag{B.0.4}$$

We now write the combination we need and then expand as usual keeping ν terms as they are, so as to simplify later calculations:

$$\begin{aligned} A^2\partial_\nu^2 A^{-2} = \frac{6}{\nu^2} &+ 3z^2 \frac{2m_*}{\hbar^2} \frac{K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \\ &+ \nu z^3 \frac{(2m_*)^{\frac{3}{2}}}{\hbar^3} \frac{K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \end{aligned} \tag{B.0.5}$$

$$
\begin{aligned}
&\approx\frac{6}{\nu^2}+\frac{3}{2}z^2\frac{2m_*}{\hbar^2}\left[-\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)-\gamma\right]\left[1-\frac{1}{4}\frac{2m_*}{\hbar^2}\nu^2z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\\
&+\frac{1}{2}\nu z^3\frac{(2m_*)^{\frac{3}{2}}}{\hbar^3}\left[\frac{\hbar}{\sqrt{2m_*}\nu z}+\frac{1}{2}\frac{\sqrt{2m_*}}{\hbar}\nu z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\\
&\times\left[1-\frac{1}{4}\frac{2m_*}{\hbar^2}\nu^2z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\\
&\approx\frac{6}{\nu^2}+c_1z^2\frac{2m_*}{\hbar^2}+c_2z^2\frac{2m_*}{\hbar^2}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+...
\end{aligned}
\tag{B.0.6}
$$

where we have well-defined constants c_1, c_2, and ν is kept as it is without further expansion. We now write down the combinations we encounter in our computations, one of them is this expression:

$$
\begin{aligned}
&-\frac{\hbar^2}{M}\left(\frac{\partial\nu}{\partial z}\right)^2\frac{1}{2}A^2\partial_\nu^2A^{-2}\\
&\approx-\frac{\hbar^2}{2M}\left[\frac{\nu^2}{4z^2}+\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^4\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+...\right]\\
&\times\left[\frac{6}{\nu^2}+\frac{2m_*}{\hbar^2}z^2+\frac{2m_*}{\hbar^2}z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+...\right]\\
&\approx-\frac{\hbar^2}{M}\frac{3}{4z^2}+O\left(\frac{m_*}{M}\nu^2\right)+O\left(\frac{m_*}{M}\nu^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right)+...\,.
\end{aligned}
\tag{B.0.7}
$$

We write the final expanded version that we use. Note that here instead of the constants in front we indicate the order of magnitude of the term in the expansion with big-O symbol. We also need the combination below, hence we write it explicitly and use the expansions we have obtained:

$$
\begin{aligned}
&-\frac{\hbar^2}{2M}\left[\frac{1}{z}\frac{\partial\nu}{\partial z}+\frac{\partial^2\nu}{\partial z^2}\right]A^2\partial_\nu A^{-2}\\
&\approx-\frac{\hbar^2}{2M}\Big[-\frac{\nu}{2z^2}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+\frac{3\nu}{4z^2}\\
&+\frac{2m_*}{\hbar^2}\nu^3+\frac{2m_*}{\hbar^2}\nu^3\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+...\Big]\\
&\times\left[-\frac{2}{\nu}+\frac{2m_*}{\hbar^2}\nu z^2+\frac{2m_*}{\hbar^2}\nu z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)+...\right]\\
&\approx\frac{\hbar^2}{M}\frac{1}{4z^2}+O\left(\frac{m_*}{M}\nu^2\right)+O\left(\frac{m_*}{M}\nu^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right)+...\,.
\end{aligned}
\tag{B.0.8}
$$

Note that the logarithmic terms by themselves are ambiguous, one should keep the next order term to find the exact expansion, however we will not be able to compute all the

corrections even at the first order due to complicated nature of these expressions, this is why we are essentially emphasizing the order of each term rather than the precise numerical factors.

Our second purpose is to find derivatives of A, with respect to z, to begin with, we look at the first derivative of this normalization constant;

$$\begin{aligned}\partial_z A =& \frac{1}{\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\frac{\partial\nu}{\partial z}\frac{1}{\sqrt{1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}} \\ &- \frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left[\frac{\frac{\sqrt{2m_*}}{\hbar}\left(z\frac{\partial\nu}{\partial z}+\nu\right)K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}\right] \\ &+ \frac{1}{4\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left[\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}\right] \\ &\times\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+K_2\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]. \end{aligned} \tag{B.0.9}$$

We consider the following term

$$\begin{aligned}&\frac{1}{4\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left[\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}\right]\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+K_2\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right] \\ &= \frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left[\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}\right] \\ &\times\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]. \end{aligned} \tag{B.0.10}$$

Here we recognized a term corresponding to $\frac{\partial\nu}{\partial z}$. As a result of these computations, the first derivative of normalization constant is found to be

$$\begin{aligned}\partial_z A =& \frac{1}{\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\frac{\partial\nu}{\partial z}\frac{1}{\sqrt{1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}} \\ &+ \frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left[\frac{\frac{2m_*}{\hbar^2}\nu|z|\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}\right]K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right). \end{aligned} \tag{B.0.11}$$

The term we are interested in is given below, by using the exact expression for A again, we get

$$\frac{1}{A}\left(\frac{1}{z}\partial_z A\right)=\frac{1}{z\nu}\frac{\partial\nu}{\partial z}+\frac{1}{2z}\left[\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)}\right]K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right). \quad \text{(B.0.12)}$$

Let us consider its small z expansion, we therefore find

$$\begin{aligned}
&\frac{1}{A}\left(\frac{1}{z}\frac{\partial A}{\partial z}\right)=\frac{1}{\nu z}\frac{\partial\nu}{\partial z}+\frac{1}{2z}\left[\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)}\right]K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\\
&\approx\frac{1}{\nu z}\left[-\frac{\nu}{2z}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3 z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\\
&+\frac{1}{4}\frac{2m_*}{\hbar^2}\nu\left[\frac{\nu}{2}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\left[1-\frac{1}{4}\frac{2m_*}{\hbar^2}\nu^2 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\\
&\times\left[-\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)-\gamma\right]\\
&\approx-\frac{1}{2z^2}+b_1\left(\frac{2m_*}{\hbar^2}\nu^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right)+b_2\left(\frac{2m_*}{\hbar^2}\nu^2\right)+\dots, \qquad \text{(B.0.13)}
\end{aligned}$$

where the coefficients b_1, b_2 can be calculated from above, since we will not compute all the higher order corrections their precise values are not important. We may therefore write the required expansion as

$$-\frac{\hbar^2}{M}\frac{1}{A}\left(\frac{1}{z}\frac{\partial A}{\partial z}\right)\approx\frac{\hbar^2}{M}\frac{1}{2z^2}+O\left(\frac{m_*}{M}\nu^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right)+O\left(\frac{m_*}{M}\nu^2\right)+\dots. \quad \text{(B.0.14)}$$

In the last part, we look at the more complicated derivative expressions of A:

$$\begin{aligned}
\partial_z A^2=&\frac{1}{2\pi}\frac{2m_*}{\hbar^2}2\nu\frac{\partial\nu}{\partial z}\frac{1}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]}\\
&-\frac{1}{2\pi}\frac{(2m_*)^{\frac{3}{2}}}{\hbar^3}\nu^2\frac{\left(z\frac{\partial\nu}{\partial z}+\nu\right)K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]^2}\\
&+\frac{1}{2\pi}\frac{(2m_*)^2}{\hbar^4}\nu^3 z\frac{\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]^2}\\
&\times\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2\pi}\frac{2m_*}{\hbar^2}2\nu\frac{\partial\nu}{\partial z}\frac{1}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]} \\
&+ \frac{1}{2\pi}\frac{(2m_*)^2}{\hbar^4}\nu^3 z\frac{\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left[1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]^2}K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&= \frac{1}{2\pi}\frac{2m_*}{\hbar^2}\nu\left[-\frac{\nu}{2z}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3 z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\left[1-\frac{1}{4}\frac{2m_*}{\hbar^2}\nu^2 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right] \\
&+ \frac{1}{8\pi}\frac{(2m_*)^2}{\hbar^4}\nu^3 z\left[\frac{\nu}{2}-\frac{1}{8}\frac{2m_*}{\hbar^2}\nu^3 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right] \\
&\times\left[1-\frac{1}{2}\frac{2m_*}{\hbar^2}\nu^2 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right]\left[-\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)-\gamma\right] \\
&= -\frac{1}{2\pi}\frac{2m_*}{\hbar^2}\frac{\nu^2}{2z}+O\left(\frac{(2m_*)^2}{\hbar^4}\nu^4 z\right)+O\left(\frac{(2m_*)^2}{\hbar^4}\nu^4 z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right)+\dots\,. \qquad \text{(B.0.15)}
\end{aligned}
$$

In our computations this term appears in the following combination, which comes from $\int \eta_+\eta_-$ term and it is denoted by (3_b) in the main text:

$$
\begin{aligned}
&-\frac{\hbar^2}{M}2A\partial_z A\frac{\pi\hbar}{2m_*}\partial_z|_\nu\left[\frac{\sqrt{2m_*}}{\nu}zK_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right] = -\frac{\hbar^2}{M}2A\partial_z A\frac{\pi\hbar}{2m_*} \\
&\times\left[\frac{\sqrt{2m_*}}{\nu}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)-\frac{2m_*}{\hbar}z\left[K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)+\frac{\hbar}{\sqrt{2m_*}\nu z}K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right]\right] \\
&= \frac{\hbar^2}{M}\left(\frac{2}{A}\partial_z A\right)A^2\frac{\pi\hbar}{2m_*}\frac{2m_*}{\hbar}zK_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&\approx O\left(\frac{m_*}{M}\nu^2\right)+O\left(\frac{m_*}{M}\nu^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right) \\
&+O\left(\frac{m_*}{M}\frac{2m_*}{\hbar^2}\nu^4 z^2\right)+O\left(\frac{m_*}{M}\frac{2m_*}{\hbar^2}\nu^4 z^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z\right)\right)\,. \qquad \text{(B.0.16)}
\end{aligned}
$$

The most complicated combinations come from the second derivative of the normalization constant A with respect to z. This straightforward, yet long computation can be simplified into nicer blocks by using some of the relations we have found. Let us recall the first derivative we have,

$$
\begin{aligned}
\partial_z A = &\frac{1}{\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\frac{\partial\nu}{\partial z}\frac{1}{\sqrt{1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}} \\
&+\frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left[\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}\right]K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\,. \qquad \text{(B.0.17)}
\end{aligned}
$$

We compute the second derivative, after tedious calculations and some simplifications,

we arrive at

$$\begin{aligned}
\partial_z^2 A = &\frac{1}{\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\frac{\partial^2\nu}{\partial z^2}\frac{1}{\sqrt{1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)}} \\
&+\frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\frac{\partial\nu}{\partial z}\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}}K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&+\frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\frac{\partial\nu}{\partial z}\frac{\frac{2m_*}{\hbar^2}\nu z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}} \\
&+\frac{1}{2\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\frac{2m_*}{\hbar^2}\frac{\left[2z^2\left(\frac{\partial\nu}{\partial z}\right)^2+\nu z^2\frac{\partial^2\nu}{\partial z^2}+5\nu z\frac{\partial\nu}{\partial z}+\nu^2\right]}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{3}{2}}} \\
&+\frac{3}{4\sqrt{2\pi}}\frac{\sqrt{2m_*}}{\hbar}\nu\left(K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^2\frac{2m_*}{\hbar^2}\frac{\frac{2m_*}{\hbar^2}\nu^2 z^2\left(z\frac{\partial\nu}{\partial z}+\nu\right)^2}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^{\frac{5}{2}}}\,.
\end{aligned} \tag{B.0.18}$$

What we need is the following combination:

$$\begin{aligned}
\frac{1}{A}\partial_z^2 A = &\frac{1}{\nu}\frac{\partial^2\nu}{\partial z^2}+\frac{1}{2}\frac{\partial\nu}{\partial z}\frac{2m_*}{\hbar^2}\left[\frac{z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)}\right]K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) \\
&+\frac{1}{2}\frac{\partial\nu}{\partial z}\frac{2m_*}{\hbar^2}\left[\frac{z\left(z\frac{\partial\nu}{\partial z}+\nu\right)}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)}\right] \\
&+\frac{1}{2}K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\frac{2m_*}{\hbar^2}\left[\frac{2z^2\left(\frac{\partial\nu}{\partial z}\right)^2+5\nu z\frac{\partial\nu}{\partial z}+\nu z^2\frac{\partial^2\nu}{\partial z^2}+\nu^2}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)}\right] \\
&+\frac{3}{4}\frac{2m_*}{\hbar^2}\left[\frac{\frac{2m_*}{\hbar^2}\nu^2 z^2\left(z\frac{\partial\nu}{\partial z}+\nu\right)^2}{\left(1+\frac{\sqrt{2m_*}}{\hbar}\nu z K_1\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^2}\right]\left(K_0\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^2\,.
\end{aligned} \tag{B.0.19}$$

In our approach, we need the small-z expansion of $\frac{1}{A}\nabla_z^2 A$ which, in cylindrical coordinates, can be expressed with the first and second z derivatives of A. As one may appreciate the expression above is fairly complicated, its exact expansion requires care and patience, since we are not actually computing the second order correction, we will only point out the types of terms we encounter in this expansion, with some undetermined coefficients in front. As a consequence, the Laplacian part of normalization is

found to be

$$-\frac{\hbar^2}{M}\frac{1}{A}\nabla_z^2 A \approx -\frac{\hbar^2}{M}\frac{1}{4z^2} + c_1\frac{m_*}{M}\nu^2 \ln\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right) + c_2\frac{m_*}{M}\nu^2 + c_3\frac{m_*}{M}\frac{2m_*}{\hbar^2}\nu^4 z^2\left(\ln\left(\frac{\sqrt{2m_*}}{\hbar}\nu z\right)\right)^2 + \dots\,, \tag{B.0.20}$$

where c_1, c_2, c_3 are constant that can be found explicitly, moreover m_* *should be replaced with* m *to this order of accuracy.* These are the results that we use in the main text. In Appendix C to illustrate the consistency of our approximations as well as to propose a scheme to compute higher order corrections we evaluate the expectation values of some of the next order terms within first order perturbation theory. This of course is an asymptotic expansion and hopefully presents a reliable description of the dynamics.

APPENDIX C: Perturbative Corrections

In order to verify the consistency of our approximations we should first show that the expectation value of z is much smaller than the spread of the light particles wave functions, which is characterized by $\zeta_0 = \frac{\hbar}{\sqrt{2m_*\epsilon}}$. This is related to z_0 that we introduced previously, one can see easily that $z_0 = \frac{2m_*}{M}\zeta_0$. For this, we need to normalize our wave function, written in terms of the variable z:

$$\Psi(z) = C\frac{2^\beta z^\beta}{(z_0(1+2\beta))^\beta}e^{-\frac{z}{z_0(1+2\beta)}}. \tag{C.0.1}$$

The normalization constant C is then found as

$$C^2 2\pi \frac{2^{2\beta}}{(z_0(1+2\beta))^{2\beta}}\int_0^\infty dz z^{2\beta+1}e^{-\frac{2z}{z_0(1+2\beta)}} = 1 \tag{C.0.2}$$

where

$$C = \sqrt{\frac{2}{\pi\Gamma(2\beta+2)z_0^2(1+2\beta)^2}}. \tag{C.0.3}$$

Next we look at the expectation value of z (within our approximation) to check the consistency of our assumption

$$\begin{aligned} < z > &= \frac{2^{2\beta+2}}{(z_0(1+2\beta))^{2\beta+2}\Gamma(2\beta+2)}\int_0^\infty dz z^{2\beta+2}e^{-\frac{2z}{z_0(1+2\beta)}} \\ &= \frac{1}{2}\frac{\Gamma(2\beta+3)}{\Gamma(2\beta+2)}z_0(1+2\beta) \\ &= \frac{e^\gamma}{2}\frac{\Gamma(2\beta+3)}{\Gamma(2\beta+2)}(1+2\beta)\frac{\hbar}{\sqrt{2m_*\epsilon}}\left(\frac{m_*}{M}\right) \ . \end{aligned} \tag{C.0.4}$$

Let us emphasize that this is a key result for the consistency of our approximations.

It is also instructive to calculate next order corrections to the binding energy of the heavy-light system as a function of the distance between the heavy centers:

$$-\nu^2 \approx -\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^\gamma z} + \frac{\epsilon^2}{2e^{2\gamma}}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right) + \dots \ . \tag{C.0.5}$$

The first term is the original potential part that we used in the effective description

of the heavy system, so let us look at the expectation value of the second term as a perturbation on our solution:

$$\begin{aligned}\left\langle \frac{\epsilon^2}{2e^{2\gamma}} \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma}\right)\right\rangle &= \frac{\epsilon^2}{2e^{2\gamma}} \frac{2^{2\beta+2}}{(z_0(1+2\beta))^{2\beta+2}\Gamma(2\beta+2)} \\ &\times \int_0^\infty dz z^{2\beta+1} e^{-\frac{2z}{z_0(1+2\beta)}} \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma}\right) \\ &= \frac{\epsilon^2}{2e^{2\gamma}}\left(\psi(2\beta+2) - \ln\left(\frac{M}{2m_*}\right) + \ln\left(\frac{(1+2\beta)e^{2\gamma}}{8}\right)\right) \\ &\approx -\frac{\epsilon^2}{2e^{2\gamma}} \ln\left(\frac{M}{m_*}\right) \ . \end{aligned} \tag{C.0.6}$$

We can easily see that this expectation value is of lower order compared to the leading order energy of the heavy particle. We emphasize that the constant terms are ambiguous as long as we keep to this order, they can be fixed if the next order terms (z without the logarithms) are also taken into account. An interesting estimate will be to calculate the expectation values of the correction terms resulting from the heavy particle relative coordinate kinetic energy term (Laplacian with respect to z) operating on the normalization constant A, the expansion of which is given in Appendix B in Equation (B.0.20). Since we have not found the precise constant in front, we compute the expectation values of each basic part separately without the constants in front:

$$\begin{aligned}(a) &= \frac{2m_*}{M}\nu^2 \approx \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^{\gamma}z} - \frac{2m_*}{M}\frac{\epsilon^2}{2e^{2\gamma}} \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma}\right) + ... \\ (b) &= \frac{2m_*}{M}\nu^2 \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z e^{\gamma}\right) \\ &\approx \frac{1}{2}\frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^{\gamma}z} \ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma}\right) - \frac{1}{4e^{2\gamma}}\frac{2m_*}{M}\epsilon^2 \ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma}\right) + ... \\ (c) &= \frac{2m_*}{M}\frac{2m_*}{\hbar^2}\nu^4 z^2 \ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z e^{\gamma}\right) \approx \frac{2m_*}{M}\frac{\epsilon^2}{e^{2\gamma}} \ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^{\gamma}\right) + ... \ . \end{aligned} \tag{C.0.7}$$

We first look at the expectation value of (a) the log-term has already been calculated above so let us focus on the expectation of the first term of (a), that we denote by a subscript as $(a)_1$,

$$\begin{aligned}< (a)_1 > &= \left\langle \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^{\gamma}z}\right\rangle = \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^{\gamma}}\frac{2^{2\beta+2}}{(z_0(1+2\beta))^{2\beta+2}\Gamma(2\beta+2)} \\ &\times \int_0^\infty dz z^{2\beta} e^{-\frac{2z}{z_0(1+2\beta)}} = \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{4\epsilon}{e^{\gamma}}\frac{\Gamma(2\beta+1)}{\Gamma(2\beta+2)z_0(1+2\beta)} = \frac{8}{e^{2\gamma}}\frac{\epsilon^2}{(1+2\beta)^2} \ , \end{aligned}$$

which is negligible to this order. In a similar way, we find the expectation value of the second term (b)

$$
\begin{aligned}
< (b) > &= \left\langle \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma z}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right)\right\rangle \\
&= \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma}\frac{2^{2\beta+2}}{(z_0(1+2\beta))^{2\beta+2}\Gamma(2\beta+2)}\int_0^\infty dz z^{2\beta}e^{-\frac{2z}{z_0(1+2\beta)}}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right) \\
&= \frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^\gamma z_0(1+2\beta)}\frac{\Gamma(2\beta+1)}{\Gamma(2\beta+2)} \\
&\left(\psi(2\beta+1)-\ln\left(\frac{M}{2m_*}\right)+\ln\left(\frac{(1+2\beta)e^{2\gamma}}{8}\right)\right) \\
&= \frac{4}{e^{2\gamma}}\frac{\epsilon^2}{(1+2\beta)^2}\left(\psi(2\beta+1)-\ln\left(\frac{M}{2m_*}\right)+\ln\left(\frac{(1+2\beta)e^{2\gamma}}{8}\right)\right) \\
&\approx -\frac{4\epsilon^2}{e^{2\gamma}}\frac{1}{(1+2\beta)^2}\ln\left(\frac{M}{m_*}\right).
\end{aligned}
\tag{C.0.8}
$$

The final expectation value is that of (c) part, it must be negligible due to m/M term and no inverse powers of z appearing in it:

$$
\begin{aligned}
< (c) > &= \left\langle \frac{2m_*}{M}\frac{\epsilon^2}{e^{2\gamma}}\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right)\right\rangle \\
&= \frac{2m_*}{M}\frac{\epsilon^2}{e^{2\gamma}}\frac{2^{2\beta+2}}{(z_0(1+2\beta))^{2\beta+2}\Gamma(2\beta+2)}\int_0^\infty dz z^{2\beta+1}e^{-\frac{2z}{z_0(1+2\beta)}}\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right) \\
&= \frac{2m_*}{M}\frac{\epsilon^2}{e^{2\gamma}}\left[\left(\psi(2\beta+2)-\ln\left(\frac{M}{2m_*}\right)+\ln\left(\frac{(1+2\beta)e^{2\gamma}}{8}\right)\right)^2+\zeta(2,2\beta+2)\right],
\end{aligned}
\tag{C.0.9}
$$

which is *negligible* to the order that we are interested in, as expected. To gain more insight, we can go one step further and calculate some of the expectation values resulting from the heavy particle kinetic energy partially operating on the light particle wave function and generating a mixed gradient term, after our simplifications, this residual term is found to be

$$
\begin{aligned}
\frac{2m_*}{M}\nu^2 z\frac{\partial\Psi}{\partial z}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\nu z e^\gamma\right) &\approx \frac{m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{2\epsilon}{e^\gamma}\frac{\partial\Psi}{\partial z}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right) \\
&\quad -\frac{2m_*}{M}\frac{\epsilon^2}{4e^{2\gamma}}z\frac{\partial\Psi}{\partial z}\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon z e^\gamma\right)+\dots .
\end{aligned}
\tag{C.0.10}
$$

We compute the expectation value of this expression (to properly identify the corrections within first order perturbation theory we must symmetrize this expression, thus

we get a term coming from the anticommutator of $\frac{\partial}{\partial z}$ and the log expression, we ignore this subtlety for now since we are not aiming for an exact computation). Let us start with the first part:

$$\begin{aligned}
&\frac{2m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma}2\pi\int_0^\infty dzz\Psi\frac{\partial\Psi}{\partial z}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\\
&=\frac{m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma}2\pi\int_0^\infty dzz\frac{\partial\Psi^2}{\partial z}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\\
&=\frac{m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma}2\pi\left[\Psi^2 z\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)|_0^\infty-\int_0^\infty dz\Psi^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)-\int_0^\infty dz\Psi^2\right]\\
&=-\frac{m_*}{M}\frac{\hbar}{\sqrt{2m_*}}\frac{\epsilon}{e^\gamma}\left[<\frac{1}{z}>+2\pi\int_0^\infty dz\Psi^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\right]\\
&\approx\frac{2\epsilon^2}{e^{2\gamma}(1+2\beta)^2}\ln\left(\frac{M}{m_*}\right).
\end{aligned}\tag{C.0.11}$$

The second part of the expansion should be small, let us see this by an explicit computation (within first order perturbation theory):

$$\begin{aligned}
&-\frac{2m_*}{M}\frac{\epsilon^2}{8e^{2\gamma}}2\pi\int_0^\infty dzz^2\frac{\partial\Psi^2}{\partial z}\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\\
&=-\frac{2m_*}{M}\frac{\epsilon^2}{8e^{2\gamma}}2\pi\left[z^2\Psi^2\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)|_0^\infty-2\int_0^\infty dzz\Psi^2\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\right.\\
&\left.-2\int_0^\infty dzz\Psi^2\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\right]\\
&=\frac{2m_*}{M}\left\langle\frac{\epsilon^2}{4e^{2\gamma}}\ln\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\right\rangle+\frac{2m_*}{M}\left\langle\frac{\epsilon^2}{4e^{2\gamma}}\ln^2\left(\frac{\sqrt{2m_*}}{2\hbar}\epsilon ze^\gamma\right)\right\rangle,
\end{aligned}\tag{C.0.12}$$

all of which are computed above and clearly of smaller order. This completes our short digression on calculating higher order corrections. As we emphasize *in principle* it is possible to compute all these corrections in first order perturbation theory, nevertheless it requires precise expansions of all the terms to first order (in terms of z) which we have not done. If we intend to go beyond the first order terms in the expansions and evaluate their contributions, the possibility of second order perturbation of the first order terms becoming equally important should be discussed. We leave these questions to the future.