Spectral comparison theorems for the Klein–Gordon equation in $d \geq 1$ dimensions

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A Thesis
In The Department
of
Mathematics and Statistics

Presented in Partial Fulfillment of the Requirements

For the Degree of
Doctor of Philosophy (Mathematics) at

Concordia University

Montréal, Quebec, Canada

December 2019

CONCORDIA UNIVERSITY

SCHOOL OF GRADUATE STUDIES

This is to certify that the thesis prepared

By: Hassan Harb

Entitled: Spectral comparison theorems for the Klein-Gordon equation in $d \geq 1$ dimensions

and submitted in partial fulfillment of the requirements for the degree of

Doctor Of Philosophy (Mathematics)

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Abstract

Spectral comparison theorems for Klein–Gordon equation in $d \geq 1$ dimensions

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We first study bound-state solutions of the Klein–Gordon equation $\varphi''(x) = \left[m^2 - \left(E - V(x)\right)^2\right]\varphi(x)$, for vector potentials which in one spatial dimension have the form $V(x) = v\, f(x)$, where $f(x) \leq 0$ is the shape of a finite symmetric central potential that is monotone non-decreasing on $[0, \infty)$ and vanishes as $x \to \infty$, and $v > 0$ is the coupling parameter.

We characterize the graph of spectral functions of the form $v = G(E)$ which represent solutions of the eigen-problem in the coupling parameter v for a given E: they are concave, and at most uni-modal with a maximum near the lower limit $E = -m$ of the energy $E \in (-m,\, m)$. This formulation of the spectral problem immediately extends to central potentials in $d > 1$ spatial dimensions. Secondly, for each of the dimension cases, $d = 1$ and $d \geq 2$, a comparison theorem is proven, to the effect that if two potential shapes are ordered $f_1(r) \leq f_2(r)$, then so are the corresponding pairs of spectral functions $G_1(E) \leq G_2(E)$ for each of the existing eigenvalues. These results remove the restriction to positive energies necessitated by earlier comparison theorems for the Klein–Gordon equation by Hall and Aliyu [49]. Corresponding results are obtained when scalar potentials $S(x)$ are also included.

We then weaken the condition for the ground states by proving that if $\displaystyle\int_0^x \left[f_2(t) - f_1(t)\right]\varphi_i(t)dt \geq 0$, the corresponding coupling parameters remain ordered, where $\varphi_i = 1, \varphi_1$ or φ_2, φ_1 and φ_2 are the bound state solutions of the Klein–Gordon equation with potentials V_1 and V_2 respectively. These results are valid for any energy $E \in (-m, m)$, but they are restricted to the ground states.

We finally present a complete recipe for finding upper and lower spectral bounds for both bounded and unbounded potentials, and we exhibit specific result for the applications for the Woods-Saxon, Gaussian, sech-squared, and Yukawa potentials in dimensions $d = 1$ and $d = 3$.

Acknowledgement

I would like to express my sincere gratitude to my supervisor Professor Richard Hall, for his tremendous support, guidance, and kindness. This work was only possible after his advice and his vast knowledge and experience, which have been a huge inspiration for me since we started doing research together. Furthermore, his financial support throughout my PhD journey helped me dedicate most of my time to focus on my studies.

I would also like to thank my parents whose love and guidance are with me in whatever I pursue. Your prayer for me was what sustained me thus far. Special notes to my brothers and sister for their continuous encouragement during my stressful times.

Finally, a special thanks to my beloved wife Zaynab, who was very understanding and supportive throughout this entire process, and has made countless sacrifices to help me get to this point. My sweetest daughter Rama, you have helped me be stronger, better and more fulfilled than I could have ever imagined. I love you and your mum to the moon and back.

To my beloved wife

Contents

List of Figures

Chapter 1

Introduction

The elementary comparison theorem of non-relativistic quantum mechanics states that if two potentials are ordered, then the respective bound-state eigenvalues are correspondingly ordered:

$$V_1 \leq V_2 \Longrightarrow E_1 \leq E_2.$$

In the non-relativistic case (Schrödinger's Equation), this is a direct consequence of the min-max principle since if the Hamiltonian $H = -\Delta + V$ is bounded from below, the discrete spectrum can be characterized variationally [4]. However, the min-max principle is not valid in a simple form in the relativistic case because the energy operators are not bounded from below [7–9]. Regarding the Klein–Gordon equation, since only a few analytical solutions are known, the existence of lower and upper bounds for the eigenvalues is important, and establishing comparison theorems for the eigenvalues of this equation is of considerable interest. We suppose that the vector potential V is written in the form $V(x) = v\, f(x)$, where $v > 0$ and $f(x)$ are defined respectively as the coupling parameter and the potential shape. The literature does provide explicit solved examples, such as the square-well potential [10, 63], the exponential potential [11, 66], the Woods-Saxon potential, and the cusp potential [12]. Based on these examples it is clear that the relation $E(v)$ is not monotonic as it is in the Dirac relativistic equation, [13–18], and indeed for Schrödinger's non-relativistic equation. Consequently, earlier comparison theorems for the Klein Gordon equation were restricted to positive energies [19, 49, 50], and some are only valid for the ground state.

In this thesis, we were able to establish general comparison theorems that are valid for all $E \in (-m, m)$, and not just for the ground state. We shall assume V represents the time component of a four-vector, with $V(x) = vf(x)$, v being the coupling parameter and the function f is the potential shape. The idea that had a profound effect on the present work and, in particular, eliminated an earlier positivity restriction for energies, was our thinking of v as a function of E. This enabled us to arrive at a *function* $v(E)$, whereas $E(v)$ is a two-valued expression.

In chapter 4 we give an explicit expression for the energy Klein–Gordon operator in dimenion $d \geq 1$, and we prove that the ground state function is decreasing on $[0, \infty)$. We then provide exact solutions for the Klein–Gordon equation with the square-well, exponential, Coulomb, and Hulthén potentials in chapter 5, which are adapted from the literature. We generalize the solution for the square-well potential to dimension $d > 3$. In chapter 6, we show that that the eigenvalue problem in the coupling parameter v leads to spectral functions of the form $v = G(E)$ which are concave, and at most uni-modal with a maximum near the lower limit $E = -m$ of the eigenenergy $E \in (-m,\, m)$. This formulation of the spectral problem immediately extends to central potentials in $d > 1$ spatial dimensions. Chapter 7 is dedicated for proving our comparison theorem in which we call a *simple general comparison theorem*, in dimension $d \geq 1$. This theorem states that

$$f_1 \leq f_2 \implies G_1(E) \leq G_2(E),$$

for all $E \in (-m, m)$ and for all ground and excited states.
Moreover, we were able to refine this theorem for the ground states in dimension $d \geq 1$, by allowing

the potential shapes to cross over in a controlled manner. We reveal the following theorems in the one - dimensional case:

1. $\int_0^\infty \big(f_2(x) - f_1(x)\big)dx \geq 0 \implies G_1(E) \leq G_2(E)$, for all $E \in (-m, m)$;
2. $\int_0^\infty \big(f_2(x) - f_1(x)\big)\varphi_i(x)dx \geq 0 \implies G_1(E) \leq G_2(E)$, for all $E \in (-m, m)$, where φ_i is the ground state function with $i = 1, 2$,

and for the $(d > 1)$ - dimensional case:

1. $\int_0^\infty \big(f_2(r) - f_1(r)\big)r^{d-1}dr \geq 0 \implies G_1(E) \leq G_2(E)$, for all $E \in (-m, m)$;
2. $\int_0^\infty \big(f_2(r) - f_1(r)\big)r^{d-1}R_i(r)dr \geq 0 \implies G_1(E) \leq G_2(E)$, for all $E \in (-m, m)$, where R_i is the ground state function with $i = 1, 2$,

In chapter 9, we prove that the energies for Coulomb-like potentials are positive, provided $v < \frac{1}{2}$. We finally exhibit a complete recipe for spectral bounds for potentials based on comparisons with the exactly soluble square-well, exponential, Coulomb, and Hulthén problems.

Chapter 2

Abstract Theory

2.1 Hilbert Space

[1–5] We provide a definition of a Hilbert space with some properties, because the space of functions in quantum mechanics is a Hilbert space. We start by defining an inner product space, or a pre-Hilbert space X.

Definition 2.1.1. Inner product space: *An inner product space X is a vector space with an inner product $\langle\cdot,\cdot\rangle$ defined on X, where $\langle\cdot,\cdot\rangle$ is a map defined as*

$$\langle\cdot,\cdot\rangle : X \times X \quad \mapsto \mathbb{C},$$

satisfying the following properties:

(i) $\langle\varphi, \psi + \xi\rangle = \langle\varphi, \psi\rangle + \langle\varphi, \xi\rangle$, *for all* $\varphi, \psi, \xi \in X$;

(ii) $\langle\varphi, \alpha\psi\rangle = \alpha\langle\varphi, \psi\rangle$ *for all* $\varphi, \psi \in X$ *and* $\alpha \in \mathbb{C}$;

(iii) $\langle\varphi, \psi\rangle = \overline{\langle\psi, \varphi\rangle}$ *for all* $\varphi, \psi \in X$;

(iv) $\langle\varphi, \varphi\rangle \geq 0$ *for all* $\varphi \in X$, *and* $\langle\varphi, \varphi\rangle = 0$ *iff* $\varphi \equiv 0$.

Definition 2.1.2. *Let $\varphi_i, \varphi_j \in X$. Then φ_i and φ_j are said to be orthogonal if $\langle\varphi_i, \varphi_j\rangle = 0$. A collection of functions $\{\varphi_i\}$, $i = 1, 2, ...$ is called an orthonormal set if $\langle\varphi_i, \varphi_i\rangle = 1$ for all i, and $\langle\varphi_i, \varphi_j\rangle = 0$ for all $i \neq j$.*

Let $S = \{\varphi_i\}_{i=1}^{N} \in X$ be an orthonormal set. Then for any $\varphi \in X$, we have:

$$\varphi = \sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i + \left(\varphi - \sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i\right).$$

But $\sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i$ and $\varphi - \sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i$ are orthogonal. Thus

$$\|\varphi^2\| = \left\|\sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i\right\|^2 + \left\|\varphi - \sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i\right\|^2,$$

and consequently, we obtain the following **Pythagorean theorem**

$$\|\varphi^2\| = \sum_{i=1}^{N}|\langle\varphi, \varphi_N\rangle|^2 + \left\|\varphi - \sum_{i=1}^{N}\langle\varphi_i, \varphi\rangle\varphi_i\right\|^2.$$

As a result we get the Bessel's inequality

$$\|\varphi\|^2 \geq \sum_{i=1}^{N}|\langle\varphi, \varphi_N\rangle|^2.$$

Corollary 2.1.1. *For any $\varphi, \psi \in X$ we have the following* **Cauchy Shwarz's inequality**

$$|\langle \varphi, \psi \rangle| \leq \|\varphi\| \, \|\psi\| \,. \tag{2.1}$$

Proof. If $\psi = 0$, then it's trivial.
Suppose that $\varphi \neq 0$. Then $\dfrac{\psi}{\|\psi\|}$ itself forms an orthonormal set. Hence, applying Bessel's inequality we get

$$\|\varphi\|^2 \geq \left| \left\langle \varphi, \frac{\psi}{\|\psi\|} \right\rangle \right|^2 = \frac{|\langle \varphi, \psi \rangle|^2}{\|\psi\|^2},$$

and the proof is complete. □

Definition 2.1.3. Hilbert Space: *A Hilbert space $\mathcal{H}$ is a complete inner product space, that is: every Cauchy sequence in $\mathcal{H}$ is convergent.*

Definition 2.1.4. *Let $\mathcal{H}$ be a Hilbert space. A basis for $\mathcal{H}$ is a maximal orthonormal subset $\beta \in \mathcal{H}$.*

Theorem 2.1.1. *Any Hilbert space $\mathcal{H}$ has an orthonormal basis, and any two bases for $\mathcal{H}$ have the same cardinality.*

The proof of this theorem is found in [2] p.44. In quantum mechanics, the space of all possible states (*wave functions*) of a particle at a given time is called the state-space. The smallest Hilbert space containing these functions in the set of square integrable functions

$$L^2(\mathcal{R}^d) = \{\varphi : \mathbb{R}^d \quad \mapsto \mathbb{R} \mid \int_{\mathbb{R}^d} |\varphi^2| < \infty\},$$

with $d \geq 1$. This is a vector space that has an inner product given by

$$\langle \varphi, \psi \rangle := \int_{\mathbb{R}^d} \varphi(x)\psi(x)\mu(dx),$$

for all $\varphi, \psi \in L^2(\mathbb{R}^d)$, in terms of which the norm is given by $||\varphi|| = \sqrt{\langle \varphi, \varphi \rangle}$. Applying the Cauchy-Schwarz's inequality we have

$$\langle \varphi, \psi \rangle \leq ||\varphi||.||\psi|| < \infty.$$

Hence $\varphi\psi \in L^2(\mathbb{R}^d)$.

2.2 Inequalities

In this section we introduce the famous Hardy's inequality which shall use in chapter 9 for studying the sign of energy-eigenvalues for Coulomb-like potentials.

Corollary 2.2.1. Hölder's inequality*[3] Let p and q be dual indices, that is $\dfrac{1}{p} + \dfrac{1}{q} = 1$, $1 \leq p \leq \infty$, and define Ω to be a measure space with measure μ. Then for any $f \in L^p(\Omega)$ and $g \in L^q(\Omega)$ we have*

$$\|fg\|_1 \leq \|f\|_p \, \|g\|_q \,, \tag{2.2}$$

where

$$L^p(\Omega) := \{\varphi : \Omega \quad \mapsto \mathbb{R} \mid \int_{\Omega} |\varphi^p| < \infty\},$$

and

$$\|f\|_p := \left(\int_{\Omega} f^p d\mu \right)^{1/p}.$$

Proof. We consider Young's inequality

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q},$$

for any $a, b \geq 0$ and $p \geq 1$, and we let $A = \left(\int_\Omega |f|^p d\mu \right)^{1/p}$, $B = \left(\int_\Omega |g|^q d\mu \right)^{1/q}$, $a = \frac{|f(x)|}{A}$, and $a = \frac{|g(x)|}{B}$. Thus

$$\frac{1}{\|f\|_p \|g\|_p} \|fg\|_1 \leq \frac{1}{p} + \frac{1}{q} = 1.$$

Hence,

$$\|fg\|_1 \leq \|f\|_p \|g\|_q .$$

□

Corollary 2.2.2. Minkowski's Inequality*[3, 26] For $f, g \in L^p(\Omega)$ we have*

$$\|f + g\|_p \leq \|f\|_p + \|g\|_p ,$$

for $p \geq 1$.

Proof. The cases $p = 1$ and $p = \infty$ follow from the triangular inequality. For $1 < p < \infty$ we have

$$|f + g|^p = |f + g|^{p-1}|f + g| \leq |f + g|^{p-1}(|f| + |g|).$$

Integrating on Ω and applying (2.2) we find that

$$\int_\Omega |f + g|^p \leq \left(\int_\Omega |f + g|^{(p-1)q} \right)^{1/q} \|f\|_p + \left(\int_\Omega |f + g|^{(p-1)q} \right)^{1/q} \|g\|_p .$$

Thus, using $(p - 1)q = p$ and $1/q = 1 - 1/p$ we get

$$\int_\Omega |f + g|^p \leq \left(\int_\Omega |f + g|^p \right)^{1-1/p} \left(\|f\|_p + \|g\|_p \right).$$

Dividing both sides by the positive term $\left(\int_\Omega |f + g|^p \right)^{1-1/p}$, we get the desired result. □

We also state the Minkowski's inequality in the integral form.
Let f be a non-negative function on $\Omega \times \Gamma$, which is $\mu \times \nu$-measurable. (Γ is a measure space with measure ν). Then

$$\int_\Gamma \left(\int_\Omega f(x, y)\mu(dx) \right)^{1/p} \nu(dy) \geq \left(\int_\Omega \left(\int_\Gamma f(x, y)\nu(dy) \right)^p \mu(dx) \right)^{1/p} . \tag{2.3}$$

Theorem 2.2.1. Hardy's Inequality*[21–25] Let $f \in L^p(0, \infty)$, $p > 1$, and $f > 0$. Then*

$$\int_0^\infty \left[\frac{1}{x} \int_0^x f(t)dt \right]^p dx \leq \left(\frac{p}{p - 1} \right)^p \int_0^\infty f^p(x)dx. \tag{2.4}$$

This inequality could be written as

$$\int_0^\infty F^p(x)dx \leq \left(\frac{p}{p - 1} \right)^p \int_0^\infty f^p(x)dx, \tag{2.5}$$

where

$$F(x) = \frac{1}{x} \int_0^x f(t)dt < \infty.$$

Proof. We first have

$$F(x) = \int_0^1 f(tx)dt.$$

Applying Minkowski's inequality for integrals (2.3) we get

$$\|F\|_p \leq \int_0^1 \|f_t\|_p \, dt,$$

where $f_t(x) = f(tx)$. Using the change the of variable $s = tx$ and applying Fubini's theorem we get

$$\|F\|_p \leq \int_0^1 \left[\int_0^1 |f(s)|^p \frac{ds}{t} \right]^{1/p} dt$$
$$\implies \|F\|_p \leq \int_0^1 t^{-1/p} dt \left[\int_0^1 |f(s)|^p ds \right]^{1/p} = \frac{p}{p-1} \|f\|_p \, .$$

Hence,

$$\|F\|_p^p \leq \left(\frac{p}{p-1} \right)^p \|f\|_p^p \, .$$

□

If we let $\varphi(x) = \int_0^x f(t)dt$, we can write the inequality (2.4) for $p = 2$ as

$$\int_0^\infty \frac{1}{x^2} \varphi^2(x) dx \leq 4 \int_0^\infty [\varphi^2(x)]' dx.$$

Applying integration by parts for the right side we get

$$\int_0^\infty \frac{1}{x^2} \varphi^2(x) dx \leq -4\varphi(0)\varphi'(0) - \int_0^\infty \varphi(x)\varphi''(x) dx.$$

Assuming that $\varphi \in C_c(0, \infty)$, set of all continuous functions with compact support in $(0, \infty)$, we obtain

$$\langle -\Delta \rangle \geq \frac{1}{4} \left\langle \frac{1}{x^2} \right\rangle. \tag{2.6}$$

This implies that the Laplacian operator is negative on $L^2(0, \infty)$, and it is the form of the inequality we will use in our later study of the eigen-energy signs for Coulomb-like potentials.

2.3 Unbounded Operators

In this section we provide some basic definitions and properties of unbounded operators on a Hilbert space, as they play a crucial role in the world of quantum mechanics. For this section we denote by $\mathcal{H}$ a Hilbert space with an inner product $\langle \cdot, \cdot \rangle$. [2, 6, 20, 27, 28]

Definition 2.3.1. *A linear operator K in $\mathcal{H}$ is a linear transformation*

$$K : D(K) \quad \mapsto \mathcal{H},$$

where $D(K) \subset \mathcal{H}$ is the domain of K. We assume that $D(K)$ is dense in $\mathcal{H}$ and we say that K is densely defined in $\mathcal{H}$.

Definition 2.3.2. *The graph of an operator K is the set of pairs*

$$\Gamma(K) := \{\langle \varphi, K\varphi\rangle \mid \varphi \in D(K)\}.$$

Thus, $\Gamma(K)$ is a subset of $\mathcal{H}\times\mathcal{H}$, which is a Hilbert space with the inner product

$$\big(\langle\varphi_1,\varphi_2\rangle, \langle\psi_1,\psi_2\rangle\big) = \langle\varphi_1,\varphi_2\rangle + \langle\psi_1,\psi_2\rangle.$$

We say that K is a closed operator if $\Gamma(K)$ is a closed subset of $\mathcal{H}\times\mathcal{H}$.

Definition 2.3.3. *An operator K on $\mathcal{H}$ is bounded if $\sup\limits_{||\varphi||=1} ||K\varphi|| < \infty$.*

Definition 2.3.4. *The adjoint of an operator K on $\mathcal{H}$ is the operator $K^* : D(K^*)$ defined by*

$$\langle K^*\psi, \varphi\rangle = \langle \psi, K\varphi\rangle,$$

for all $\varphi \in D(K)$ and $\psi \in D(K^*)$ where

$$D(K^*) := \{\psi \in \mathcal{H} \mid \exists \psi^* \in \mathcal{H}, \langle K\varphi, \psi\rangle = \langle \varphi, \psi^*\rangle \ , \forall \varphi \in D(K) \quad and \quad K^*\varphi = \psi^*\}.$$

Definition 2.3.5. *An operator K on $\mathcal{H}$ is called Hermitian (or symmetric), if $D(K) \subset D(K^*)$ and $K\varphi = K^*\varphi$, for all $\varphi \in D(K)$. Moreover, if $\langle\varphi, K\varphi\rangle \geq 0$ for all $\varphi \in D(K)$, we say that K is a positive operator, and if $\langle\varphi, K\varphi\rangle > 0$ for all $\varphi \in D(K)$ and $\varphi \neq 0$, we say that K is positive definite.*

If K is Hermitian with $D(K) = D(K^*)$ and $K = K^*$, we say that K is a self adjoint operator.

Definition 2.3.6. *The spectrum of an operator K on $\mathcal{H}$ is the set*

$$\sigma(K) := \{\lambda \in \mathcal{C} \mid K - \lambda \quad \textit{is not invertible}\}.$$

Then, λ is an eigenvalue of K.

The point (discrete) spectrum of K is the set $\sigma_P(K)$ of all λ such that λ is an isolated eigenvalue of K with a finite multiplicity.

2.4 The min-max variational principle

The min-max principle, known as *Fischer-Courant theorem*, is very useful for estimating the discrete spectrum of Schrödinger operators, since not all the problems in non-relativistic quantum mechanics can be analytically solved. [2, 6, 27, 29, 30]

Theorem 2.4.1.

Let H be a self-adjoint operator that is bounded from below, on a Hilbert space $\mathcal{H}$, with a discrete spectrum $E_1 \leq E_2 \leq ... \leq E_n$. We denote by $\mathcal{D}_n$ an arbitrary n-dimensional subspace in $\mathcal{H}$. Then

$$E_n = \inf_{\mathcal{D}_n} \sup_{\psi\in\mathcal{D}_n\cap D(\mathcal{H})} \frac{\langle\varphi, H\varphi\rangle}{\langle\varphi,\varphi\rangle} \tag{2.7}$$

$$= \min_{\mathcal{D}_n} \max_{\psi\in\mathcal{D}_n\cap D(\mathcal{H})} \frac{\langle\varphi, H\varphi\rangle}{\langle\varphi,\varphi\rangle} \tag{2.8}$$

$$= \sup_{\mathcal{D}_n} \inf_{\psi\in\mathcal{D}_n\cap D(\mathcal{H})} \frac{\langle\varphi, H\varphi\rangle}{\langle\varphi,\varphi\rangle} \tag{2.9}$$

$$= \max_{\mathcal{D}_n} \min_{\psi\in\mathcal{D}_n\cap D(\mathcal{H})} \frac{\langle\varphi, H\varphi\rangle}{\langle\varphi,\varphi\rangle}. \tag{2.10}$$

The ratio $\dfrac{\langle \varphi, H\varphi\rangle}{\langle \varphi, \varphi\rangle}$ is called the *Rayleigh quotient*, and the values E_n are their corresponding eigenvalues. This theorem is the main idea of the Rayleigh-Ritz (or variation) method. If $\mathcal{D}_n \subset D(H)$, then the corresponding eigenvalues $E_1(\mathcal{D}_n) \leq E_2(\mathcal{D}_n) \leq \ldots \leq E_n(\mathcal{D}_n)$, provide upper bounds $\big(E_1(\mathcal{D}_n) \geq E_1\big)$.

The Variational Method: We first assume that φ is normalized, i.e. $\|\varphi\| = 1$. Since $\langle H\rangle = \langle \varphi, H\varphi\rangle \geq E_n$ (2.7), then the Schrödinger operator is bounded from below. Thus we can find an upper bound for the least energy-eigenvalue of H (the ground state energy), and consequently, characterize the H-spectrum variationally, by choosing a convenient trial function.

Example: We find an upper bound for the operator $H = -\Delta + vx^2$ in one dimension, by choosing the trial function

$$\varphi(x) = \frac{N}{x^2 + b^2} \in L^2(\mathbb{R}),$$

where N is the normalization constant, $v > 0$, and $b > 0$ is an adjusting parameter. Since $\|\varphi\| = 1$, then

$$1 = N^2 \int_{-\infty}^{\infty} \frac{1}{(x^2+b^2)^2} dx \quad \Longrightarrow \; N = \sqrt{\frac{2b^3}{\pi}}.$$

We have $\langle H\rangle = \langle -\Delta\rangle + \langle vx^2\rangle$. Then

(i) $\langle -\Delta\rangle = N^2 \displaystyle\int_{-\infty}^{\infty} \frac{1}{(x^2+b^2)} \frac{d^2}{dx^2}\left(\frac{1}{(x^2+b^2)}\right) dx = \frac{b^3}{\pi} \int_{-\infty}^{\infty} \frac{2(3x^2-b^2)}{(x^2+b^2)^4} dx = \frac{1}{2b^2}.$

(ii) $\langle vx^2\rangle = v^2 N^2 \displaystyle\int_{-\infty}^{\infty} \frac{x^2}{(x^2+b^2)^2} dx = v^2 b^2.$

Thus,

$$\langle H\rangle = \frac{1}{2b^2} + v^2 b^2.$$

We now minimize $\langle H\rangle$ with respect to the parameter b. Then,

$$\frac{\partial H}{\partial b} = -\frac{1}{b^3} + 2v^2 b = 0.$$

$$\Longrightarrow \quad b = \sqrt[4]{\frac{1}{2v^2}}.$$

Hence,

$$\langle H\rangle_{\min} = \frac{1}{2\sqrt{\dfrac{1}{2v^2}}} + v^2\sqrt{\frac{1}{2v^2}} = v\sqrt{2}.$$

This result is verified since we know the exact value for the ground state energy, which is v. [38].

We now state the **Comparison theorem for non-relativistic quantum mechanics**, which is a direct consequence of the min-max principle.

Theorem 2.4.2. *[2, 4, 35] Let H_a and H_b be two self-adjoint operators such that $H_a \leq H_b$, that is to say: $\langle \varphi, H_a\varphi\rangle \leq \langle \varphi, H_b\varphi\rangle$ for all $\varphi \in D(H_a) \cap D(H_b)$. Then the eigenvalues of H_a are smaller than those of H_b.*

Proof. Let $E_n(a)$ and $E_n(b)$ be the respective eigenvalues of H_a and H_b in the ascending order, and choose $\varphi \in D(H_a) \cap D(H_b)$. Then by the min-max principle we have:

$$\begin{aligned} E_n(a) &= \inf_{D(H_a)} \sup_{\varphi \in D(H_a) \cap D(H_b)} \frac{\langle \varphi, H_a \varphi \rangle}{\langle \varphi, \varphi \rangle} \\ &\leq \inf_{D(H_b)} \sup_{\varphi \in D(H_a) \cap D(H_b)} \frac{\langle \varphi, H_b \varphi \rangle}{\langle \varphi, \varphi \rangle} \\ &= E_n(b). \end{aligned}$$

□

2.5 Schrödinger Operators

We first recall the Hamiltonian equation in classical mechanics [43]

$$H = \frac{P^2}{2m} + V,$$

where p is the momentum and V is the potential function. this represents the total energy E. Passing to quantum mechanics, we do the following replacements:

$$P \to -i\hbar\nabla \quad \text{and} \quad E \to i\hbar\frac{\partial}{\partial t},$$

which leads to the so called *Schrödinger equation*

$$i\hbar\frac{\partial\varphi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\Delta + V(x) \right] \varphi(x,t). \tag{2.11}$$

Assuming that $\hbar = 2m = 1$ (2.11) reads

$$H\varphi = E\varphi, \tag{2.12}$$

where H

$$H = -\Delta + V,$$

is the linear operator called *Schrödinger operator*. We shall consider the class of potentials V to be the negative non-decreasing functions $C_0^\infty(\mathbb{R}^d)$, $d \geq 1$. [6, 31–33, 36, 37, 67, 77] The comparison theorem (**theorem** 2.4.2) is stated as

$$V_a \leq V_b \implies E_a \leq E_b,$$

where E_a and E_b are respective eigenvalues of $H_a = -\Delta + V_a$ and $H_b = -\Delta + V_b$.

2.6 The Heisenberg uncertainty principle

This is one of the fundamental implications of the quantum theory. It means that it is impossible for the position and the momentum of a particle cannot be accurately measured at the same time. [39]

We first define the coordinate multiplication ad the momentum operators over $L^2(\mathbb{R}^d)$ as

$$x_j : \quad \varphi(x) \to x_j\varphi_j(x),$$

with $d \geq 1$, where x_j is the j-th component of the coordinate x in the state φ, and

$$p_j : \varphi(x) \to -i\hbar\nabla_j\big(\varphi(x)\big),$$

where $i^2 = -1$ and $\hbar$ is the reduced Planck's constant.

We recall that commutator operator is

$$[A, B] := AB - BA,$$

where A and B are two operators.

Lemma 2.6.1. *If A and B are two self adjoint operators then*

$$\langle \varphi, i[A, B]\varphi \rangle = -2Im\langle A\varphi, B\varphi \rangle.$$

Proof. $\langle \varphi, i[A, B]\varphi \rangle = \langle \varphi, i(AB - BA)\varphi \rangle = i\Big(\langle \varphi, AB\varphi \rangle - \langle \varphi, BA\varphi \rangle \Big) = i\Big(\langle A\varphi, B\varphi \rangle - \langle B\varphi, A\varphi \rangle \Big)$
$= i\Big[\langle A\varphi, B\varphi \rangle - \overline{\langle A\varphi, B\varphi \rangle} \Big] = -2\mathrm{Im}\langle A\varphi, B\varphi \rangle.$ □

Theorem 2.6.1. Heisenberg uncertainty principle *We define the dispersions of x_j and p_j in a state φ as*

$$(\Delta x_j)^2 := \langle \big(x_j - \langle x_j \rangle\big)^2 \rangle,$$

and

$$(\Delta p_j)^2 := \langle \big(p_j - \langle p_j \rangle\big)^2 \rangle,$$

where $\langle x_j \rangle = \langle \varphi, x_j\varphi \rangle$ and $\langle p_j \rangle = \langle \varphi, p_j\varphi \rangle$ are the respective expected values of x_j and p_j. Then for any state φ such that $\|\varphi\| = 1$ we have

$$(\Delta x_j)(\Delta p_j) \geq \hbar/2.$$

Proof. We assume, for simplicity, that $\langle x \rangle = \langle p \rangle = 0$. A simple calculation gives the following canonical relation

$$\frac{i}{\hbar}[p_j, x_j] = 1.$$

Then

$$1 = \langle \varphi, \varphi \rangle = \langle \varphi, \frac{i}{\hbar}[p_j, x_j]\varphi \rangle = -\frac{2}{\hbar}\mathrm{Im}\langle p_j\varphi, x_j\varphi \rangle \leq -\frac{2}{\hbar}\Big| \langle p_j\varphi, x_j\varphi \rangle \Big|.$$

Hence, applying (2.1) we get

$$1 \leq \frac{2}{\hbar} \|p_j\varphi\| \, \|x_j\varphi\| \,,$$

and we obtain the desired result. □

2.7 Formulation of a relativistic quantum theory

In order to develop a more correct quantum theory, it should satisfy the principles of **special relativity**. That is to say: laws of motion valid in one inertial system (a coordinate system in which Newton's laws of motion are valid), must be true in all other inertial systems. Mathematically speaking, this means that a relativistic quantum theory must satisfy the *Lorentz invriance* property, which we shall now define. [40–42]

Definition 2.7.1. Lorentz transformation *Consider a four-vector x. we define $x' := \Lambda x$ to be the Lorentz transformation of x, where Λ is the following 4×4-matrix*

$$\Lambda = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

γ is defined as the Lorentz factor and

$$\gamma := \frac{1}{\sqrt{1-\beta^2}},$$

with $0 < \beta < 1$.

We say that a quantity A is Lorentz invariant if $A' = A$ where A' is the Lorentz transform of A.

Example: We consider the four-vector

$$v = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix},$$

which represents the space-time coordinates in a given inertial system (c is a constant which represents the speed of light in vacuum). We compute the coordinates of v', the Lorentz transform of v. Thus

$$v' = \Lambda v.$$

We want to verify the Lorentz invariance of the quantity $-c^2t^2 + x^2$. Then

$$\begin{aligned} -c^2(t')^2 + (x')^2 &= -(\gamma ct - \beta\gamma x)^2 + (\gamma x - \beta\gamma ct)^2 \\ &= (\beta^2 - 1)\gamma^2(c^2t^2 - x^2) \\ &= -c^2t^2 + x^2. \end{aligned}$$

Hence, the quantity $-c^2(t')^2 + (x')^2$ is Lorentz invariant.

2.7.1 Construction of the relativistic Klein–Gordon equation

We first define the contravariant form of a four-vector x as

$$x^\mu := \{x^0, x^1, x^2, x^3\} = \{ct, x, y, z\},$$

which describes the space-time coordinates, where the time-like component is denoted as the zero component. We also define the covariant form of x as

$$x_\mu := \{ct, -x, -y, -z\} = \{x_0, x_1, x_2, x_3\}.$$

We can transform from one form into the other by applying the following relations

$$x^\mu = g^{\mu\nu}x_\nu \quad \text{and} \quad x_\mu = g_{\mu\nu}x^\nu,$$

where

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \text{and} \quad g^{\mu\nu} = (g^{-1})_{\mu\nu}.$$

We also define the covariant and contravariant forms of the four-momentum vector as

$$p_\mu = i\hbar \frac{\partial}{\partial x^\mu} \quad \text{and} \quad p^\mu = i\hbar \frac{\partial}{\partial x_\mu},$$

respectively. Thus,

$$p^\mu p_\mu = -\hbar^2 \frac{\partial}{\partial x_\mu} \frac{\partial}{\partial x^\mu} = -\hbar^2 \Box,$$

where

$$\Box := \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta = \frac{E^2}{c^2} - \Delta,$$

is the so called d'Alembertian operator.
The Klein–Gordon equation for free particles is defined as

$$p^\mu p_\mu \psi = m_0^2 c^2 \psi, \tag{2.13}$$

where m_0 is the rest mass of the particle. Thus, we can write (2.13) as

$$\left(\frac{\partial^2}{c^2 \partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \frac{m_0^2 c^2}{\hbar^2} \right) \psi = 0.$$

This equation verifies the Lorentz covariance; that is to say its form is preserved while changing the coordinate system. Solutions for this equation are of the form

$$\psi = \exp\big(-\frac{i}{\hbar} p_\mu x^\mu \big) = \exp\left[\frac{i}{\hbar} (p \cdot x - Et) \right],$$

where $p = (p_x, p_y, p_z)$ and $x = (x^1, x^2, x^3)$.

Since $p^\mu p_\mu = \dfrac{E^2}{c^2} - \Delta$, then the equation $p^\mu p_\mu = m_0^2 c^2$ gives the energy relativistic operator

$$E = \pm \sqrt{m_0^2 c^2 - \Delta}. \tag{2.14}$$

We will reformulate (2.13) for $d \geq 1$ in the next chapter.

We now provide an example which shows that the Klein–Gordon energy operators are not necessarily bounded from below, for which we try to apply the variational method explained in **section** 2.4. We use the one-dimensional equation (3.1) defined in the chapter 2

$$\varphi''(x) = \left[m^2 - \big(E - V(x) \big)^2 \right] \varphi(x),$$

and we choose

$$\varphi(x) = N e^{-b|x|}$$

as a trial function, where $b > 0$ is a parameter and N is a normalization constant. Since $\|\varphi\| = 1$, then

$$\varphi(x) = \sqrt{b} e^{-b|x|} \in L^2(\mathbb{R}).$$

We consider the cut-off Coulomb potential [44, 45]

$$V(x) = -\frac{1}{|x| + a},$$

where $a > 1$. Multiplying this equation by φ and applying integration by parts we get

$$\langle \Delta \rangle = m^2 - E^2 + 2E \langle V \rangle - \langle V^2 \rangle. \tag{2.15}$$

We have:

(i)

$$\langle \Delta \rangle = \int_{-\infty}^{\infty} -b^3 e^{-2b|x|} dx = -b^2.$$

(ii)

$$\langle V \rangle = \int_{-\infty}^{\infty} -\frac{be^{-2b|x|}}{|x|+a} dx = 2\int_{0}^{\infty} -\frac{be^{-2bx}}{x+a} dx.$$

Using the change of variable $u = 2bx + 2ab$ we get

$$\langle V \rangle = -2be^{2ab} \int_{2ab}^{\infty} \frac{e^{-u}}{u} du = -(2b)e^{2ab} E_1(2ab),$$

where E_n is the exponential integral function [47]

$$E_n(z) = \int_{1}^{\infty} \frac{e^{-zt}}{t^n} dt.$$

(iii)

$$\langle V^2 \rangle = \int_{-\infty}^{\infty} \frac{be^{-2b|x|}}{(|x|+a)^2} dx = 2\int_{0}^{\infty} \frac{be^{-2bx}}{(x+a)^2} dx.$$

Applying integration by parts $\left(u = e^{-2bx} \text{ and } dv = \dfrac{2b}{(x+a)^2}\right)$, then using the change of variable $u = 4bx + 4ab$ we find that

$$\langle V^2 \rangle = \frac{(2b)(e^{2ab})E_2(2ab)}{a}.$$

Thus, (2.15) becomes

$$-b^2 = m^2 - E^2 - 4(E)(b)(e^{2ab})E_1(2ab) - \frac{2b}{a}(e^{2ab})E_2(2ab),$$

We now minimize the energy E with respect to b. Thus,

$$\begin{aligned} -2b = -2(E)\frac{dE}{db} - 4\frac{dE}{db}(b)(e^{2ab})E_1(2ab) - 4(E)(e^{2ab})E_1(2ab) - 4(E)(b)(e^{2ab})\frac{\partial}{\partial b}E_1(2ab) \\ -\frac{2}{a}(e^{2ab})E_2(2ab) - \frac{2b}{a}(2ae^{2ab})E_2(2ab) - \frac{2b}{a}(e^{2ab})\frac{\partial}{\partial b}E_2(2ab). \end{aligned}$$

Letting $\dfrac{\partial E}{\partial b} = 0$ we get

$$\begin{aligned} -b = -4(E)(e^{2ab})E_1(2ab) - 2(E)(b)(e^{2ab})\frac{\partial}{\partial b}E_1(2ab) - \frac{1}{a}(e^{2ab})E_2(2ab) \\ -\frac{b}{a}(2ae^{2ab})E_2(2ab) - \frac{b}{a}(e^{2ab})\frac{\partial}{\partial b}E_2(2ab). \end{aligned}$$

Thus

$$E = \frac{-be^{-2ab} + \dfrac{1}{a}E_2(2ab) + \big(2b\big)E_2(2ab) + \dfrac{b}{a}\dfrac{\partial}{\partial b}E_2(2ab)}{-2\big(1+ab\big)E_1(2ab) - \big(2b\big)\dfrac{\partial}{\partial b}E_1(2ab)}.$$

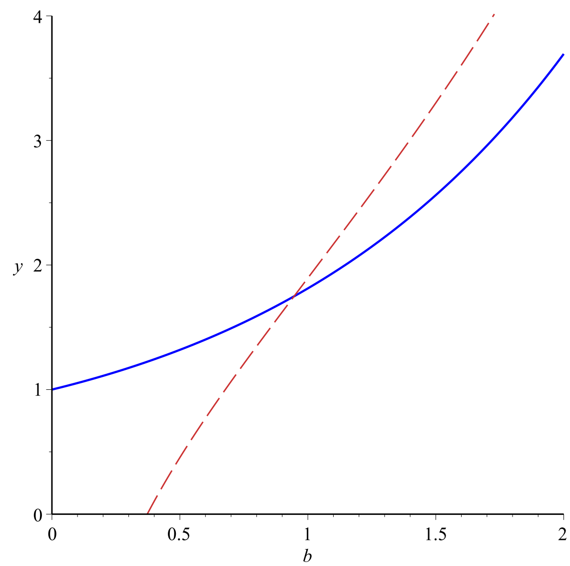


Figure 2.1: Graphs of functions $h(b) = \dfrac{e^b}{1+0.5b}$ full line, and $g(b) = E_1(b)$ dashed line.They intersect at $x \approx 0.946$.

Setting the denominator equal to zero we get

$$(1+ab)E_1(2ab) = -b\frac{\partial}{\partial b}E_1(2ab) = e^{2ab}.$$

We choose $a = 0.5$ and sketch the graphs of the functions

$$h(b) = \frac{e^b}{1+0.5b},$$

and

$$g(b) = E_1(b)$$

in figure1. We find that $b \approx 0.946$. This implies that the energy operator for the Klein–Gordon equation with the potential function $f(x) = -\dfrac{1}{|x|+0.5}$ is not bounded below, which means that a simple variational principle for characterizing the spectrum of the Klein–Gordon equation as in the Schrödinger case is no more possible. Hence, using suitable comparison theorems is very helpful. These theorems are based on the dependence of the eigen-energy E on the coupling constant $v > 0$; i.e $E = E(v)$, for which we express the potential function V as $V(x) = vf(x)$. However, all the previous theorems [48–50] were restricted to positive energies due to the lack of monotonicity caused by the *two-valued expression* $E(v)$. What we have did in our work was studying the Klein–Gordon problem in the eigenvalue v, and thus creating the *spectral functions* $v(E)$. We shall completely characterize these graphs in **chapter** 6.

2.8 The numerical shooting method

The shooting method is a numerical method for solving a differential equation boundary problem. It reduces it to an initial value problem [51–55].

Consider the following boundary value problem

$$\frac{d^2y}{dt^2} = f\left(t, y, \frac{dy}{dt}\right),$$

where $t \in [a, b]$ with the boundary conditions

$$\begin{cases} y(a) = \alpha \\ y(b) = \beta. \end{cases}$$

Assuming that $y'(a) = A$ the boundary conditions are reduced to

$$\begin{cases} y(a) = \alpha \\ \left.\dfrac{dy}{dt}\right|_a = A, \end{cases}$$

where the constant A must be chosen so that y satisfies the right hand boundary condition $y(b) = \beta$. The shooting method gives an iterative procedure with which we can determine the constant A. Figure 2.2 illustrates the solution of the boundary value problem given two distinct values of A. In one case, the value of $A = A_1$ gives a value for the initial slope which is too low to satisfy the boundary condition $y(b) = \beta$, whereas the value of $A = A_2$ is too large to satisfy this condition. However, A_1 and A_2 suggest the next guess: we have to adjust the value of A in the reduced conditions and find an A which will lead to a solution that satisfies the given boundary conditions. The basic algorithm is as follows:

(i) Solve the differential equation using any known method with initial conditions $y(a) = \alpha$ and $y'(a) = A$;

(ii) Evaluate the solution $y(t)$ at $t = b$ and compare this value with the target value $y(b) = \beta$.

(iii) Adjust the value of A (either bigger or smaller) until a desired level of accuracy is achieved.

In our applications, instead of the initial slope A, the adjustable parameter is the eigenvalue $v = v(E)$, given that the calculated wave function has the correct number of nodes for the eigenvalue sought, and it approaches 0 near infinity.

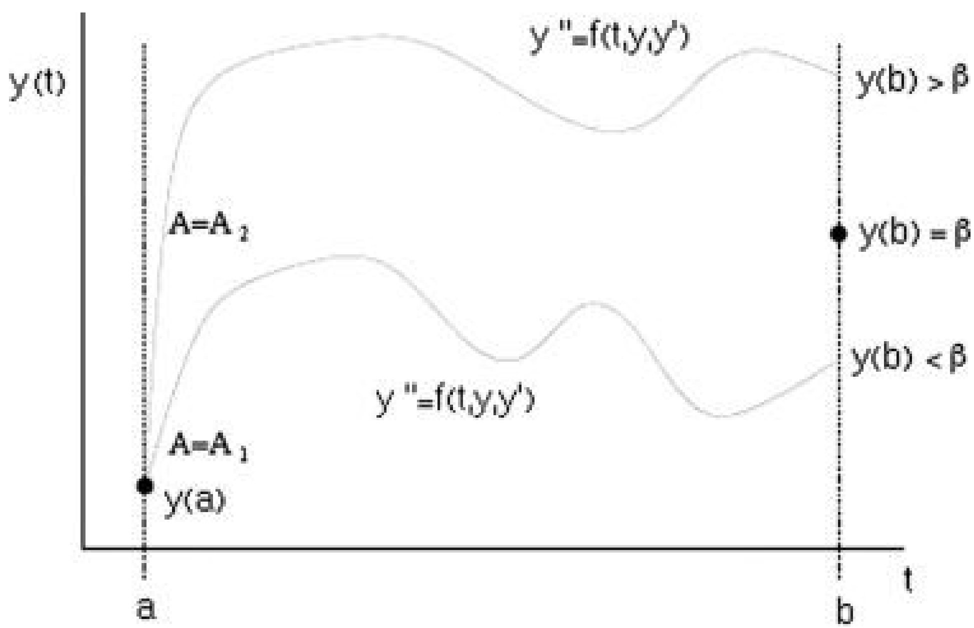


Figure 2.2: shows the solutions of the boundary value problem with $y(a) = \alpha$ and $y'(a) = A$. Here, two values of A are used to illustrate the solution's behavior and its lack of matching the correct boundary value $y(b) = \beta$.

Chapter 3

The Klein–Gordon equation

3.1 Klein–Gordon equation in dimension $d = 1$

The Klein–Gordon equation in one dimension is given by:

$$\varphi''(x) = \left[m^2 - \left(E - V(x)\right)^2\right]\varphi(x), \quad x \in \mathbb{R}. \tag{3.1}$$

where φ'' denotes the second order derivative of φ with respect to x, natural units $\hbar = c = 1$ are used, and E is the energy of a spinless particle of mass m. We suppose that the potential function V is expressed as $V(x) = vf(x)$ with $v > 0$ and f satisfies the following conditions:

1. $V(x) = vf(x), x \in \mathbb{R}$, where $v > 0$ is the coupling parameter and $f(x)$ is the potential shape;
2. f is even $f(x) = f(-x)$;
3. f is not identically zero, and is non-positive, that is $f(x) \leq 0$;
4. f is attractive, that is f is monotone non-decreasing over $[0, \infty)$;
5. f vanishes at infinity, i.e $\lim\limits_{x\to\pm\infty} f(x) = 0$.

We also assume that $V(x) = vf(x)$ is in this class $\mathcal{P}$ of potentials, for which the Klein–Gordon equation (3.1) has at least one discrete eigenvalue E, and that equation (3.1) is the eigen-equation for the eigenstates.

3.2 Klein–Gordon equation in dimension $d > 1$

The Klein–Gordon equation in d dimensions is given by

$$\Delta_d\Psi(r) = [m^2 - (E - V(r))^2]\Psi(r),$$

where natural units $\hbar = c = 1$ are used and E is the discrete energy eigenvalue of a spinless particle of mass m. We suppose here that the vector potential function $V(r)$, $r = ||\mathbf{r}||$, is a radially-symmetric Lorentz vector potential (the time component of a space-time vector), which belongs to the class $\mathcal{P}_d$ with the following properties:

1. $V(r) = vf(r), r \in [0, \infty)$, where $v > 0$ is the coupling parameter and $f(r)$ is the potential shape;
2. f is not identically zero and non-positive;
3. f is attractive, that is f is monotone non-decreasing over $[0, \infty)$;
4. f is not more singular than $r^{-(d-2)}$, $r \in [0, \infty)$, that is $\lim\limits_{r\to 0} r^{(d-2)} f(r) = A, \quad -\infty < A \leq 0$;

5. f vanishes at infinity, i.e $\lim_{r\to\infty} f(r) = 0$.

This is a wider potential class than $\mathcal{P}$, since it contains Coulomb and Coulomb - like potentials, such as the Yukawa and the Hulthén potentials. The operator Δ_d is the d-dimensional Laplacian. Hence, the wave function for $d > 1$ can be expressed as $\Psi(r) = R(r)Y_{l_{d-1,\dots,l_1}}(\theta_1, \theta_2, ..., \theta_{d-1})$, where $R \in L^2(\mathbb{R}^d)$ is a radial function and $Y_{l_{d-1,\dots,l_1}}$ is a normalized hyper-spherical harmonic with eigenvalues $l(l + d - 1)$, $l = 0, 1, 2, ...$ [61] The radial part of the above Klein–Gordon equation can be written as:

$$\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}R(r)\right) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{l(l+d-2)}{r^2}\right]R(r),$$

where R satisfies the second-order linear differential equation

$$R''(r) + \frac{d-1}{r}R'(r) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{l(l+d-2)}{r^2}\right]R(r). \tag{3.2}$$

Applying the change of variable $R(r) = r^{-\frac{d-1}{2}}\varphi(r)$, we obtain the following reduced second-order differential equation:

$$\varphi''(r) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2}\right]\varphi(r), \tag{3.3}$$

where

$$Q = \frac{1}{4}(2l + d - 1)(2l + d - 3),$$

with $l = 0, 1, 2, ...$ and $d = 2, 3, 4, ...$, which is the radial Klein-Gordon equation for $d > 1$ dimensions. The reduced wave function φ satisfies $\varphi(0) = 0$ and $\lim_{r\to\infty}\varphi(x) = 0$ [59].

We also define the Klein–Gordon equation with a scalar potential S [62]:

$$\Delta_d\Psi(r) = [\big(m + S(r)\big)^2 - \big(E - V(r)\big)^2]\Psi(r), \tag{3.4}$$

where S satisfies either

i S is non-negative ($S \geq 0$);

ii S is non-increasing on $[0, \infty)$;

iii S vanishes at infinity; i.e $\lim_{r\to\infty} S(r) = 0$,

or

i S is non-positive and bounded by $-m$, i.e, $-m \leq S \leq 0$;

ii S is non-decreasing on $[0, \infty)$;

iii S vanishes at infinity; i.e $\lim_{r\to\infty} S(r) = 0$.

Applying the same change of variable $R(r) = r^{-\frac{d-1}{2}}\varphi(r)$, we obtain the following second order radial equation

$$\varphi''(r) = \left[\big(m + S(r)\big)^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2}\right]\varphi(r). \tag{3.5}$$

Chapter 4

Discrete energies and bound states of the Klein–Gordon equation

4.1 Klein–Gordon bound states in dimension $d = 1$

Let φ be a bound state solution for equation (3.1). Then $\varphi \in L^2(\mathbb{R})$. Since $\lim_{x\to\pm\infty} f(x) = 0$, then equation (3.1) has the asymptotic form

$$\varphi''(x) = (m^2 - E^2)\varphi(x),$$

at infinity, with solutions $\varphi(x) = C_1 e^{\sqrt{k}|x|} + C_2 e^{-\sqrt{k}|x|}$, where C_1 and C_2 are constants of integration, and $k = m^2 - E^2$. The radial wave function of φ vanishes at infinity; thus, $C_1 = 0$. Since $\varphi \in L^2(\mathbb{R})$, then $k > 0$ which means that

$$|E| < m. \tag{4.1}$$

Suppose that $\varphi(x)$ is a solution of (3.1). Then by direct substitution we conclude that $\varphi(-x)$ is another solution of (3.1). Thus, by using linear combinations, we see that all the solutions of this equation may be assumed to be either even or odd. Hence, if φ is even then $\varphi'(0) = 0$, and if φ is odd then $\varphi(0) = 0$. Since $\varphi \in L^2(\mathbb{R})$ then $\int_{-\infty}^{+\infty} \varphi^2 dx < \infty$. This means that the wave functions can be normalized and consequently we shall assume that φ satisfies the normalization condition

$$||\varphi||^2 = \int_{-\infty}^{\infty} \varphi^2(x)dx = 1. \tag{4.2}$$

4.1.1 Properties of the bound states of the Klein-Gordon equation in dimension $d = 1$

Lemma 4.1.1. *If φ is the node-free (ground) state, then φ'' changes its sign only once over $[0, \infty)$.*

Proof. Let $\varphi''(x) = 0$. Then from equation (3.1) we get $m^2 - \big(E - V(x)\big)^2 = 0$, which means that $V(x) = E - m$ or $V(x) = E + m$. Since $|E| < m$ and $V(x) \le 0$, then $V \ne E + m$. Hence, $V(x) = E - m$ and $\varphi''(x) = 0 \Longleftrightarrow x = V^{-1}(E - m)$, where V^{-1} is the inverse of the monotone function V.

1. V **is unbounded near** 0**:** Since V is unbounded near 0, then $\varphi'' < 0$ near 0, and since V vanishes at ∞, equation (3.1) becomes $\varphi'' = (m^2 - E^2)\varphi > 0$. Hence, φ is concave on $\big[0, V^{-1}(E - m)\big)$ and convex on $\big(V^{-1}(E - m), \infty\big)$.

2. V **is bounded; that is:** $V_0 \le V \le 0$**:**

   Since φ is an even state, then $\varphi'(0) = 0$, which means that $y = \varphi(0)$ is an equation of the tangent line to φ at $x = 0$.

If φ is convex near 0, then φ'' must change it sign at some $x_1 \in [0,\infty)$ since we know that φ vanishes near ∞. However, equation (3.1) becomes $\varphi'' = (m^2 - E^2)\varphi > 0$ near ∞, which means that φ is convex near ∞. Thus φ'' should again change its sign at some $x_2 \in [x_1,\infty)$. This means that φ has two inflection points on $[0,\infty)$, which is a contradiction. Hence, φ is concave on $\big[0, V^{-1}(E-m)\big)$ and convex on $\big(V^{-1}(E-m),\infty\big)$.

□

Lemma 4.1.2. *φ'' changes its sign at least once over $[0,\infty)$, for any excited state φ.*

Proof. Using the parity of φ, it is sufficient to study the sign of φ'' on the interval $[0,\infty)$. If V is unbounded near 0, then $\varphi'' < 0$ near 0 and $\varphi'' > 0$ near ∞. If V is bounded; that is $V_0 \le V \le 0$ where $V_0 = V(0)$, then we divide the proof into the following two cases:

1. φ **has only one node:** Suppose that φ has one node α, then $\varphi''(x) = 0 \iff x = \alpha$ or $x = V^{-1}(E-m)$. If $\varphi(x) > 0$ for $x > \alpha$, then φ should attain a maximum value since it vanishes near ∞, and thus $\varphi'' < 0$. However, by the same condition that φ vanishes near ∞, φ'' should change its sign one more time. This means that $V^{-1}(E-m) \in \big(\alpha,\infty\big)$. Therefore

   (A) if $\varphi(x) > 0$ for $x > \alpha$, then $\varphi''(x) < 0$ for $x \in \big(\alpha, V^{-1}(E-m)\big)$, and $\varphi''(x) > 0$ for $x \in (0,\alpha) \cup \big(V^{-1}(E-m),\infty\big)$;

   (B) if $\varphi(x) < 0$ for $x > \alpha$, then $\varphi''(x) > 0$ for $x \in \big(\alpha, V^{-1}(E-m)\big)$, and $\varphi''(x) < 0$ for $x \in (0,\alpha) \cup \big(V^{-1}(E-m),\infty\big)$.

2. φ **has n nodes,** $n \ge 2$**:**

   Suppose that φ has n nodes, $x = \alpha_1, \alpha_2, ..., \alpha_n$, $n \ge 2$. Then

   $$\varphi''(x) = 0 \iff m^2 - \big(E - V(x)\big)^2 = 0 \text{ or } \varphi(x) = 0,$$

   which means that

   $$x = \alpha_1, \alpha_2, ..., \alpha_n \text{ or } V^{-1}(E-m).$$

   We shall now study the concavity of φ over the interval (α_{n-1},∞) : If $\varphi(x) > 0$ on $\big(\alpha_{n-1},\alpha_n\big)$, then φ must attain a maximum value at some $x_0 \in \big(\alpha_{n-1},\alpha_n\big)$ and φ is concave on $\big(\alpha_{n-1},\alpha_n\big)$. For $x > \alpha_n$, φ changes both its sign and concavity. Thus φ becomes convex and negative for $x > \alpha_n$. However, since α vanishes near ∞, then φ'' vanishes and changes its sign one more time somewhere after its last node. This implies that $V^{-1}(E-m) \in \big(\alpha_n,\infty\big)$, and therefore $\varphi''(x) < 0$ for $x \in \big(\alpha_{n-1},\alpha_n\big) \cup \big(V^{-1}(E-m),\infty\big)$, and $\varphi''(x) > 0$ for $x \in \big(\alpha_n, V^{-1}(E-m)\big)$. By the same reasoning, if $\varphi(x) < 0$ on (α_{n-1},α_n), then $\varphi''(x) > 0$ for $x \in \big(\alpha_{n-1},\alpha_n\big) \cup \big(V^{-1}(E-m),\infty\big)$, and $\varphi''(x) < 0$ for $x \in \big(\alpha_n, V^{-1}(E-m)\big)$.

□

Lemma 4.1.3. *The ground state of the klein–Gordon equation is non-increasing on $x \in [0,\infty)$, for all $|E| < m$.*

Proof. Since $\varphi'(0) = 0$, $\varphi''(x) < 0$ on $\big[0, V^{-1}(E-m)\big)$, $\varphi''(x) > 0$ on $\big(V^{-1}(E-m),\infty\big)$, and $\lim\limits_{x\to\infty} \varphi(x) = 0$, hence φ is non-increasing on $[0,\infty)$. □

4.1.2 Discrete energies in dimension $d = 1$

We first write equation (3.1) as

$$\big(\varphi(x)\big)E^2 - \big(2vf(x)\varphi(x)\big)E + \big(\varphi''(x) - m^2\varphi(x) + v^2 f^2(x)\varphi(x)\big) = 0.$$

This is a quadratic equation in E. Then

$$E = vf(x) \pm \frac{\sqrt{v^2 f^2(x)\varphi^2(x) - \big(\varphi(x)\varphi''(x) - m^2\varphi^2(x) + v^2 f^2(x)\varphi^2(x)\big)}}{\varphi(x)}$$

Then

$$E = vf(x) - \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}, \tag{4.3}$$

or

$$E = vf(x) + \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}, \tag{4.4}$$

In solution (4.3), φ'' cannot change its sign because if $\varphi''(x) < 0$, then

$$vf(x) - \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}} \leq -\sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}} < -m,$$

and we already know that $|E| < m$. Hence, since we have shown in lemmas **2.1.1** and **2.1.2** that φ'' must change its sign, then E can only take the second solution (4.4).

4.1.3 Klein–Gordon bound states in dimension $d > 1$ except for $d = 2$, $l = 0$

In this section, we use the reduced Klein–Gordon equation stated in (3.3), with φ satisfying $\varphi(0) = 0$, to study the properties of all states except the s-states of the 2-dimensional case, that is to say for $d = 2$ and $l = 0$.
Let φ be a bound state for equation (3.2). Since V vanishes at ∞, then (3.2) becomes

$$\varphi''(r) = (m^2 - E^2)\varphi(r)$$

near infinity, which means that $|E| < m$ by the same reasoning as used for equation (5.37). Since $\varphi \in L(\mathbb{R}^d)$, then φ can be normalized, and we shall assume the normalization condition

$$\int_0^\infty \varphi^2(r)dr = 1.$$

Lemma 4.1.4. *φ'' should change its sign at least once, for any state φ.*

Proof. 1. φ **is a node-free state:**

$\varphi''(r) = 0 \Longleftrightarrow m^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2} = 0$, and near ∞, $\varphi'' = (m^2 - E^2)\varphi > 0$, which means that φ is convex near ∞.

If φ is concave near 0, then the theorem is proved.

If φ is convex near 0, then φ'' should change its sign at least at some r_1, r_2, solutions of the equation $m^2 - \big((E - V(r)\big)^2 + \frac{Q}{r^2} = 0$, in order to be positive near ∞.

2. φ **has one node:**

Suppose that φ has one node α, then $\varphi''(r) = 0 \Longleftrightarrow r = \alpha$ or $r = r_1, r_2, ..., r_n$, where the $r_i's$ are roots of the equation $m^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2} = 0$, $i = 1...n$.

Let's study the sign of φ'' for $r > \alpha$:

If $\varphi(r) > 0$, then due to the fact that φ vanishes at ∞, it should attain a maximum value over the interval (α, ∞) becoming concave near α^+. And due to the same fact, φ'' should change its sign at least once over (α, ∞), implying that there exists $r_i \in (\alpha, \infty)$. If $\varphi(r) < 0$, then we can also prove this lemma by the same reasoning.

3. φ **has** n **nodes,** $n \geq 2$**:**

   Suppose that φ has n nodes, $\alpha_1, \alpha_2, ..., \alpha_n$ with $n \geq 2$.

   Then $\varphi''(r) = 0 \Longleftrightarrow m^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2} = 0$ or $\varphi = 0$, which means:

   $r = \alpha_1, \alpha_2, ..., \alpha_n, r_1, r_2, ..., r_n$, where the $r_i' s$ are the solutions of the equation

   $m^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2} = 0$, $i = 1, 2, ..., n$.

   We will study the concavity of φ over the interval (α_{n-1}, α_n):

   If there exists some $r_i \in (\alpha_{n-1}, \alpha_n)$, then φ'' changes its sign at least once over (α_{n-1}, α_n)

   If there isn't any inflection point of α between α_{n-1} and α_n, then φ'' doesn't change its sign on (α_{n-1}, α_n); however, since φ vanishes at ∞, then there must be at least one inflection point $r_i \in (\alpha_{n-1}, \alpha_n)$, which means that φ changes its concavity at least once over (φ_{n-1}, ∞).

□

4.1.4 Discrete energies in dimension $d > 1$ except for $d = 2$ and $l = 0$

The expression (3.3), written as

$$\big(\varphi(r)\big)E^2 - \big(2vf(r)\varphi(r)\big)E + \left(\varphi''(r) - m^2\varphi(r) + v^2 f^2(r)\varphi(r) - \frac{Q}{r^2}\varphi(r)\right) = 0,$$

is a quadratic equation in E.

Thus,

$$E = vf(r) \pm \sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}.$$

If $\varphi''(r) < 0$, then $vf(r) - \sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}} < -m$, which means that E cannot take this value since $|E| < m$. Hence, since we have shown that φ must change its sign at least once for any bound state, then

$$E = vf(r) + \sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}. \tag{4.5}$$

4.2 2-dimensional s-states

The reduced Klein–Gordon equation (3.3) reads

$$\varphi'' = \left[m^2 - \big(E - V(r)^2\big) - \frac{1}{r^2}\right]\varphi(r).$$

Thus $E = vf(r) \pm \sqrt{m^2 - \frac{1}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}$. Eliminating the solution $E = vf(r) - \sqrt{m^2 - \frac{1}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}$ fails because of the existence of the term $-\frac{1}{r^2}$. Thus, we use the non-reduced form of the Klein–Gordon radial equation, namely

$$R''(r) + \frac{d-1}{r}R'(r) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{l(l+d-2)}{r^2}\right]R(r),$$

where $d = 2$, $l = 0$, and $\displaystyle\int_0^\infty R^2(r) r^{d-1} dr = 1$. Hence,

$$R''(r) + \frac{1}{r}R'(r) = \left[m^2 - \big(E - V(r)\big)^2\right]R(r). \tag{4.6}$$

Lemma 4.2.1. *Consider the Klein–Gordon equation (3.2). Then there exists an interval* $J \subset [0,\infty)$ *such that* $-\dfrac{R''(r)}{R(r)} - \dfrac{R'(r)}{rR(r)} > 0$.

Proof. 1. R **is a node-free state:**

$$R''(r) = 0 \iff m^2 - \big(E - V(r)\big)^2 - \frac{R'(r)}{rR(r)} = 0 \iff V(r) = E \pm \sqrt{m^2 - \frac{R'}{rR(r)}}.$$

If R is decreasing near 0, then $-\dfrac{R'(r)}{rR(r)} > 0$ near 0.

If R is increasing near 0, then it must attain a maximum value at some $r_0 \in [0,\infty)$ and end up decreasing since $\lim\limits_{r\to\infty} R(r) = 0$. Thus, $-\dfrac{R'}{rR(r)} > 0$ on (r_0,∞).

Hence, in both cases R must be decreasing on a subset (r_0,∞) of $[0,\infty)$, and $\sqrt{m^2 - \dfrac{R'(r)}{rR(r)}} > m$ on this subset interval.

Therefore, V cannot take the value $E + \sqrt{m^2 - \dfrac{R'(r)}{rR(r)}}$ since V is non-positive and

$$R''(r) = 0 \iff V(r) = E - \sqrt{m^2 - \frac{R'(r)}{rR(r)}}. \tag{4.7}$$

Let r_i be a root of equation (4.7).

If $r_i \in (r_0,\infty)$, then $J = (r_0, r_i)$.

If $r_i \notin (r_0,\infty)$, then there must exist at least another inflection point $r_j \in (r_0,\infty)$ because R vanishes at infinity, which also implies that $R > 0, R' < 0$, and $R'' < 0$ on (r_0, r_j). Therefore, $J = (r_0, r_j)$.

2. R **is an excited State:** Suppose that R has n nodes $\alpha_1, \alpha_2, ...\alpha_n$ and consider the interval (α_n,∞).

Then

$$R'' = 0 \iff m^2 - \big(E - V(r)\big)^2 - \frac{R'(r)}{rR(r)} = 0. \tag{4.8}$$

If R is increasing near α^+, then it should attain a maximum value at some $r_0 \in (\alpha_n,\infty)$, become decreasing, and change its concavity at $r_i \in (r_0,\infty)$, where r_i is a root of equation (4.8), since $\lim_{x\to\infty} R(r) = 0$. Hence, $R > 0, R' < 0$, and $R'' < 0$ on (r_0, r_i) and therefore $J = (r_0, r_i)$.

If R is decreasing near α^+, then by the same reasoning we conclude that $R < 0, R' > 0$, and $R'' > 0$ on (r_0, r_i) and $J = (r_0, r_i)$.

□

4.2.1 Discrete energies for the 2-dimensional s-states

Writing equation (4.6) as

$$\big(R(r)\big)E^2 - 2\big(vf(r)R(r)\big)E + \big(R''(r) + \frac{1}{r}R'(r) + v^2 f^2(r)R(r) - m^2 R(r) = 0,$$

we obtain a quadratic equation of E. Thus

$$E = vf(r) \pm \sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}. \tag{4.9}$$

Since we have proven the existence of an interval J such that $-\dfrac{R''(r)}{R(r)} - \dfrac{R'(r)}{rR(r)} > 0$, and since $|E| < m$, then the option $E = vf(r) - \sqrt{m^2 - \dfrac{R''(r)}{R(r)} - \dfrac{R'(r)}{rR(r)}}$ in expression (4.9) is falsified.

Therefore

$$E = vf(r) + \sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}. \tag{4.10}$$

4.2.2 Klein–Gordon bound states for $d > 1$

Lemma 4.2.2. *The ground state eigenfunction of the Klein–Gordon equation is non-increasing for $r \in [0, \infty)$ and $|E| < m$.*

Proof. For $l = 0$, equation (3.2) can be written as

$$R'(r) = r^{-(d-1)} \int_0^r F(t)R(t)t^{d-1}dt \tag{4.11}$$

where

$$F(t) = m^2 - \big(E - vf(t)\big)^2.$$

Replacing E by the expression (4.10) and using this in $F'(t) = \dfrac{dF}{dt}$ we find

$$F'(t) = 2vf'(t)\big(E - vf(t)\big) = 2\left[\sqrt{m^2 - \frac{R''(t)}{R(t)} - \frac{R'(t)}{tR(t)}}\right]vf'(t) \geq 0.$$

Thus we have reached the same result as in [60], but extended to $|E| < m$. Hence, $R'(r) \leq 0$ for all $r \in [0, \infty)$ and $|E| < m$. □

Chapter 5

Some exact solutions of the Klein–Gordon equation

5.1 Klein–Gordon equation with the square-well potential

5.1.1 One dimensional case

Consider the Klein–Gordon equation in dimension $d = 1$:

$$\varphi''(x) = [m^2 - \big(E - g(x,t)\big)^2]\varphi(x),$$

and the square-well potential

$$g(r,t) = \begin{cases} -v_0, & |x| \le t \\ 0, & \text{elsewhere} \end{cases},$$

where $v_0 > 0$. For $x < -t$, we get: $\varphi''(x) = (m^2 - E^2)\varphi(x)$. Thus, $\varphi(x) = Ae^{-kx} + Be^{kx}$ with $k^2 = m^2 - E^2$. Since φ vanishes at $-\infty$, then $A = 0$ and $\varphi(x) = Be^{kx}$. Similarly, for $x > t$ we obtain $\varphi(x) = Ce^{-kx}$. For $|x| \le t$, $\varphi''(x) + w^2\varphi(x) = 0$ with $w = \sqrt{(E+v_0)^2 - m^2}$. Then $\varphi(x) = D\sin(wx) + E\cos(wx)$. Since,as shown in section 4.1, all the solutions are either even or odd, then the even solution is

$$\varphi(x) = \begin{cases} Be^{kx}, & x < -t \\ E\cos(wx), & |x| \le t \\ Ce^{-kx}, & x > t \end{cases},$$

and the odd solution is

$$\varphi(x) = \begin{cases} Be^{kx}, & x < -t \\ D\sin(wx), & |x| \le t \\ Ce^{-kx}, & x > t \end{cases}.$$

Regarding the even solution, since φ is required to be continuously differentiable at t, then

$$E\cos(wt) = Ce^{-kt}, \tag{5.1}$$

and

$$-Ew\sin(wt) = -Cke^{-kt}. \tag{5.2}$$

Dividing equations 5.2 by 5.1 we obtain the eigenvalue equation

$$w\tan wt = k. \tag{5.3}$$

Similarly, the eigenvalue equation for the odd states reads

$$w\cot(wt) = -k. \tag{5.4}$$

These equations allow us to compute the eigenvalue v_0 given the energy E.

5.1.2 $d > 1$ dimensional cases

The radial part of the Klein–Gordon equation reads [61]

$$R''(r) + \frac{d-1}{r}R'(r) = \left[m^2 - \big(E - g(r,t)\big)^2 + \frac{l(l+d-2)}{r^2}\right]R(r), \tag{5.5}$$

where $l = 0, 1, 2, ...$ and

$$g(r,t) = \begin{cases} -v_0, & r \leq t \\ 0, & \text{elsewhere} \end{cases}$$

with $v_0 > 0$. For $d = 3$, the eigenvalue equation is [63]:

$$\frac{j_l'(k_i t)}{j_l(k_i t)} = \frac{h_l^{(1)\prime}(ikt)}{h_l^{(1)}(ikt)}, \tag{5.6}$$

where $k_i^2 = (E + v_0)^2 - m^2$, $k^2 = m^2 - E^2$, $i^2 = -1$, j_l is the spherical Bessel function of the first kind, and $h_l^{(1)}$ is the Hankel function of the first kind. In particular, the eigenvalue equation for the s-states ($l = 0$) is [63]:

$$k_i \cot(k_i t) = -k.$$

To generalize for any d-dimensional case, we consider the reduced form of the radial part of the Klein–Gordon equation (3.3). For $r < t$, we write it as

$$r^2\varphi'' + [k_i^2 r^2 - Q]\varphi(r) = 0.$$

Changing the variable r into $\sigma = k_i r$ we obtain the following differential equation:

$$\sigma^2\varphi''(\sigma) + [\sigma^2 - \nu(\nu+1)]\varphi(\sigma) = 0,$$

where $\nu = \frac{2l+d-3}{2}$. This is the Ricatti-Bessel equation with solution $\varphi(\sigma) = C_1\sigma j_\nu(\sigma) + C_2\sigma y_\nu(\sigma)$ [64], where y_ν is the spherical Bessel function of the second kind. Since we have an irregular point at $\sigma = 0$, then $C_2 = 0$. For $r > t$ we obtain the differential equation

$$r^2\varphi''(r) + [-k^2 r^2 - Q]\varphi(r) = 0.$$

Using the change of variable $\sigma = ikr$ we obtain

$$\sigma^2\varphi''(\sigma) + [\sigma^2 - \nu(\nu+1)]\varphi(\sigma) = 0,$$

whose general solution is [64] $\varphi(\sigma) = W_1\sigma h^{(1)}(\sigma) + W_2\sigma h^{(2)}(\sigma)$, where $h^{(2)}$ is the Hankel function of the second kind. Since $\varphi \in L^2(\mathbb{R})$, then $W_2 = 0$. Since φ is continuously differentiable at $r = t$, then the corresponding eigenvalue equation is

$$\frac{[(k_i t)j_l(k_i t)]'}{(k_i t)j_l(k_i t)} = \frac{[(ikt)h_l^{(1)}(ikt)]'}{(ikt)h_l^{(1)}(ikt)}. \tag{5.7}$$

5.2 Klein–Gordon equation with the exponential potential

5.2.1 One-dimensional case

The exact solution can be found in [65].

Consider the Klein–Gordon equation (3.1) and the exponential potential $V(x) = -ve^{-\frac{|x|}{a}}$, with $v = \dfrac{g}{2a}$. Letting $q^2 = m^2 - E^2$ we obtain the following equation for $x > 0$

$$\left[\frac{d^2}{dx^2} + 2E\big(\frac{g}{2a}\big)e^{-\frac{x}{a}} + \big(\frac{g}{2a}\big)^2 e^{-\frac{2x}{a}} - q^2\right]\varphi(x) = 0. \tag{5.8}$$

We define the new variable $y = e^{-\frac{x}{a}}$. Thus equation (5.8) becomes

$$\left[y^2\frac{d^2}{dy^2} + y\frac{d}{dy} + (agEy + \frac{g^2}{4}y^2 - a^2q^2)\right]\varphi(y) = 0. \tag{5.9}$$

Using the solution $\varphi(y) = y^r\Psi(y^s)$ with $r = -\frac{1}{2}$ and $s = 1$, (8.7) transforms into

$$\left[\frac{d^2}{dy^2} + \frac{g^2}{4} + \frac{agE}{y} + \left(\frac{\frac{1}{4} - a^2q^2}{y^2}\right)\right]\Psi(y) = 0. \tag{5.10}$$

Then, applying the change of variables $z = iy$ ($i^2 = -1$) and $w = gz$, equation (5.10) transforms into

$$\left[\frac{d^2}{dw^2} + \frac{-1}{4} + \frac{k}{w} + \left(\frac{\frac{1}{4} - \mu^2}{w^2}\right)\right]\Psi(y) = 0, \tag{5.11}$$

where $\mu^2 = a^2q^2$ and $k = -iaE$. This is identified as the Whittaker differential equation [64] whose solutions vanishing at infinity can be written in terms of the confluent hyper-geometric functions

$$M_{k\mu}(w) = e^{-\frac{w}{2}}w^{\mu+\frac{1}{2}}M\left(\mu - k + \frac{1}{2}, 2\mu + 1; w\right). \tag{5.12}$$

Finally, we write the wave-function in terms of x, $x > 0$, as

$$\varphi_+ = A_+\exp\left(-\frac{ig}{2}e^{-\frac{x}{a}} - qx\right)(ig)^{aq+\frac{1}{2}} \times M(\alpha, \gamma; ige^{-\frac{x}{a}}), \tag{5.13}$$

where $\alpha = aq + iaE + 0.5$ and $\gamma = 2aq + 1$, and A_+ is the normalization constant.
By the symmetry of the potential we can deduce the wave-function for $x < 0$

$$\varphi_- = A_-\exp\left(-\frac{ig}{2}e^{\frac{x}{a}} + qx\right)(ig)^{aq+\frac{1}{2}} \times M(\alpha, \gamma; ige^{\frac{x}{a}}), \tag{5.14}$$

with A_- being the normalization constant.
In order to obtain the eiqenvalue equations, we use the fact that the wave-functions are continuously differentiable at the origin. For even states we get $A_+ = A_-$. Using the identity [64]

$$\frac{dM}{dw} = \frac{\alpha}{\gamma}M(\alpha + 1, \gamma + 1; w), \tag{5.15}$$

and matching the derivatives, we obtain the following eigenvalue equation

$$\frac{M(\alpha + 1, \gamma + 1; ig)}{M(\alpha, \gamma; ig)} = \frac{ig - 2aq}{2(\alpha/\gamma)ig}. \tag{5.16}$$

Regarding the odd states, we have $\varphi(0) = 0$. Hence we obtain the following eigenvalue equation

$$M(\alpha, \gamma; ig) = 0. \tag{5.17}$$

5.2.2 3-dimensional case

We reveal the exact solution of the s-states found in [66]. Thus the Klein–Gordon equation (3.3) with the potential $V(r) = -ve^{-\frac{r}{a}}$ reads

$$\left[\frac{d^2}{dr^2} + m^2 - (E + ve^{-\frac{r}{a}})^2\right]\phi(r) = 0. \tag{5.18}$$

Applying the change of variable $\varphi(r) = e^{\frac{r}{2a}}w(t)$ and the substitution $t = 2ivae^{-\frac{r}{a}}$ we get

$$\frac{d^2w}{dt^2} + \left[-\frac{1}{4} - \frac{iEa}{t} + \frac{1/4 - p^2a^2}{t^2}\right]w(t) = 0, \tag{5.19}$$

with $p^2 = m^2 - E^2$. This is the Whittaker differential equation [64]whose solution in terms of t is

$$w(t) = Ne^{-t/2}t^{1/2+\mu}{}_1F_1(\frac{1}{2} + \mu - \lambda, 1 + 2\mu; t), \tag{5.20}$$

where $\lambda = -iEa$, $\mu = pa$, and N is the normalization constant. Thus, the ground state wave function in terms of r reads

$$R(r) = Ne^{-r/2a}W_{\lambda,\mu}\left(2ivae^{-r/a}\right), \tag{5.21}$$

Where $W$is the Whittaker function. Using $\varpi(0) = 0$ we obtain the eigenvalue equation

$${}_1F_1\left(\frac{1}{2} + \mu - \lambda, 1 + 2\mu; 2iva\right) = 0, \tag{5.22}$$

where ${}_1F_1$ is the confluent hypergeometric function. This equation determines the energies of the s-states given the coupling parameter v.

5.3 3-dimensional Klein–Gordon equation with the Coulomb potential

An analytical solution is found in [67] and [68]. We use the following 3-dimensional Klein–Gordon radial equation

$$\left[-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{r^2}\right]\Psi(r) = \left[(E - V(r))^2 - m^2\right]\Psi(r), \tag{5.23}$$

where $V(r) = -\frac{v}{r}$. Applying the change of variable $\Psi(r) = \frac{R(r)}{r}$ we get

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \left(E - V(r)\right)^2 - m^2\right]R(r) = 0, \tag{5.24}$$

which becomes

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1) - v^2}{r^2} + \frac{2Ev}{r} - m^2 + E^2\right]R(r) = 0. \tag{5.25}$$

Using the re-scaling parameters

$$\beta = 2\sqrt{m^2 - E^2},$$

$$\mu = \sqrt{(l + \frac{1}{2})^2 - v^2},$$

and

$$\lambda = \frac{2vE}{\beta},$$

and applying the change of variable $\rho = \beta r$, equation (5.25) transforms into

$$\left[\frac{d^2}{d\rho^2} - \frac{\mu^2 - 1/4}{\rho^2} + \frac{\lambda}{\rho} - \frac{1}{4}\right]R(\rho) = 0. \tag{5.26}$$

We now study the behavior of the $R(\rho)$ near 0 and ∞.

1. For $\rho \to \infty$, equation (5.26) behaves like

$$\left[\frac{d^2}{d\rho^2} - \frac{1}{4}\right] R(\rho) = 0, \tag{5.27}$$

which means that $R(\rho) = Ae^{-\rho/2} + be^{+\rho/2}$ near ∞. Normalizing the wave function requires $b = 0$. Thus,

$$R(\rho) = Ae^{-\rho/2}, \tag{5.28}$$

for sufficiently large ρ.

2. For $\rho \to 0$, we can neglect the last two terms of equation (5.26), thus

$$\left[\frac{d^2}{d\rho^2} - \frac{\mu^2 - 1/4}{\rho^2}\right] R(\rho) = 0. \tag{5.29}$$

Then

$$R(\rho) = C\rho^s, \tag{5.30}$$

with

$$Cs(s-1)\rho^{s-2} - C(\mu^2 - \frac{1}{4})\rho^{s-2} = 0,$$

which gives $s = \frac{1}{2} \pm \sqrt{\frac{1}{4} + \mu^2 - \frac{1}{4}} = \frac{1}{2} \pm \mu$.

In order to preserve integrability of the wave function near 0, we fix $s = \frac{1}{2} + \mu$. By the definition of μ, we observe that for $l = 0$, only real wave functions exist for $v < \frac{1}{2}$. Combining (5.28) and (5.30) we choose

$$R(\rho) = N\rho^{1/2+\mu} e^{-\rho/2} f(\rho), \tag{5.31}$$

where N is the normalization constant, and $f(\rho)$ is a polynomial of finite order in ρ since it should be constant for $\rho \to 0$, and it should guarantee the normalization for $\rho \to \infty$. Inserting (5.31) in (5.26) we obtain the following differential equation for $f(\rho)$

$$\frac{d^2 f}{d\rho^2} + \left(\frac{2\mu+1}{\rho} - 1\right)\frac{df}{d\rho} - \frac{\mu + 1/2 - \lambda}{\rho} f(\rho) = 0. \tag{5.32}$$

For simplification we let $2\mu + 1 = c$ and $\mu + \frac{1}{2} - \lambda = a$ so that

$$\frac{d^2 f}{d\rho^2} + \left(\frac{c}{\rho} - 1\right)\frac{df}{d\rho} - \frac{a}{\rho} f(\rho) = 0. \tag{5.33}$$

We solve this differential equation by using a power series expansion

$$f(\rho) = \sum_{n'=0}^{\infty} a_{n'} (\rho)^{n'}. \tag{5.34}$$

Inserting (5.34) in (5.33) yields

$$\sum_{n'=2}^{\infty} a_{n'} n'(n'-1)\rho^{n'-2} + c\sum_{n'=1}^{\infty} n' a_{n'} \rho^{n'-2} - \sum_{n'=1}^{\infty} n' a_{n'} \rho^{n'-1} - a\sum_{n'=0}^{\infty} a_{n'} \rho^{n'-1} = 0. \tag{5.35}$$

Setting $a_0 = 1$ and comparing the coefficients of equal powers in ρ gives

$$a_1 = \frac{a}{c}$$

$$a_2 = \frac{a_1(a+1)}{2(c+1)}$$

$$\vdots$$

$$a_m = \frac{a_m - 1(a+m-1)}{m(c+m-1}.$$

Hence

$$f(\rho) = 1 + \frac{a}{c}\rho + \frac{a}{c}\frac{a_1(a+1)}{2(c+1)}\frac{\rho^2}{2} + \ldots = \sum_{n'=0}^{\infty} \frac{(a)_{n'}}{(c)_{n'}}\frac{\rho^{n'}}{n'!}, \tag{5.36}$$

where $(a)_{n'}$ is the pochammer notation. This is the confluent hypergeometric function ${}_1F_1(a,c;\rho)$. Since

$${}_1F_1(a,c;\rho\to\infty) = \frac{\Gamma(c)}{\Gamma(a)}\rho^{a-c}e^{\rho}, \tag{5.37}$$

diverges, then the normalization condition requires that the series should be finite. If $a+n'=0$ holds, then all terms of higher order, $m > n'$, vanish. Thus, since $\mu + \frac{1}{2} - \lambda = a$ then

$$\lambda = \mu + \frac{1}{2} + n' = \frac{vE}{\sqrt{m^2 - E^2}}. \tag{5.38}$$

Therefore we have got an explicit expression for E

$$E = \frac{m}{\sqrt{1 + \frac{v^2}{\left[n' + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - v^2}\right]^2}}}. \tag{5.39}$$

5.4 3 - dimensional Klein–Gordon equation with the Hulthén potential

There are exact solutions offered for the s- states of the 3- dimensional Klein–Gordon equation with the Hulthén potential, in [69, 70] We consider the equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + (E-V)^2 - m^2\right]R(r) = 0, \tag{5.40}$$

with $l=0$, $m=1$, and $V(r) = -v\frac{e^{-r/a}}{1-e^{-r/a}}$ [71–73]. We define the function $w(r)$ as

$$R(r) = e^{-pr}\left[1 - e^{-r/a}\right]^{\lambda+1}w(r), \tag{5.41}$$

where $p^2 = 1 - E^2$ and

$$\lambda(\lambda+1) = -v^2a^2, \tag{5.42}$$

which gives

$$\lambda = \frac{1}{2} + \sqrt{\frac{1}{4} - v^2a^2}. \tag{5.43}$$

Thus λ should be real with $\lambda > -1/2$ in order to obtain a bound state. Applying the change of variable $t = 1 - e^{-r/a}$ we obtain the following differential equation

$$t(1-t)\frac{d^2w}{dt^2} + \Big[2(\lambda+1) - (3+2\lambda+2pa)t\Big]\frac{dw}{dt} + \Big[2Eva^2 - (\lambda+1)(1+2pa)\Big]w(t) = 0. \tag{5.44}$$

Hence $w(t) = {}_2F_1(a', b, c; t)$ [64] with

$$a' = \lambda + 1 + pa - \Big[\lambda(\lambda+1) + p^2a^2 + 2vEa^2\Big]^{1/2}, \tag{5.45}$$

$$b = \lambda + 1 + pa + \Big[\lambda(\lambda+1) + p^2a^2 + 2vEa^2\Big]^{1/2}, \tag{5.46}$$

and

$$c = 2(\lambda+1). \tag{5.47}$$

Consequently,

$$R(r) = Ne^{-pr}\big[1 - e^{-r/a}\big]^{\lambda+1}{}_2F_1(a', b, c; 1 - e^{-r/a}), \tag{5.48}$$

with N being the normalization constant. With the transformation formula [64] for the hypergeometric function ${}_2F_1$, the radial wave function can be expressed as

$$\begin{aligned} R(r) = Ne^{-pr}\big[1 - e^{-r/a}\big]^{\lambda+1}.\Bigg[&\frac{\Gamma(c)\Gamma(c-a'-b)}{\Gamma(c-a')\Gamma(c-b)}{}_2F_1(a', b, a'+b-c+1; e^{-pr})e^{-pr} \\ &+\frac{\Gamma(c)\Gamma(a'+b-c)}{\Gamma(a')\Gamma(b)}{}_2F_1(c-a', c-b, c-a'-b+1; e^{-pr})e^{pr}\Bigg]. \end{aligned} \tag{5.49}$$

Since $R(r) \in L^2(\mathbb{R})$, then the term containing e^{pr} should be eliminated. This requires that

$$\frac{\Gamma(c)\Gamma(a'+b-c)}{\Gamma(a')\Gamma(b)} = 0,$$

which holds if

$$(n_r + a')(n_r + b) = 0, \tag{5.50}$$

where $n_r = 0, 1, 2...$
Defining $n = n_r + 1$ and substituting (5.45) and (5.46) in (5.50) we get the following relation

$$2Eva^2 + \lambda(\lambda+1) - 2pa(n+\lambda) - (n+\lambda)^2 = 0. \tag{5.51}$$

We now study the necessary condition for having a bound state. Using the fact that as $E \to 1$, $p \to 0$, we find from (5.51)

$$2va^2 > (n+\lambda)^2 - \lambda(\lambda+1).$$

Applying (7.12) we get the following condition

$$2va^2 > (n+\lambda)^2 + v^2a^2. \tag{5.52}$$

We observe that the ground state is characterized by $n = 1$. Using (5.43) in (5.52) we obtain

$$\sqrt{\frac{1}{4} - v^2a^2} < 2va^2 - \frac{1}{2}.$$

This gives a lower bound for the coupling constant, that is $v < \dfrac{1}{2a}$. Squaring both sides we get $(1+4a^2)v^2 - 2v > 0$ which gives the following upper bound $v > \dfrac{2}{1+4a^2}$. Therefore

$$\frac{2}{1+4a^2} < v < \frac{1}{2a}. \tag{5.53}$$

Moreover, regarding (5.52) as a quadratic equation in the quantum number$n$

$$n^2 + (2\lambda)n + (\lambda^2 + v^2a^2 - 2va^2) < 0, \tag{5.54}$$

we can extract the following condition:

$$1 \leq n < -\lambda + a\sqrt{2v - v^2}. \tag{5.55}$$

We now find an explicit expression for the discrete energy E for s-states. Writing (5.51) as

$$2Eva^2 - a^2v^2 - (n+\lambda)^2 = 2a(n+\lambda)\sqrt{1-E^2}.$$

Squaring both sides and using relation (5.42) we obtain the following quadratic equation in E

$$4a^2\left[a^2v^2 + (n+\lambda)^2\right]E^2 - 4va^2\left[a^2v^2 + (n+\lambda)^2\right]E + \left[a^2v^2 + (n+\lambda)^2\right] - 4a^2(n+\lambda)^2 = 0. \tag{5.56}$$

Therefore

$$E = \frac{v}{a} + \frac{n+\lambda}{2a}\sqrt{\frac{4a^2}{a^2v^2 + (n+\lambda)^2} - 1}. \tag{5.57}$$

Chapter 6

General features of the spectral curve $v = G(E)$

6.1 One-dimensional case

Definition 6.1.1. *We denote by* $\langle f \rangle$ *and* $\langle f^2 \rangle$ *the mean values of* f *and* f^2 *respectively, where*

$$\langle \varphi, \psi \rangle = \int_{-\infty}^{\infty} \varphi(x)\psi(x)dx,$$

is the inner product on $L^2(\mathbb{R})$*, that is*

$$\langle f \rangle = \langle \varphi, f\varphi \rangle = \int_{-\infty}^{\infty} f(x)\varphi^2(x)dx,$$

and

$$\langle f^2 \rangle = \langle \varphi, f^2\varphi \rangle = \int_{-\infty}^{\infty} f^2(x)\varphi^2(x)dx.$$

Lemma 6.1.1.

$$2E\langle f \rangle < v\langle f^2 \rangle, \forall |E| < m. \tag{6.1}$$

Proof. Expanding equation (3.1) we get:

$$\varphi''(x) = (m^2 - E^2)\varphi(x) + 2Evf(x)\varphi(x) - v^2 f^2(x)\varphi(x).$$

Multiplying both sides by φ and integrating over $\mathbb{R}$ we obtain:

$$\int_{-\infty}^{\infty} \varphi''(x)\varphi(x)dx = m^2 - E^2 + 2Ev\langle f \rangle - v^2\langle f^2 \rangle.$$

After applying integration by parts and using the fact that φ vanishes at $\pm\infty$, the left-hand side of the last equation becomes $-\int_{-\infty}^{\infty} \left(\varphi'(x)\right)^2 dx$. Thus, $-\int_{-\infty}^{\infty} \left(\varphi'(x)\right)^2 dx + E^2 - m^2 = 2Ev\langle f \rangle - v^2\langle f^2 \rangle$. Since the left-hand side is negative, we have the desired result. □

We now define the operator K as:

$$K = -\frac{\partial^2}{\partial x^2} + 2Evf - v^2 f^2. \tag{6.2}$$

If φ is solution of the Klein–Gordon equation (3.1), then we have:

$$K\varphi = (E^2 - m^2)\varphi, \tag{6.3}$$

and it follows

$$\langle \varphi, K\varphi \rangle = \langle \varphi, (E^2 - m^2)\varphi \rangle = E^2 - m^2. \tag{6.4}$$

We observe that the domain of K is $D_K = H^2(\mathbb{R})$, where $H^2(\mathbb{R})$ is the Sobolev space defined as follows:

$$H^2(\mathbb{R}) = \{\varphi \in L^2(\mathbb{R}) : \varphi', \varphi'' \in L^2(\mathbb{R})\}.$$

Since $||K\varphi|| = |E^2 - m^2| \cdot ||\varphi|| \leq m^2||\varphi||$ for all $\varphi \in D_K$, then K is a bounded operator. This implies that K is continuous. We also observe that K is symmetric, that is to say: $\langle \varphi, K\psi \rangle = \langle K\varphi, \psi \rangle$. We now consider a family of Klein–Gordon spectral problems where $v = v(E)$ is a function of E. Let φ_E denote the partial derivative of φ with respect to E. If we differentiate the normalization integral (4.2) partially with respect to E, we obtain the orthogonality relation $\langle \varphi, \varphi_E \rangle = 0$. Furthermore, differentiating equation (6.4) with respect to E we obtain:

$$\langle \varphi_E, K\varphi \rangle + \langle \varphi, K_E\varphi \rangle + \langle \varphi, K\varphi_E \rangle = 2E. \tag{6.5}$$

The symmetry of K and the orthogonality of φ and φ_E imply that

$$\langle \varphi, K\varphi_E \rangle = \langle \varphi_E, K\varphi \rangle = (E^2 - m^2)\langle \varphi_E, \varphi \rangle = 0.$$

Then by using the expression

$$K_E = 2vf + 2Ev_Ef - 2vv_Ef^2 \tag{6.6}$$

in equation (6.5), we obtain the key equation for our theorem in this section, namely:

$$v_E = \frac{E - v\langle f \rangle}{E\langle f \rangle - v\langle f^2 \rangle}. \tag{6.7}$$

Theorem 6.1.1. *If $E \geq v\langle f \rangle$, then $E_1 \leq E_2 \Rightarrow v(E_1) \geq v(E_2)$; and if $E < v\langle f \rangle$, then $E_1 < E_2 \Rightarrow v(E_1) < v(E_2)$.*

Proof. If $E \geq 0$, then $v_E \leq 0$, and the theorem holds immediately. On the other hand, if $E < 0$, then by (6.1), $E\langle f \rangle < 2E\langle f \rangle < v\langle f^2 \rangle$, which means that $E\langle f \rangle - v\langle f^2 \rangle < 0$. Thus $v\langle f \rangle \leq E < 0 \Rightarrow v_E \leq 0$, and $E < v\langle f \rangle \Rightarrow v_E > 0$. Therefore, the theorem has been proven. $\square$

Theorem 6.1.2. *The spectral curve $v(E) = G(E)$ is concave for all $|E| < m$.*

Proof. Suppose that for any $|E_i| < m$, φ_i is the corresponding wave function, $\langle f_i \rangle = \int_{-\infty}^{+\infty} f(x) \cdot (\varphi_i)^2 dx$, and $\langle f_i^2 \rangle = \int_{-\infty}^{+\infty} f^2(x) \cdot (\varphi_i)^2 dx$. Let the maximum value of $G(E)$ be equal to v_{cr}. By **theorem 6.1.1**, the corresponding value of E is $E_{cr} = v_{cr}\langle f_{cr} \rangle$. Consider the point $A\big(E_{cr}, v_{cr}\langle f_{cr} \rangle\big)$ and fix the point $B\big(E_n, v_n\big)$ on the spectral curve $G(E)$, where $v_n = G(E_n)$, such that $E_n \neq E_{cr}$ and $E_n \in (-m, m)$. Then

$$(AB) : G_c(E) = v_{cr} + \frac{v_{cr} - v_n}{v_{cr}\langle f_{cr} \rangle - E_n}\big(E - v_{cr}\langle f \rangle\big).$$

Assume, without loss of generality, that $E_{cr} < E_n$, and consider the function $t(E) = G(E) - G_c(E)$ where $E \in [E_{cr}, E_n]$. Then $t'(E) = \dfrac{dt}{dE} = \dfrac{E - v\langle f \rangle}{E\langle f \rangle - v\langle f^2 \rangle} + \dfrac{v_n - v_{cr}}{v_{cr}\langle f_{cr} \rangle - E_n}$, which vanishes at the point $\big(E_m, G(E_m)\big)$ with

$$E_m = \frac{v_mE_n\langle f_m \rangle - v_mv_{cr}\langle f_m \rangle\langle f_{cr} \rangle + v_mv_{cr}\langle f_m^2 \rangle - v_mv_n\langle f_m^2 \rangle}{E_n - v_{cr}\langle f_{cr} \rangle + \langle f_m \rangle\big(v_{cr} - v_n\big)}$$

$$= \frac{v_m\langle f_m \rangle\big(E_n - v_{cr}\langle f_{cr} \rangle\big) + v_m\langle f_m \rangle^2(v_{cr} - v_n) + v_m\langle f_m^2 \rangle(v_{cr} - v_n) - v_m\langle f_m \rangle^2(v_{cr} - v_n)}{E_n - v_{cr}\langle f_{cr} \rangle + \langle f_m \rangle\big(v_{cr} - v_n\big)}.$$

Hence

$$E_m = v\langle f_m\rangle + \frac{v_m\big(v_{cr} - v_n\big)\big(\langle f_m^2\rangle - \langle f_m\rangle^2\big)}{E_n - v_{cr}\langle f_{cr}\rangle + \langle f_m\rangle\big(v_{cr} - v_n\big)}. \tag{6.8}$$

Since $t'(E_{cr}) > 0$ and $t(E_{cr}) = t(E_n) = 0$, then the point $\big(E_m, G(E_m)\big)$ must be a maximum point of $t(E)$ over the interval $[E_{cr}, E_n]$ and $t(E) \geq 0$ over $[E_{cr}, E_n]$. This means that the chord $[AB]$ is always beneath the spectral curve $G(E)$ over $[E_{cr}, E_n]$ and the proof is complete. □

We observe that φ is not necessarily required to be a node-free state, this means that the previous theorem is valid for all states, ground state and any excited state.

6.2 $(d \geq 1)$-dimensional case

Definition 6.2.1. *We denote by $\langle f\rangle$ and $\langle f^2\rangle$ the mean values of f and f^2 respectively, where*

$$\langle \varphi, \psi\rangle = \int_0^\infty \varphi(r)\psi(r)r^{d-1}dr,$$

is the inner product on $L^2(\mathbb{R}^d)$, that is

$$\langle f\rangle = \langle \varphi, f\varphi\rangle = \int_0^\infty f(r)\varphi^2(r)r^{d-1}dr,$$

and

$$\langle f^2\rangle = \langle \varphi, f^2\varphi\rangle = \int_0^\infty f^2(r)\varphi^2(r)r^{d-1}dr.$$

We define the operator

$$K = -\frac{\partial^2}{\partial r^2} + 2Evf - v^2f^2 + \frac{Q}{r^2}. \tag{6.9}$$

We have

$$\langle K\rangle = \langle (E^2 - m^2)\varphi, \varphi\rangle = E^2 - m^2.$$

As in the previous section, K is bounded and symmetric with $D_K = H^2(\mathbb{R}^d)$. We consider the same family of Klein–Gordon spectral problems with $v = v(E)$ Since $K_E = 2vf + 2Ev_Ef - 2vv_Ef^2$, then we obtain the same relation as in the one-dimensional case,

$$v_E = \frac{E - v\langle f\rangle}{E\langle f\rangle - v\langle f^2\rangle}.$$

Theorem 6.2.1. *If $E \geq v\langle f\rangle$, then $E_1 \leq E_2 \Rightarrow v(E_1) \leq v(E_2)$, and if $E < v\langle f\rangle$, then $E_1 < E_2 \Rightarrow v(E_1) > v(E_2)$.*

Proof. Same as **theorem 6.1.1**. □

Theorem 6.2.2. *The spectral curve $G(E)$ is concave for all $|E| < m$*

Proof. Same as **theorem 6.1.2** □

We observe that as in the one-dimensional case, this theorem does not require the radial wave function to be node-free; it's valid for both ground and excited states.

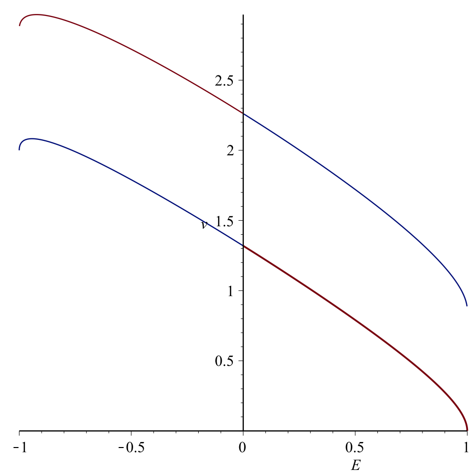


Figure 6.1: Graphs of the function $v(E)$ in the square-well potential in one dimension, for the ground state and the first excited state.

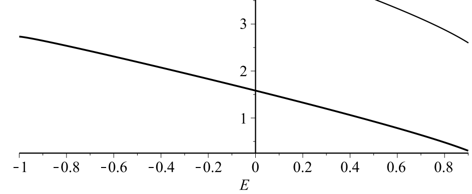


Figure 6.2: Graphs of the function $v(E)$ in the Woods-Saxon potential shape $f(x) = -\dfrac{1}{1+e^{b(|x|-1)}}$ in one dimension, with $b = \frac{20}{7}$, for the ground state, the first excited state, and the second excited state. The graphs are plotted using a numerical shooting method of our own.

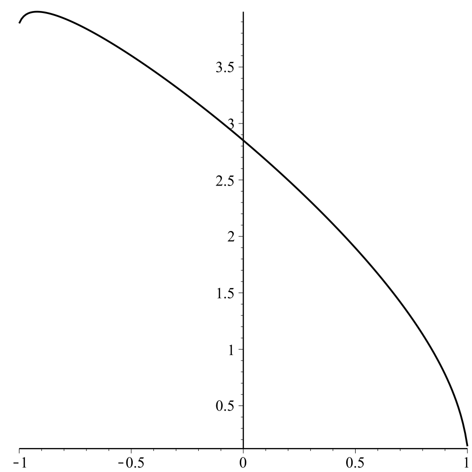


Figure 6.3: Graph of the function $v(E)$ in the exponential potential $f(x) = -Ae^{-qx}$ in one dimension, for the ground state, where the values $A = 1$ and $q = \dfrac{10}{3}$ is applied.

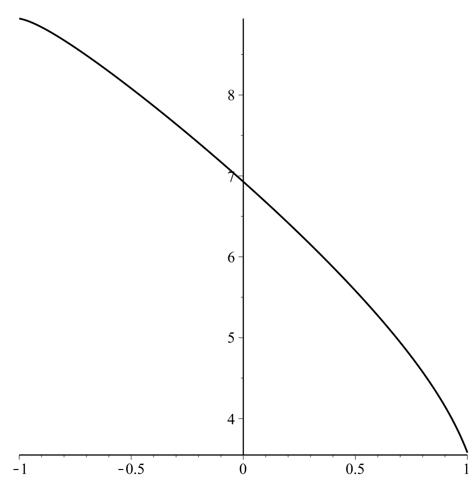


Figure 6.4: Graph of the function $v(E)$ in the soft-core potential [75, 76] $V(r) = vf(r)$ with $f(r) = \dfrac{-1}{(r^p + c^p)^{1/p}}$ in dimension $d = 3$, for the ground state, where the values $p = 3$ and $c = 0.6$ is applied.

Chapter 7

The simple general comparison theorems for potential shapes in $d \geq 1$ dimension

7.1 One-dimensional case

We consider the Klein–Gordon equation (3.1) with $V(x)$ a potential function that belongs to the class $\mathcal{P}$ defined in **section 3.1**. In this section, we consider the parameter $a \in [0,1]$ and the two potential shapes f_1 and f_2 with $f = f(a,x) = f_1(x) + a\big[f_2(x) - f_1(x)\big]$, where $f_1 \leq f_2 \leq 0$. Hence $f \leq 0$, attractive, even, vanishes at infinity, $f(0,x) = f_1(x)$ when $a = 0$, and $a = 1$ when $f(1,x) = f_2(x)$, and

$$\frac{\partial f}{\partial a} = f_2(x) - f_1(x) \geq 0. \tag{7.1}$$

Hence, f is monotone non-decreasing in the parameter a. The idea in this section is to study the variations of the coupling v with respect to a, provided $v = v(a)$ and the value of E is given as a constant, that is $\frac{\partial E}{\partial a} = 0$, and $-m < E < m$. We again consider the symmetric bounded operator K in (6.2), and we define φ_a to be the partial derivative of φ with respect to a. Differentiating equation (6.4) with respect to a we get:

$$\langle \varphi_a, K\varphi \rangle + \langle \varphi, K_a\varphi \rangle + \langle \varphi, K\varphi_a \rangle = 0 \tag{7.2}$$

Applying the partial derivative with respect to a to equation (4.2) and using the symmetry of K, we obtain the new orthogonality relation

$$\langle \varphi_a, K\varphi \rangle = \langle \varphi, K\varphi_a \rangle = (E^2 - m^2)\langle \varphi_a, \varphi \rangle = 0. \tag{7.3}$$

We also have:

$$K_a = 2Ev_a f + 2Ev(f_2 - f_1) - 2vv_a f^2 - 2v^2 f(f_2 - f_1),$$

with v_a defined as $\frac{\partial v}{\partial a}$. Equation (7.2) becomes:

$$Ev_a\langle f \rangle + Ev\int_{-\infty}^{\infty}\Big(f_2(x) - f_1(x)\Big)\varphi^2(x)dx - vv_a\langle f^2 \rangle - v^2\int_{-\infty}^{\infty} f\Big(f_2(x) - f_1(x)\Big)\varphi^2(x)dx = 0.$$

This leads us to the following relation:

$$v_a = \frac{vI}{E\langle f \rangle - v\langle f^2 \rangle}, \tag{7.4}$$

where

$$I = \int_{-\infty}^{\infty}\Big(f_2(x) - f_1(x)\Big)\Big(vf(x) - E\Big)\varphi^2(x)dx. \tag{7.5}$$

Lemma 7.1.1. *The integral I defined in relation (7.5) is non-positive for any state φ.*

Proof. Replacing the E with expression (4.4) in (7.5) we obtain

$$I = \int_{-\infty}^{\infty} -\big(f_2(x) - f_1(x)\big)\sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}\varphi^2(x)dx \leq 0. \tag{7.6}$$

□

Theorem 7.1.1.

$$f_1(x) \leq f_2(x) \Rightarrow v_1 \leq v_2,$$

for all $x \in [0, \infty)$.

Proof. Consider the relation (7.4). If $E \geq 0$, then $E\langle f\rangle - v\langle f^2\rangle < 0$, and if $E < 0$, then using the relation (6.1) we also get the same result. Thus, the denominator of equation (7.4) is negative for all $|E| < m$. Since we also proved in **lemma 7.1.1** that $I \leq 0$, then $v_a \geq 0$ for all $a \in [0, 1]$ and $E \in (-m, m)$. This result completes the proof of the theorem. □

7.2 $d > 1$-dimensional case except for $d = 2$ and $l = 0$

We consider the Klein–Gordon equation (3.3) with $V(r)$ a radially symmetric potential function that belongs to the class $\mathcal{P}_d$ defined in **section 3.2**. We also define the parameter $a \in [0, 1]$ and the two potential shapes f_1 and f_2 with $f = f(a, r) = f_1(r) + a\big[f_2(r) - f_1(r)\big]$, where $f_1 \leq f_2 \leq 0$. Hence $f \leq 0$, attractive, vanishes at infinity, $f(0, r) = f_1(r)$ when $a = 0$, and $a = 1$ when $f(1, r) = f_2(r)$, and

$$\frac{\partial f}{\partial a} = f_2(r) - f_1(r) \geq 0. \tag{7.7}$$

Hence, f is monotone non-decreasing in the parameter a. We then assume that $v = v(a)$, fix E, and derive the operator K defined in (6.9) with respect to a to obtain a relation similar to (7.2). Following the same procedure as in **section 5.1** we find the relation

$$v_a = \frac{vI}{E\langle f\rangle - v\langle f^2\rangle}, \tag{7.8}$$

where

$$I = \int_0^{\infty} \Big(f_2(r) - f_1(r)\Big)\Big(vf(r) - E\Big)\varphi^2(r)dx. \tag{7.9}$$

Lemma 7.2.1. *The integral I defined in relation (7.9) is non-positive for any state φ and for all $d > 1$, except for the s-states of $d = 2$, that is: when $d = 2$ and $l = 0$.*

Proof. Using relation (4.5) in (7.9) we get:

$$I = -\int_0^{\infty} \big(f_2(r) - f_1(r)\big)\sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}\varphi^2(r)dr \leq 0.$$

□

Theorem 7.2.1.

$$f_1(r) \leq f_2(r) \Longrightarrow v_1 \leq v_2,$$

for all $r \in [0, \infty)$ and $d > 1$, except for the s-states for $d = 2$, that is, when $d = 2$ and $l = 0$.

Proof. Same proof as **theorem 7.1.1** □

7.3 Case of two-dimensional s-states

We use the Klein–Gordon equation (4.6) and the symmetric operator

$$K = -\frac{\partial^2}{\partial r^2} - \frac{\partial}{\partial r} + 2Evf - v^2 f^2.$$

Then

$$\langle K \rangle = E^2 - m^2. \tag{7.10}$$

Differentiating (7.10) with respect to the parameter a we get

$$\langle R_a, KR \rangle + \langle R, K_a R \rangle + \langle R, KR_a \rangle = 0, \tag{7.11}$$

where $K_a = \frac{\partial K}{\partial a}$. But

$$\frac{\partial}{\partial a}\left[\int_0^\infty R^2(r)dr\right] = 2\int_0^\infty R(r)\frac{\partial R(r)}{\partial a} = 0.$$

Then we obtain the orthogonality relation $\langle R, R_a \rangle = \langle R_a, R \rangle = 0$. Therefore, $\langle R_a, KR \rangle = \langle R, KR_a \rangle = (E^2 - m^2)\langle R, R_a \rangle = 0$, with $R_a = \frac{\partial R}{\partial a}$. We also have $K_a = 2Ev_a f + 2Ev(f_2 - f_1) - 2vv_a f^2 - 2v^2 f(f_2 - f_1)$, where $v_a = \frac{\partial v}{\partial a}$. Thus, using K_a in equation (7.11) we obtain

$$v_a = \frac{v\left[\int_0^\infty \big(f_2(r) - f_1(r)\big)\big(vf(r) - E\big)R^2(r)\right]}{E\langle f \rangle - v\langle f^2 \rangle} \tag{7.12}$$

Theorem 7.3.1. *For the s-states of $d = 2$ we have*

$$f_1(r) \leq f_2(r) \Longrightarrow v_1 \leq v_2,$$

for all $r \in [0, \infty)$.

Proof. Using the expression (4.5) in equation (7.12) we get

$$v_a = \frac{v\int_0^\infty -\left[(f_2(r) - f_1(r))\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}R^2(r)\right]dr}{\int_0^\infty \left[\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}R^2(r)\right]f(r)dr} \geq 0,$$

for all $r \in [0, \infty)$. Hence, the proof is complete. □

7.4 Special cases with scalar potentials

We consider the Klein–Gordon equation (3.5), and we discuss two special cases.

Definition 7.4.1. *Consider equation (3.5). If $V = S$, then we have a spin symmetry, and if $V = -S$, then we have a pseudo-spin symmetry.*

Theorem 7.4.1. *Consider the Klein–Gordon equation (3.5) for $d > 1$ with a spin symmetry case. That is to say $S(r) = V(r) = vf(r)$. Then*

$$f_1(r) \leq f_2(r) \implies v_1 \leq v_2.$$

Proof. Since $S(r) = V(r) = vf(r)$ on $[0, \infty)$, then (3.5) reads

$$\varphi''(r) = \big[m^2 - E^2 + 2(E+m)vf\big]\varphi. \tag{7.13}$$

We define the operator

$$K = -\Delta + 2vf(v+m) + \frac{Q}{r^2}.$$

Thus $K\varphi = (E^2 - m^2)\varphi$ and $\langle K_a \rangle = 0$, with a being the same parameter defined in section 7.2 and

$$K_a = 2v_a f(E+m) + 2v(f_2 - f_1)(E+m).$$

Hence,

$$v_a = \frac{v\displaystyle\int_0^\infty \big(f_1(r) - f_2(r)\big)\varphi^2(r)dr}{\langle f \rangle},$$

and the proof is complete. □

Theorem 7.4.2. *Consider the Klein–Gordon equation (3.5) for $d > 1$ with a pseudo-spin symmetry case. That is to say $S(r) = -V(r) = -vf(r)$. Then*

$$f_1(r) \leq f_2(r) \implies v_1 \leq v_2.$$

Proof. Same as theorem 7.4.1. □

Chapter 8

The refined general comparison theorems for potential shapes in $d \geq 1$ dimension

In this chapter we provide stronger versions of the general comparison theorem $f_1 \leq f_2 \implies G_1(E) \leq G_2(E)$, by allowing the potential shapes to cross over with still preserving the ordering of the coupling parameters. However, these theorems are restricted to the ground state, and they are valid for all $E \in (-m, m)$.

8.1 One-dimensional case

We consider the Klein–Gordon equation (3.1) with $V(x)$ a potential function that belongs to the class $\mathcal{P}$ defined in **section 3.1**. We also consider the parameter $a \in [0, 1]$ and the two potential shapes f_1 and f_2 with $f = f(a, x) = f_1(x) + a\big[f_2(x) - f_1(x)\big]$, where $f_1 \leq f_2 \leq 0$, as in chapter 7. Thus the relation (7.1) is still valid. We assume that the coupling parameter v is a function of a, $\big(v = v(a)\big)$ and the value of E is given as a constant, that is $\frac{\partial E}{\partial a} = 0$, and $-m < E < m$. We again consider the symmetric bounded operator K in (6.2), and we define φ_a to be the partial derivative of φ with respect to a. Using relations (7.2), (7.3), and

$$K_a = 2Ev_a f + 2Ev(f_2 - f_1) - 2vv_a f^2 - 2v^2 f(f_2 - f_1), \tag{8.1}$$

we get

$$Ev_a \int_0^\infty f\varphi^2(x)dx + Ev \int_0^\infty \Big(f_2(x) - f_1(x)\Big)\varphi^2(x)dx - vv_a \int_0^\infty f^2\varphi^2(x)dx$$
$$-v^2 \int_0^\infty f\Big(f_2(x) - f_1(x)\Big)\varphi^2(x)dx = 0.$$

This leads us to the following relation:

$$v_a = \frac{vJ}{E\displaystyle\int_0^\infty f(x)\varphi^2(x)dx - v\int_0^\infty f^2\varphi^2(x)dx}, \tag{8.2}$$

where

$$J = \int_0^\infty \Big(f_2(x) - f_1(x)\Big)\Big(vf(x) - E\Big)\varphi^2(x)dx. \tag{8.3}$$

Theorem 8.1.1. *For any two potentials $f_1,\ f_2 \in \mathcal{P}$ we have:*

$$\mu(x) = \int_0^x [f_2(t) - f_1(t)]dt \geq 0 \quad x \in [0, \infty) \implies G_1(E) \leq G_2(E), \tag{8.4}$$

for any ground state energy E.

Proof. Applying integration by parts to (8.3) we get

$$J = (vf(x) - E)\varphi^2(x)\mu(x)\Big|_0^\infty - \int_0^\infty \big[vf'(x)\varphi^2(x) + 2(vf(x) - E)\varphi(x)\varphi'(x)\big]\mu(x)dx.$$

Regarding that $\lim_{x\to\infty} \varphi(x) = 0$ and $\mu(0) = 0$, we get

$$J = -\int_0^\infty \big[vf'(x)\varphi^2(x) + 2(vf(x) - E)\varphi(x)\varphi'(x)\big]\mu(x)dx.$$

Substituting E by (4.4) we conclude that $J \leq 0$.
Therefore, following **Lemma 6.1.1.** $v_a \geq 0$, and the theorem is proven. □

We now state a stronger version of the above theorem, which can be applied in case we know one of the ground states φ_1 or φ_2:

Theorem 8.1.2. *For any potentials $f_1,\ f_2 \in \mathcal{P}$ we have:*

$$\rho(x) = \int_0^x [f_2(t) - f_1(t)]\varphi_j(t)dt \geq 0 \quad x \in [0, \infty) \implies G_1(E) \leq G_2(E),$$

for $j = 1, 2$ and for any ground state energy E.

Proof. Suppose, *w.l.o.g*, that $j = 1$. Applying the operator $\dfrac{\partial}{\partial a}$ to the expression (6.3) we get

$$K_a\varphi + K\varphi_a = (E^2 - m^2)\varphi_a. \tag{8.5}$$

We then multiply (8.5) by φ_1 and apply the inner product to get

$$\langle\varphi_1, K_a\varphi\rangle = -\langle\varphi_1, K\varphi_a\rangle + \langle(E^2 - m^2)\varphi_1, \varphi_a\rangle,$$

which implies that

$$\langle\varphi_1, K_a\varphi\rangle = -\langle\varphi_1, K\varphi_a\rangle + \langle K\varphi_1, \varphi_a\rangle. \tag{8.6}$$

Since K is symmetric, then $\langle\varphi_1, K\varphi_a\rangle = \langle K\varphi_1, \varphi_a\rangle$. Then relation (8.6) becomes

$$\langle\varphi_1, K_a\varphi\rangle = 0. \tag{8.7}$$

Using (8.1) we obtain

$$v_a = \frac{v\,\langle\varphi_1, (f_2 - f_1)(vf - E)\varphi\rangle}{\langle\varphi_1, f(E - vf)\varphi\rangle}. \tag{8.8}$$

By (4.4) we observe that the denominator of (8.8) is negative. Applying integration by parts to the numerator changes it into

$$\big(vf(x) - E\big)\varphi(x)\rho(x)\Big|_0^\infty - \int_0^\infty \big[vf'(x)\varphi(x) + \big(vf(x) - E\big)\varphi'(x)\big]\rho(x)dx. \tag{8.9}$$

Since $\lim_{x\to\infty}(x) = 0$ and $\rho(0) = 0$ then (8.9) becomes

$$-\int_0^\infty \Big[vf'(x)\varphi(x) + \big(vf(x) - E\big)\varphi'(x)\Big]\rho(x)dx \leq 0.$$

Therefore $v_a \geq 0$ and the proof is complete. □

8.2 $d > 1$-dimensional case

In this section we shall use the Klein–Gordon radial equation (3.2) and we assume that the normalization condition for bound states is

$$\int_0^\infty R^2(r)r^{d-1}dr = 1. \tag{8.10}$$

Differentiating (8.10) with respect to a we obtain the orthogonality relation $\langle R_a, R\rangle = \langle R, R_a\rangle = 0$. We also define $f(r,a) = af_1(r) + (1-a)f_2(r)$, $f_1, f_2 \in \mathcal{P}_d$, and we consider the operator

$$K = -\frac{\partial^2}{\partial r^2} - \frac{\partial}{\partial r} + 2Evf - v^2 f^2. \tag{8.11}$$

By the same reasoning for the one-dimensional case we obtain the relation

$$v_a = \frac{vJ}{E\langle f\rangle - v\langle f^2\rangle}, \tag{8.12}$$

where

$$J = \int_0^\infty \Big(f_2(r) - f_1(r)\Big)\Big(vf(r) - E\Big)r^{(d-1)}R^2(r)dr, \tag{8.13}$$

$\langle f\rangle = \int_0^\infty f(r)R^2(r)r^{d-1}dr$, and $\langle f^2\rangle = \int_0^\infty f^2(r)R^2(r)r^{d-1}dr$. Using (4.10) relation (8.12) reads

$$v_a = \frac{vJ}{\int_0^\infty \left[\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}R^2(r)\right]r^{d-1}f(r)dr}. \tag{8.14}$$

Theorem 8.2.1. *If f_1, $f_2 \in \mathcal{P}_d$ such that $(f_2 - f_1)$ has t^{d-1}-weighted area, then:*

$$\eta(r) = \int_0^r [f_2(t) - f_1(t)]t^{d-1}dt \geq 0 \quad r \in [0,\infty) \implies G_1(E) \leq G_2(E), \tag{8.15}$$

where E is the ground state energy.

Proof. Integrating (8.13) by parts we get

$$J = (vf(r) - E)R^2(r)\eta(r)\Big|_0^\infty - \int_0^\infty \Big[vf'(r)R^2(r) + 2\big(vf(r) - E\big)R(r)R'(r)\Big]\eta(r)dr.$$

Using $\lim\limits_{x\to\infty} R(r) = 0$ and $\eta(0) = 0$ we obtain

$$J = -\int_0^\infty \Big[vf'(r)R^2(r) + 2\big(vf(r) - E\big)R(r)R'(r)\Big]\eta(r)dr.$$

Hence, relation (8.14) is non-negative and the theorem is proved. □

As in the one-dimensional case, we state a stronger version of the previous refining theorem:

Theorem 8.2.2. *For any two potentials $f_1, f_2 \in \mathcal{P}_d$ we have:*

$$\sigma(r) = \int_0^r [f_2(t) - f_1(t)]t^{d-1}R_j(t)dt \geq 0 \quad r \in [0,\infty) \implies G_1(E) \leq G_2(E), \tag{8.16}$$

for $j = 1, 2$, where E is the ground state energy E.

Proof. In the same manner of the proof of the one-dimensional theorem we arrive to the following formula

$$v_a = \frac{v\langle R_1, (f_2 - f_1)(vf - E)R\rangle}{\langle R_1, f(E - vf)R\rangle}, \tag{8.17}$$

which is equal to

$$\frac{-\displaystyle\int_0^\infty \Big[vf'(r)R(r) + \big(vf(r) - E\big)R'(r)\Big]\sigma(r)dr}{\displaystyle\int_0^\infty R_1(r)\Bigg[\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}\Bigg]R(r)r^{d-1}f(r)dr} \geq 0. \tag{8.18}$$

Hence we have reached our desired result. □

8.3 Special cases with scalar potentials

Consider the Klein–Gordon equation (3.5). We shall prove the refined theorems for the spin-symmetric and spin-pseudo-symmetric cases.

Theorem 8.3.1. Spin symmetric case *Assume that we have $V(r) = S(r)$ on $[0, \infty)$. If f_1, $f_2 \in \mathcal{P}_d$ such that $(f_2 - f_1)$ has t^{d-1}-weighted area, then:*

$$\eta(r) = \int_0^r [f_2(t) - f_1(t)]t^{d-1}dt \geq 0 \quad r \in [0, \infty) \implies G_1(E) \leq G_2(E), \tag{8.19}$$

where E is the ground state energy.

Proof. We use the operator $K = -\Delta + 2vf(m + E) + \dfrac{Q}{r^2}$. Then

$$v_a = \frac{-vJ}{\langle f\rangle},$$

with $J = \displaystyle\int_0^\infty \big(f_2(t) - f_1(t)\big)\varphi^2(t)dt$. Integrating J by parts and using $\lim_{r\to\infty}\varphi(r) = 0$, we get

$$J = \int_0^\infty 2\varphi(t)\varphi'(t)\eta(t)dt. \tag{8.20}$$

Then $J \leq 0$ since the ground state is decreasing on $[0, \infty)$. Therefore $v_a \geq 0$, and the proof is complete. □

Theorem 8.3.2. Spin symmetric case *Assume that we have $V(r) = S(r)$ on $[0, \infty)$. Then for any two potentials $f_1, f_2 \in \mathcal{P}_d$ we have:*

$$\sigma(r) = \int_0^r [f_2(t) - f_1(t)]t^{d-1}\varphi_j(t)dt \geq 0 \quad r \in [0, \infty) \implies G_1(E) \leq G_2(E), \tag{8.21}$$

for $j = 1, 2$, where E is the ground state energy E.

Proof. Similar to the case $d = 1$. □

Chapter 9

Sign of Coulomb-like energy eigenvalues in dimension $d \geq 3$

In this section we study the sign of the energy eigenvalues of a certain class of Coulomb-like potentials. We consider the reduced Klein–Gordon equation (3.3), and we assume the following normalization condition for bound states

$$\int_0^\infty \varphi^2(r)dr = 1.$$

Theorem 9.0.1. *Let $f \in \mathcal{P}_d$ such that $f(r) = -\dfrac{w(r)}{r}$ with $w(r)$ non-increasing, $w(0) \leq 1$, and $\lim_{r\to\infty} w(r) = 0$. Then the corresponding ground state energy E of equation (3.3) is positive for $v < \dfrac{d-2}{2}$.*

Proof. Multiplying equation (3.3) by φ and integrating over $[0,\infty)$ we get

$$-2Ev\,\langle f\rangle = \langle -\Delta\rangle + m^2 - E^2 + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle - v^2\left\langle f^2\right\rangle. \tag{9.1}$$

Using Hardy's inequality $\left(\langle -\Delta\rangle \geq \left\langle \dfrac{(d-2)^2}{4r^2}\right\rangle\right)$ ([77]), equation (9.1) becomes

$$-2Ev\,\langle f\rangle \geq \left\langle \frac{(d-2)^2}{4r^2}\right\rangle + m^2 - E^2 + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle - v^2\left\langle f^2\right\rangle.$$

Since $m^2 - E^2 > 0$ for all $E \in (-m,m)$ and $v < \dfrac{d-2}{2}$ then

$$-2Ev\,\langle f\rangle > \frac{(d-2)^2}{4}\left\langle \frac{1}{r^2} - f^2\right\rangle + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle \tag{9.2}$$

Replacing $f(r)$ by $\dfrac{w(r)}{r}$ and using $d \geq 3$ in (9.2) we conclude that

$$-2Ev\,\langle f\rangle > \frac{1}{4}\left\langle \frac{1-w^2(r)}{r^2}\right\rangle + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle \geq 0.$$

Hence, $E > 0$. $\square$

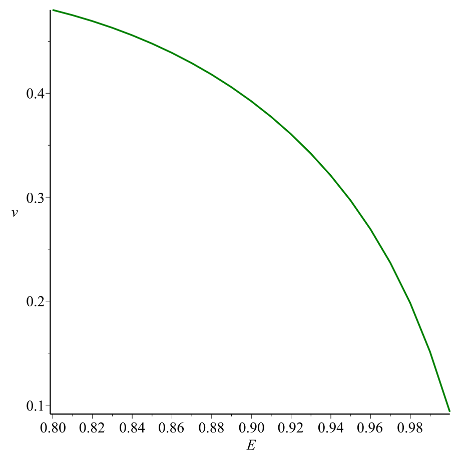


Figure 9.1: Spectral curve $u = G(e)$ for the Klein–Gordon equation with the Coulomb potential shape $f(r) = -\dfrac{1}{r}$. $E > 0$ for $v < 0.5$.

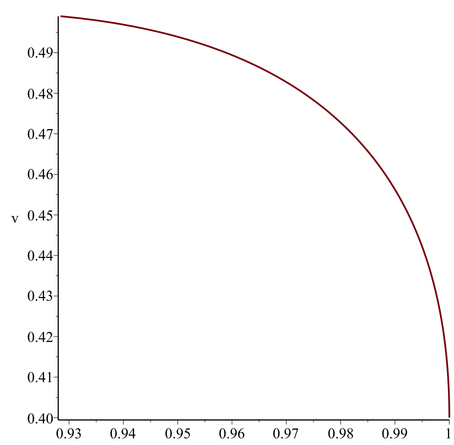


Figure 9.2: Spectral curve $u = G(e)$ for the Klein–Gordon equation with the Hulthén potential shape $f(r) = -\dfrac{1}{e^r - 1}$. $E > 0$ for $v < 0.5$.

Chapter 10

Spectral bounds for general potential shapes

In this section we exhibit a complete recipe for finding square-well potential bounds for any *bounded and unbounded* potential shape f in the classes $\mathcal{P}$ and $\mathcal{P}_d$ defined in sections 3.1 and 3.2 respectively, and consequently, spectral bounds for the coupling v, provided the energy is fixed. We have chosen the square-well and exponential potentials for the bounded case and Coulomb and Hulthén potentials for the unbounded case because we know the corresponding analytical solutions for the Klein–Gordon problem.

10.1 Square-Well and exponential spectral bounds for general bounded potentials

We exhibit a complete recipe for finding square-well potential bounds for any *bounded* potential shape f in the class $\mathcal{P}$ defined in **section** 3.1, and consequently, spectral bounds for the coupling v, provided the energy is fixed. We have chosen the square-well potential because we know the analytical solution for the Klein–Gordon problem with this potential. Before showing this solution, we state the following lemma:

Lemma 10.1.1. *Consider the d-dimensional Klein–Gordon equation ($d \geq 1$)*

$$\varphi''(r) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{Q}{r^2}\right]\varphi(r), \tag{10.1}$$

where $V(r) = vf(r)$ and f belongs to the class of potential shapes defined in the previous sections. We define $s > 0$ and E_1 to be the new energy corresponding to the potential $V_1(r) = v(f(r) - s)$. Then $|E + vs| < m$ and $E_1 = E - vs$.

Proof. For $r \to +\infty$, the Klein–Gordon equation becomes $\varphi''(r) = \left[m^2 - \big(E + vs\big)^2\right]\varphi(r)$; thus, $\varphi(r) = C_1 e^{kr} + C_2 e^{-kr}$ with $k = \sqrt{m^2 - (E + vs)^2}$. Since φ vanishes at ∞, then $C_1 = 0$, and since $\varphi \in L^2(\mathbb{R})$, then $|E+vs| < m$. Moreover, we can write (10.1(as: $\varphi''(r) = \left[m^2 - \big(E - vs - V(r) + vs\big)^2 + \frac{Q}{r^2}\right]\varphi(r) = \left[m^2 - \big(E - vs - v(f(r) - vs)\big)^2 + \frac{Q}{r^2}\right]\varphi(r) = \left[m^2 - \big((E - vs) - V_1(r)\big)^2 + \frac{Q}{r^2}\right]\varphi(r)$. Therefore, $E_1 = E - vs$. $\square$

10.1.1 General spectral bounds in the simple comparison theorem

Consider an attractive potential $V(r) = vf(r)$, where f is a bounded potential shape in the class defined in the previous sections. We want to find the best square-well spectral bounds for the graph $v = G(E)$. We define the downward vertically-shifted square-well potential

$$g(r,t_1) = \begin{cases} f(0), & r \leq t_1 \\ f(t_1), & \text{elsewhere} \end{cases},$$

, and the square-well potential

$$g(r,t_2) = \begin{cases} f(t_2), & r \leq t_2 \\ 0, & \text{elsewhere} \end{cases}.$$

Thus, $g(r,t_1) \leq f(r) \leq g(r,t_2)$ for all $r \geq 0$, and for each pair of contact points $\{t_1, t_2\}$. We observe that $f(r)$ has infinite families of lower and upper bounds $G_L^{(t_1)}(E) \leq G(E) \leq G_U^{(t_2)}(E)$, where $G_L^{(t_1)}(E)$ and $G_U^{(t_2)}(E)$ are the respective spectral functions $v_L(E)$ and $v_U(E)$. The final step is to optimize over the parameter t in order to obtain the best square-well spectral bounds for $G(E)$, that is

$$G_L(E) = \max_{t_1>0} G_L^{(t_1)}(E) \leq G(E) \leq G_U(E) = \min_{t_2>0} G_U^{(t_2)}(E). \tag{10.2}$$

These functions are extracted from the eigenvalue equations 5.3 and 5.4 for the one-dimensional case, and from 5.6 and 5.7 in the higher dimensional cases.
We first consider a square-well potential with depth A and semi-width b in dimension $d = 1$, and we define the new variables $e = Eb$, $u = Ab$, $\mu = mb$, and $t = b\left[(E+A)^2 - m^2\right]^{\frac{1}{2}}$. Then from equation 5.3 the ground state solution becomes:

$$e(t) = \pm\left[\mu^2 - \left(t \cdot \tan(t)\right)^2\right]^{\frac{1}{2}} \text{ and } u(t) = (t^2 + \mu^2)^{\frac{1}{2}} - e(t).$$

For definiteness, we now assume $\mu = 1$. We observe that $e = 0$ when $t = t_0 \approx 0.860334$. The graph depicting $u = G(e)$ is shown in Figure 10.1:

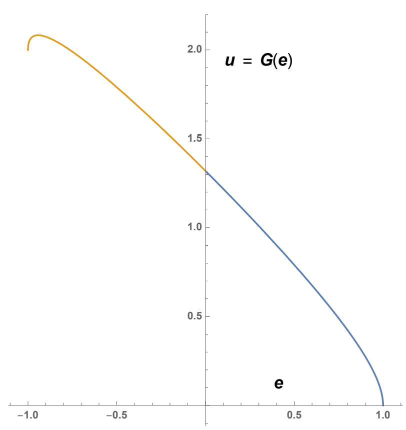


Figure 10.1: Spectral curve $u = G(e)$ for the Klein–Gordon equation with the square-well potential.

Example: The Woods-Saxon potential in 1-dimension

We consider the Woods-Saxon potential $V(x) = vf(x)$, where $f(x) = -1\left(1 + e^{\frac{(|x|-1)}{q}}\right)^{-1}$, and $q > 0$ is a range parameter [56]. We are interested in finding an upper bound and a lower bound for the coupling parameter v, for any given value of $|E| < m$ and for $q = 0.005$. Since we have shown the analytical

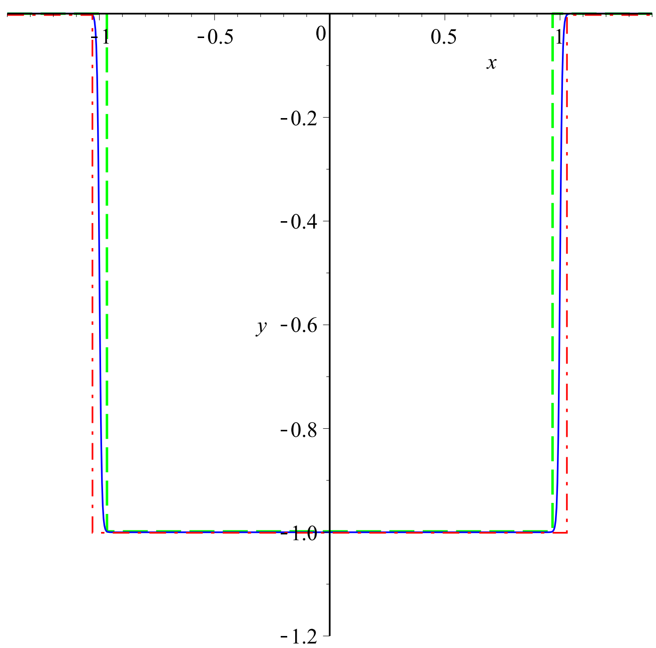


Figure 10.2: Graphs for the potential shapes (i) $g_u(x, 0.9675) = -0.9984$ for $|x| < 0.9675$, and 0 elsewhere; (ii) $f(x) = -1\left(1 + e^{\frac{(|x|-1)}{0.005}}\right)^{-1}$; (iii) $g_l(x, 1.03) = -1.001$ for $|x| < 0.9675$, and -0.0025 elsewhere.

solution for the Klein–Gordon differential equation with the square-well potential, we shall use a square-well potential as an upper bound for f, and another downward vertically-shifted square-well as a lower bound. We define the functions

$$g_u(x, 0.9675) = \begin{cases} -0.9984, & |x| \leq 0.9675 \\ 0, & \text{elsewhere} \end{cases},$$

and

$$g_l(x, 1.03) = \begin{cases} -1.001, & |x| \leq 1.03 \\ -0.0025, & \text{elsewhere} \end{cases}.$$

Since $f_l(x) \leq f(x) \leq f_u(x)$ for all $x \in (-\infty, +\infty)$, then according to **theorem** 7.1.1, we conclude that $G_L(E) = v_l \leq v \leq G_U(E) = v_u$, where v_l and v_u are the respective couplings for f_l and f_u. For example, if we fix $E = -0.512574196$, we get $v_u = 1.81478$ and $v_l = 1.79017$. Hence we conclude that $1.79017 \leq v \leq 1.81478$. This result has been verified numerically, using our own shooting method realized in Maple, and with which we find $v = 1.80494$. The graphs of f_l, f, and f_u are shown in figure 10.2, and the spectral curves of $G_L(E)$, $v = G(E)$, and $G_U(E)$ are shown in figures 10.3, 10.4, and 10.5.

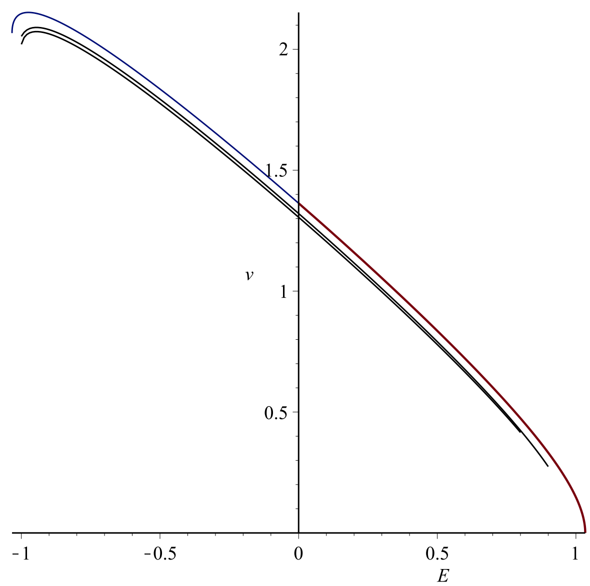


Figure 10.3: Graphs for spectral bounds $G_L(E), G(E)$, and ${}_U(E)$ for potential shapes (i) $g_x(x, 0.9675) = -0.9984$ for $|x| < 0.9675$, and 0 elsewhere; (ii) $f(x) = -1\left(1 + e^{\frac{(|x|-1)}{0.005}}\right)^{-1}$; (iii) $g_x(x, 1.03) = -1.001$ for $|x| < 0.9675$, and -0.0025 elsewhere. $(-1 < E < 1)$.

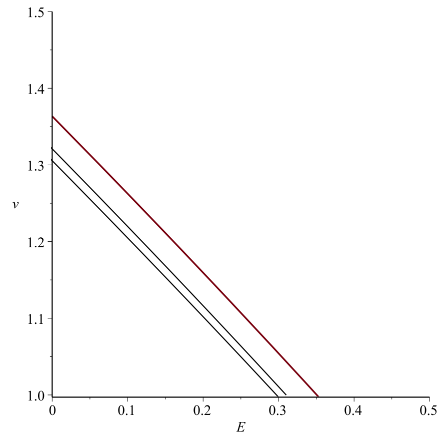


Figure 10.4: Graphs for spectral bounds $G_L(E), G(E)$, and ${}_U(E)$ for potential shapes (i) $g_x(x, 0.9675) = -0.9984$ for $|x| < 0.9675$, and 0 elsewhere; (ii) $f(x) = -1\left(1 + e^{\frac{(|x|-1)}{0.005}}\right)^{-1}$; (iii) $g_x(x, 1.03) = -1.001$ for $|x| < 0.9675$, and -0.0025 elsewhere. $(0 < E < 0.5)$.

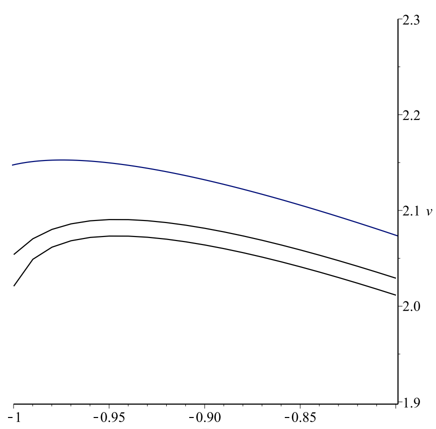


Figure 10.5: Graphs for spectral bounds $G_L(E), G(E)$, and ${}_U(E)$ for potential shapes (i) $g_x(x, 0.9675) = -0.9984$ for $|x| < 0.9675$, and 0 elsewhere; (ii) $f(x) = -1\left(1 + e^{\frac{(|x|-1)}{0.005}}\right)^{-1}$; (iii) $g_x(x, 1.03) = -1.001$ for $|x| < 0.9675$, and -0.0025 elsewhere. $(-1 < E < -0.8)$.

10.1.2 General spectral bounds in the refined comparison theorem

The refined comparison theorems allow us to find better spectral bounds than those found by applying the simple version, since the potential shapes are allowed to cross over even more than once in a controlled way. we provide a method for finding the best lower and upper spectral bounds for any bounded potential shape f. We use the square-well potential and the exponential potential as a lower bound and an upper bound respectively. We have chosen the square-well and the exponential potentials because we know the exact solutions of the Klein–Gordon equation with each of these potentials as we have seen in **chapter** 5.

Consider an attractive potential $V \in \mathcal{P}$ such that $V(r) = vf(r)$. Let $V_1(r) = v_1 f_1(r)$ be the square-well potential such that

$$f_1(x) = \begin{cases} f(0), & |x| \leq t \\ 0, & \text{elsewhere} \end{cases},$$

with

$$\int_0^t \big(f(r) - f_1(r)\big) dr > 0,$$

and

$$\int_0^\infty \big(f(r) - f_1(r)\big) dr = 0.$$

We also consider the exponential potential $V_2(r) = v_2 f_2(r)$ with $f_2(r) = -e^{-qr}$, $q > 0$, which intersects with f at $r = \alpha$ such that

$$\int_0^\alpha \big(f_2(r) - f(r)\big) dr > 0,$$

and

$$\int_0^\infty \big(f_2(r) - f(r)\big) dr = 0.$$

Hence, for any eigenenergy $E \in (-m, m)$ we have $G_L(E) \leq G(E) \leq G_U(E)$ where G_L, G, and G_U are the respective graphs of the spectral functions $v_1(E), v(E)$, and $v_U(E)$ respectively.

Applications

1. Let $V(x) = vf(x)$ be the Gaussian potential where $f(x) = -e^{-qx^2}$, and $q > 0$ is a range parameter. We want to find a lower and an upper bound for the coupling constant v, for any given eigenenergy $E \in (-m, m)$ and $q = -0.8$. We choose the square-well potential $V_1(x) = v_1 f_1(x)$ and the exponential potential $V_2(x) = v_2 f_2(x)$ with

$$f_1(x) = \begin{cases} -1, & |x| \leq \frac{\sqrt{5\pi}}{4} \\ 0, & \text{elsewhere} \end{cases},$$

and

$$f_2(x) = -e^{-\frac{4}{\sqrt{5\pi}}x}.$$

We have $\int_0^{\frac{\sqrt{5\pi}}{4}} \big(f(x) - f_1(x)\big) dx \approx 0.20816$ and $\int_0^\infty \big(f(x) - f_1(x)\big) dx = 0$(figure 10.6). On the other hand, f and f_2 cross over at $x_0 \approx 0.8$ (figure 10.7) with $\int_0^{x_0} \big(f_2(x) - f(x)\big) dx \approx 0.15253$ and $\int_0^\infty \big(f_2(x) - f(x)\big) dx = 0$. We fix $E = -0.0377$ and we deduce that $v_1 \leq v \leq v_2$ where $v_1 = 1.36$ and $v_2 = 1.9$. We have numerically verified this result by using our own shooting method realized in Maple, and with which we find $v = 1.581$. The graphs of $v_1(E), v(E)$, and $v_2(E)$ are shown in figure 10.8.

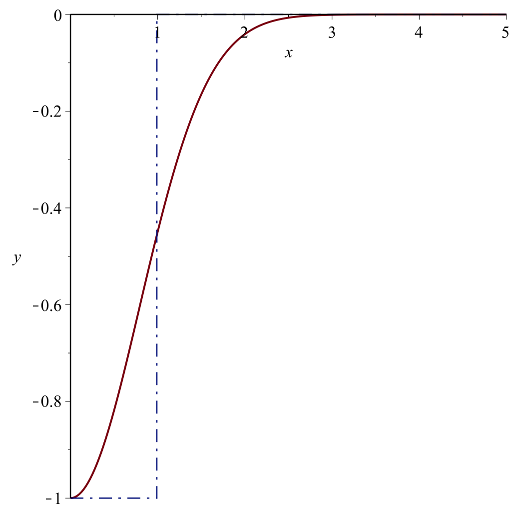


Figure 10.6: Potential Shapes $f_1(x) = -1$ if $|x| \leq \frac{\sqrt{5\pi}}{4}$ and 0 elsewhere, dashed lines and $f(x) = -Ae^{-qx^2}$ full line, where $A = 1$ and $q = 0.8$ were applied.

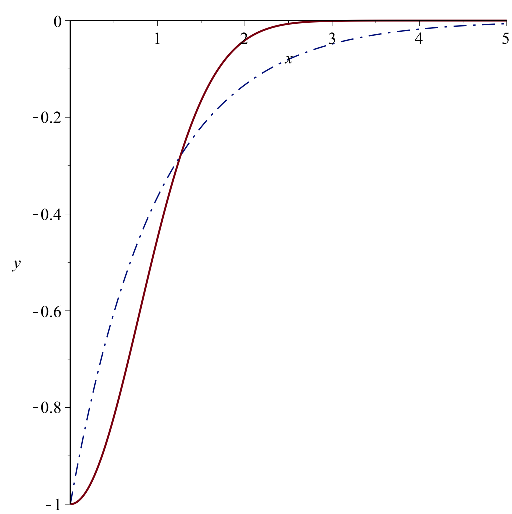


Figure 10.7: Potential Shapes $f(x) = -Ae^{-qx^2}$ full line and $f_2(x) = -Be^{-ax}$ dashed lines, where $q = 0.8$, $a = \frac{4}{\sqrt{5\pi}}$, and $A = B = 1$ were applied.

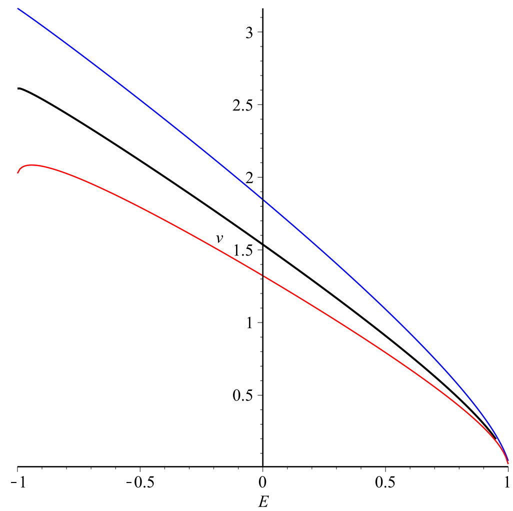


Figure 10.8: Graphs for $v_1(E), v(E)$, and $v_2(E)$ corresponding to $f_1(x) = -1$ if $|x| \leq \frac{\sqrt{5\pi}}{4}$ and 0 elsewhere, $f(x) = -e^{-0.8x^2}$, and $f_2(x) = -e^{-\frac{4x}{\sqrt{5\pi}}}$ respectively, for $-1 < E < 1$.

2. In this example we consider the sech-squared potential $V(x) = vf(x)$ where $f(x) = -\dfrac{\beta}{(e^{-qx} + e^{qx})^2}$. [78–81] We find the spectral bounds for $\beta = 3$ and $q = 0.35$. We choose the exponential potentials $V_1(x) = v_1 f_1(x)$ and $V_2(x) = v_2 f_2(x)$ such that

$$f_1(x) = -e^{-0.46666x},$$

and

$$f_2(x) = -0.75e^{-0.35x}.$$

This example shows that the refinement theorem is still valid even if the corresponding potential shapes cross over more than once, as long as the integral of their difference is convergent. Figures 10.9 and 10.10 show how the relative graphs of f_1, f, and f, f_2 cross over, with

$$\int_0^\infty \big(f(x) - f_1(x)\big)dx = \int_0^\infty \big(f_2(x) - f(x)\big)dx = 0.$$

We fix $E = -0.314$ and we get $v_1 = 1.9 \leq v \leq v_2 = 2.39$. We verify this result numerically and find that $v = 2.0943$. The graphs of v_1, v, and v_2 are shown in figure 10.11.

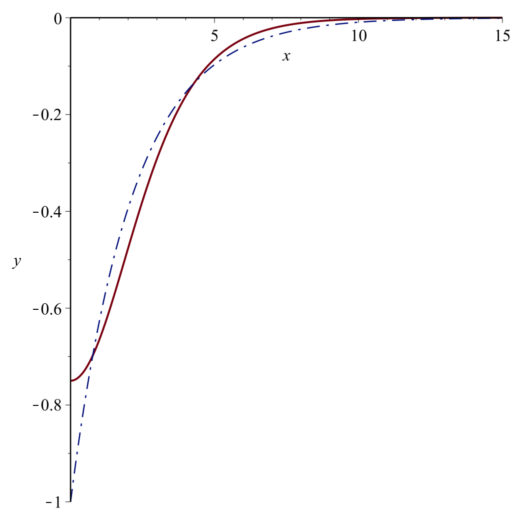


Figure 10.9: Potential Shapes $f_1(x) = -Ae^{-qx}$ dashed lines and $f(x) = -\dfrac{\beta}{(e^{-0.35x} + e^{0.35x})^2}$ full line, where $q = 0.35$, $C = b = 1$, and $A = 1$ were applied.

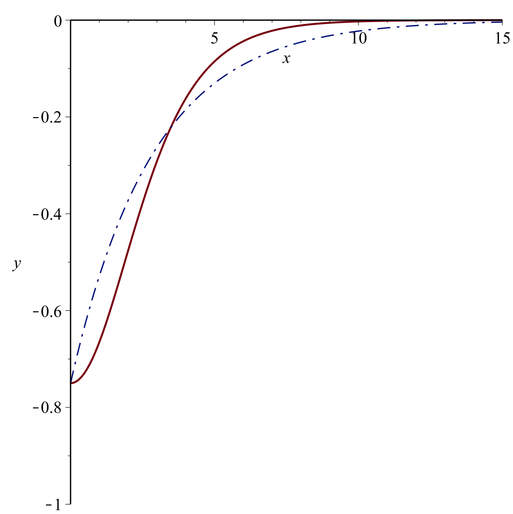


Figure 10.10: Potential Shapes $f_2(x) = -Ae^{-qx}$ dashed lines and $f(x) = -\dfrac{\beta}{(e^{-0.35x} + e^{0.35x})^2}$ full line, where $q = 0.35$ and $A = 0.75$ were applied.

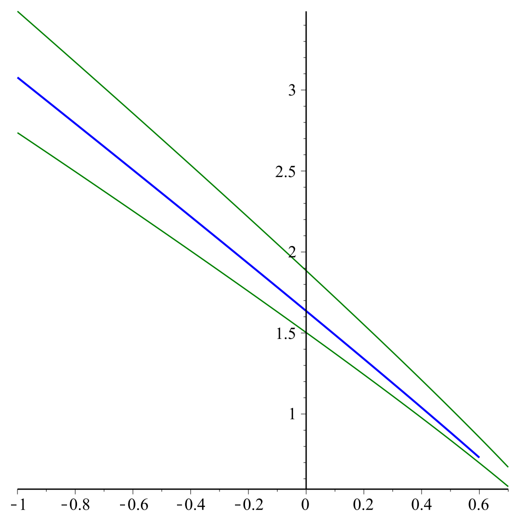


Figure 10.11: Graphs for $v_1(E), v(E)$, and $v_2(E)$ corresponding to $f_1(x) = -e^{-0.46666x}$, $f(x) = -\dfrac{\beta}{(e^{-0.35x} + e^{0.35x})^2}$, and $f_2(x) = -0.75e^{-0.35x}$ respectively, for $-1 < E < 1$.

3. We now consider the Woods Saxon potential $V(x) = vf(x)$ with $f(x) = -1\left(1 + e^{\frac{|x|-1}{0.1}}\right)^{-1}$ [56]. We use the square well potential $V_l(x) = v_l f_l(x)$ with

$$f_1(x) = \begin{cases} -1, & |x| \leq 1 \\ 0, & \text{elsewhere} \end{cases},$$

and the exponential potential $V_u(x) = v_u f_u(x)$ with

$$f_u(x) = -e^{-0.75|x|},$$

The potential shapes f_l and f intersect at $x_l = 1$ (figure 10.12), f and f_u intersect at $x_u \approx 1.0128$ (figure 10.13), and

$$\int_0^{x_l} \big(f(x) - f_l(x)\big)dx > 0,$$

and

$$\int_0^{x_u} \big(f_u(x) - f(x)\big)dx > 0.$$

If we fix $E = 0.5$, we get $v_l = 0.976$ and $v_u = 0.79$. Applying the shooting numerical method we verify that $v_l \leq v = 0.8136 \leq v_u$ (figure 10.14).

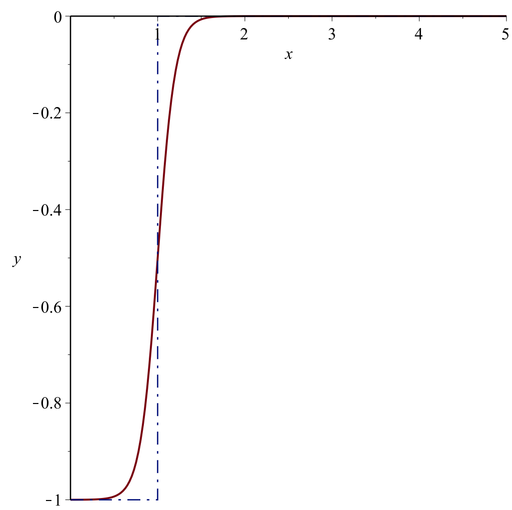


Figure 10.12: Potential Shapes $f_l(x) = 1$ if $|x| \leq 1$ and 0 elsewhere dashed lines and $f(x) = -1\left(1 + e^{\frac{|x|-1}{0.1}}\right)^{-1}$ full line.

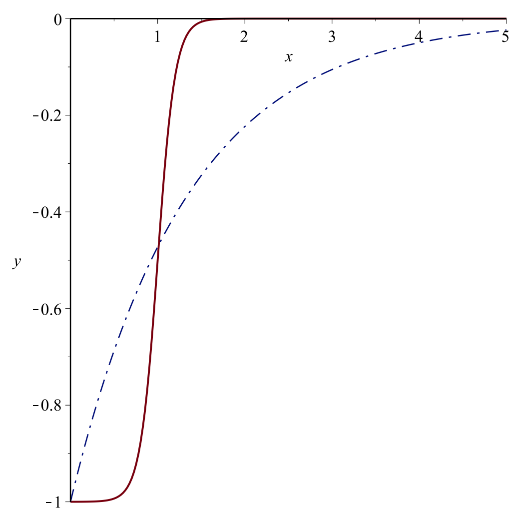


Figure 10.13: Potential Shapes $f_u(x) = -e^{-0.75x}$ dashed lines and $f(x) = -1\left(1 + e^{\frac{|x|-1}{0.1}}\right)^{-1}$ full line.

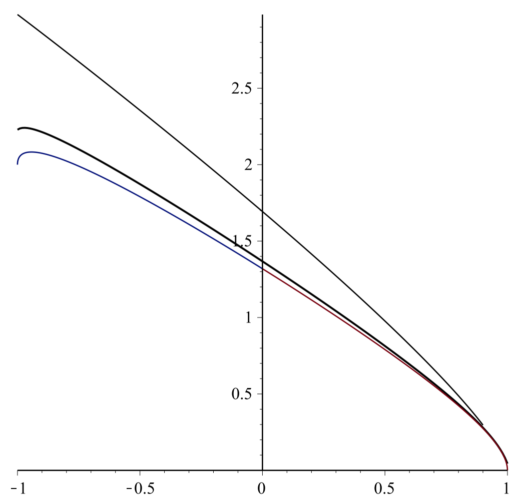


Figure 10.14: Graphs of v_l, v, and v_u, corresponding to $f_u(x) = -e^{-0.75x}$, $f(x) = -1\left(1 + e^{\frac{|x|-1}{0.1}}\right)^{-1}$ and $f_u(x) = -e^{-0.75|x|}$ respectively.

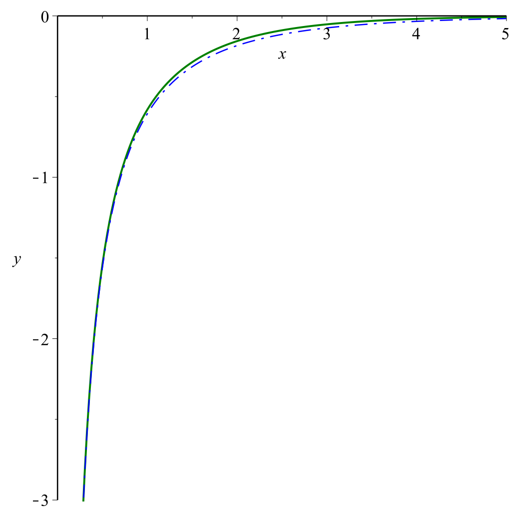


Figure 10.15: Potential Shapes $f_1(r) = -\frac{1}{e^{1.001r}-1}$ full line and $f(r) = -\frac{e^{-ar}}{r}$ dashed lines, where $a = 0.5$ was applied.

10.1.3 Hulthén and Coulomb Spectral Bounds for Singular Potentials

Since we know the exact solutions of the Klein–Gordon equation with the Coulomb and Hlthén potentials as shown in chapter 5, we can find spectral bounds for any singular potential in $\mathcal{P}_d$.

The Yukawa Potential in dimension $d = 3$

1. Consider the Yukawa potential $V(r) = vf(r)$ with $f(r) = -\frac{e^{-ar}}{r}$ [57] , where $a > 0$ is a range parameter. We shall find a lower and an upper bound for the coupling constant v, for any $E \in (-m, m)$, for $a = 0.5$. We choose the Hulthén potentials $V_1(r) = v_1 f_1(r)$ and $V_2(r) = v_2 f_2(r)$ [74] where

$$f_1(r) = -\frac{1}{e^{1.001r}-1},$$

and

$$f_2(r) = -\frac{1}{e^{0.966r}-1}.$$

We fix $E = 0.96$ and obtain $v_1 = 0.4895$ and $v_2 = 0.4799$. Since $f_1(r) > f(r)$ for $r \in [0, \infty)$ as shown in figure (10.12), then according to our simple general comparison theorem [58], we find that $v_1 > v$. On the other hand, f and f_2 cross over at $r_0 \approx 1.2$ as shown in the right graph of figure (10.13), with $\int_0^{r_0} \big(f_2(r) - f(r)\big) r^2 dx = 0.0108 > 0$. Hence, applying our refined version of the general comparison theorem, we obtain $v > v_2$. We have numerically verified this result by finding that $v = 0.4834$. The graphs of $v_1(E), v(E)$, and $v_2(E)$ are shown in figure (10.14).

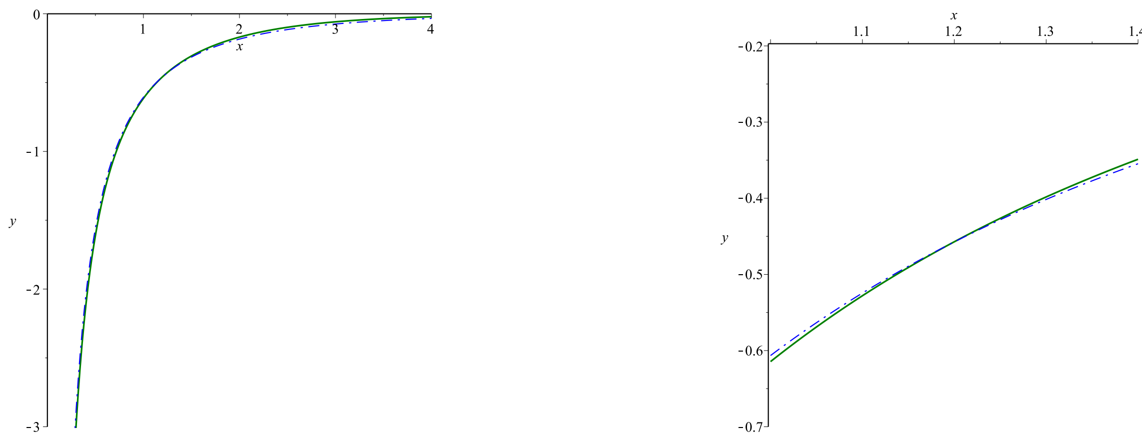


Figure 10.16: Left graph: potential shape $f_2(r) = -\dfrac{1}{e^{0.966r}-1}$ solid line and $f(r) = -\dfrac{e^{-ar}}{r}$ dashed lines. They intersect at $r_0 \approx 1.2$ as shown in the right graph. $a = 0.5$ was applied.

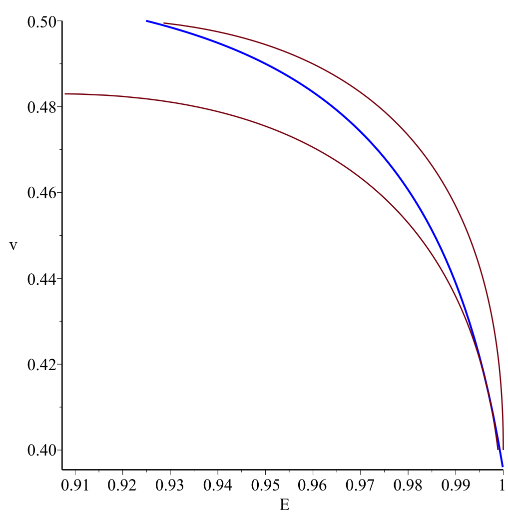


Figure 10.17: Graphs for $v_1(E), v(E)$, and $v_2(E)$ corresponding to $f_1(r) = -\dfrac{1}{e^{1.001r}-1}$, $f(r) = -\dfrac{e^{-0.5r}}{r}$, and $f_2(r) = -\dfrac{1}{e^{0.966r}-1}$ respectively, for $-1 < E < 1$.

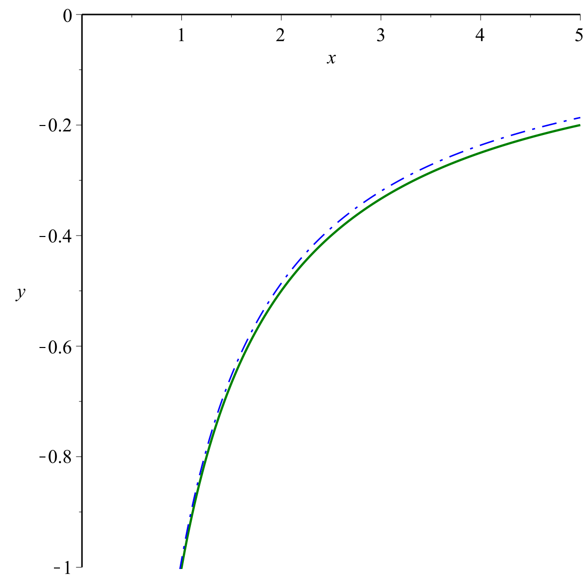


Figure 10.18: Potential Shapes $f_l(x) = -\dfrac{1}{r}$ dashed lines and $f(x) = -\dfrac{e^{-qr}}{r}$ full line, where $q = 0.014$ was applied.

2. We now consider another example for the Yukawa potential for which the range parameter is small, for which we use Coulomb spectral bounds. We let $f(r) = -\dfrac{e^{-0.014r}}{r}$, and we consider the Coulomb potentials $V_l(r) = v_l f_l(r)$ and $V_u(r) = v_u f_u(r)$ with

$$f_l(r) = -\frac{1}{r},$$

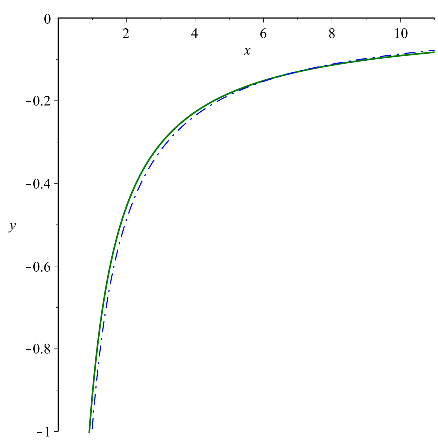
and

$$f_u(r) = -\frac{0.91}{r}.$$

Since $f_l(r) < f(r)$ for all $r \geq 0$ (figure 10.15), then applying the simple comparison theorem we deduce that $G_l(E) = v_l < v = G(E)$ for all $|E| < m$. We now let φ_u be the exact solution of the Klein–Gordon equation with the potential $V_u(r)$. The graphs of $f_u(r).\varphi_u(r)$ and $f(r).\varphi_u(r)$ cross over at $r \approx 6.85$ (figure 10.16) with

$$\int_0^{6.85} \big[f_u(r) - f(r)\big] r^2 \varphi(r) dr \approx 0.406 > 0.$$

Thus, applying **theorem** 8.2.1 we conclude that $G(E) = v < v_u = G_u(E)$. To verify that, we fix $E = 0.9$ and find that $v_l = 0.392$ and $v_u = 0.431$. We also numerically estimated the value of v and got $v = 0.399$.



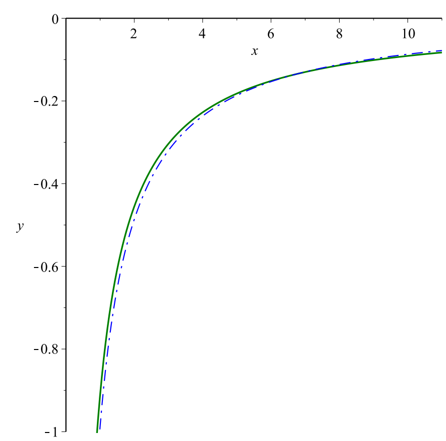


Figure 10.19: Left graph: potential shape $f_u(r) = -\dfrac{0.91}{r}$ solid line and $f(r) = -\dfrac{e^{-qr}}{r}$ dashed lines. Right graph: $f_u(r)\varphi_u(r)$ solid line and $f(r)\varphi_u(r)$ dashed lines. $q = 0.014$ was applied.

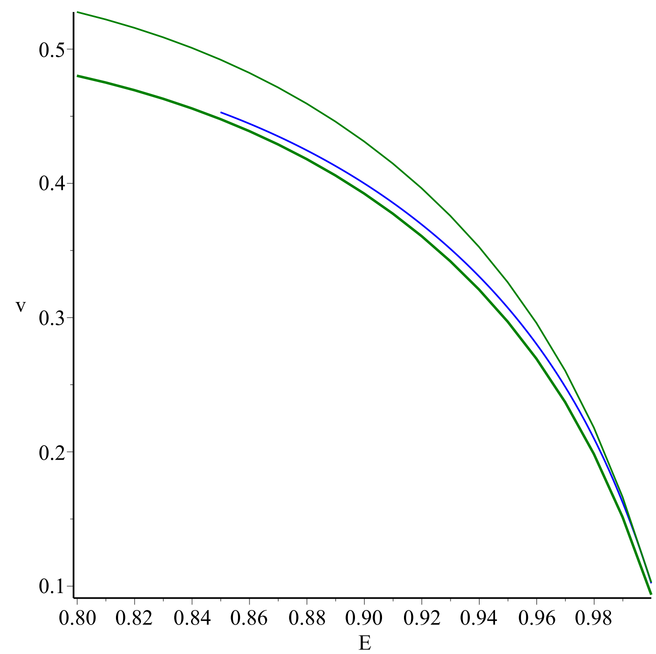


Figure 10.20: Spectral graphs v_l, v and v_u corresponding to $f_l(r) = -\dfrac{1}{r}, f(r) = -\dfrac{e^{-0.014r}}{r}$ full line, and $f_u(r) = -\dfrac{0.91}{r}$.

Chapter 11

Conclusion

The radial reduced eigen-equations for a one-particle potential model might in suitable units be written, fo the non-relativistic and Klein–Gordon cases, respectively, as

- (NR)

$$\varphi''(r) = \left[2m\big(vf(r) - E\big) + \frac{Q}{r^2}\right]\varphi(r);$$

- (KG)

$$\varphi''(r) = \left[m^2 - \big(E - vf(r)\big)^2 + \frac{Q}{r^2}\right]\varphi(r),$$

where $Q = \frac{1}{4}(2l + d - 1)(2l + d - 3)$, the potential shape $f(r) < 0$, and coupling parameter $v > 0$. We note that a slightly different formulation of the Klein–Gordon equation is required if $d = 2$ and $l = 0$. By familiarity with well-known Schrödinger examples, or by a variational analysis of them we expect, for suitable $v > v_0 > 0$, to find bound states with non-relativistic energies $E(v)$ having monotonic behavior $E'(v) < 0$ if the potential shape $f(r)$ is negative. However, these assumptions are not correct for the corresponding Klein–Gordon eigenvalues. This makes it difficult to design physically realistic models for relativistic problems.

In this thesis, we first represent the relation between the coupling v and the discrete eigenvalue E by writing v as a function $v = G(E)$ of E for $-m < E < m$. The spectral curve $v = G(E)$ is concave, and at most unimodal with a maximum close to $E = -m$. A bridging parameter $a \in [0, 1]$ is introduced such that $f = f_1 + a(f_2 - f_1)$. By studying the dependence of v on a for each fixed value of E, we establish the comparison theorem $f_1 \le f_2 \Longrightarrow G_1(v) \le G_2(v)$. These results are valid for all negative and positive energies, and for both ground and excited states. They allow us to devise spectral approximations in much the same way as is possible for the corresponding Schrödinger problem where the discrete spectrum can be defined variationally and the concomitant comparison theorems follow almost automatically by means of variational arguments.

Moreover, we exhibit a refined version of the comparison theorem still for nodeless states, by weakening the condition $f_1(r) \le f_2(r)$ to $\int_0^x \big[f_2(t) - f_1(t)\big]dt \ge 0$ for $d = 1$, and $\int_0^r \big[f_2(t) - f_1(t)\big]t^{d-1}dt \ge 0$ for $d \ge 3$, on $[0, \infty)$. We also prove that if we know one of the wave functions φ_1 or φ_2, we can replace the new condition by $\int_0^x \big[f_2(t) - f_1(t)\big]\varphi_i(t)dt \ge 0$ for $d = 1$, and $\int_0^r \big[f_2(t) - f_1(t)\big]t^{d-1}\varphi_i(t)dt \ge 0$ for $d \ge 3$, with $i = 1, 2$. The latter conditions provide us with a stronger theorem because, since the ground state is non-increasing on $[0, \infty)$, the potential shapes are even allowed to cross over more while preserving the ordering of the coupling parameters $v_1 = v_1(E)$ and $v_2 = v_2(E)$, for any energy

$E \in (-m, m)$.

We then prove that for any potential whose shape $f(r)$ is no more singular than $r^{-(d-2)}$, $(d \geq 3)$, with $f(r) = -\dfrac{w(r)}{r}$, where $w(r)$ is non-increasing on $[0, \infty)$ and $w(0) \leq 1$, the lowest eigen-energy is always positive for $v < \dfrac{1}{2}$. As an application to our refined theorem, we have constructed upper and lower bounds for the discrete spectrum generated by any given central negative bounded potential, by using the exact solutions of the Klein–Gordon equation with the square-well and the exponential potentials.

Finally, as an illustration, we are able to use the exact solution of the square-well, exponential, Coulomb, and Hulthén problems to construct upper and lower bounds for the discrete Klein–Gordon spectrum generated by any given member of the class of bounded and unbounded Coulomb - like negative potentials.

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Appendix A

Published Paper

EPJ Plus

Eur. Phys. J. Plus (2019) **134**: 449 DOI 10.1140/epjp/i2019-12833-5

General comparison theorems for the Klein-Gordon equation in d dimensions

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Società Italiana di Fisica Springer

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THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

General comparison theorems for the Klein-Gordon equation in d dimensions

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Received: 17 April 2019 / Revised: 8 June 2019
Published online: 17 September 2019

Abstract. We study bound-state solutions of the Klein-Gordon equation $\varphi''(x) = [m^2 - (E - v\, f(x))^2]\varphi(x)$, for bounded vector potentials which in one spatial dimension have the form $V(x) = v\, f(x)$, where $f(x) \le 0$ is the shape of a finite symmetric central potential that is monotone non-decreasing on $[0, \infty)$ and vanishes as $x \to \infty$. Two principal results are reported. First, it is shown that the eigenvalue problem in the coupling parameter v leads to spectral functions of the form $v = G(E)$ which are concave, and at most uni-modal with a maximum near the lower limit $E = -m$ of the eigenenergy $E \in (-m, m)$. This formulation of the spectral problem immediately extends to central potentials in $d > 1$ spatial dimensions. Secondly, for each of the dimension cases, $d = 1$ and $d \ge 2$, a comparison theorem is proven, to the effect that if two potential shapes are ordered $f_1(r) \le f_2(r)$, then so are the corresponding pairs of spectral functions $G_1(E) \le G_2(E)$ for each of the existing eigenvalues. These results remove the restriction to positive eigenvalues necessitated by earlier comparison theorems for the Klein-Gordon equation.

1 Introduction

The elementary comparison theorem of non-relativistic quantum mechanics states that if two potentials are ordered, then the respective bound-state eigenvalues are correspondingly ordered:

$$V_1 \le V_2 \Longrightarrow E_1 \le E_2.$$

In the non-relativistic case (Schrödinger's Equation), this is a direct consequence of the min-max principle since the Hamiltonian $H = -\Delta + V$ is bounded from below, and the discrete spectrum can be characterized variationally [1]. However, the min-max principle is not valid in a simple form in the relativistic case because the energy operators are not bounded from below [2–4]. Regarding the Klein-Gordon equation, since only a few analytical solutions are known, the existence of lower and upper bounds for the eigenvalues is important, and establishing comparison theorems for the eigenvalues of this equation is of considerable interest. We suppose that the vector potential V is written in the form $V(x) = v\, f(x)$, where $v > 0$ and $f(x)$ are defined respectively as the coupling parameter and the potential shape. The literature does provide explicit solved examples, such as the square-well potential [5,6], the exponential potential [7, 8], the Woods-Saxon potential, and the cusp potential [9]. Based on these examples it is clear that the relation $E(v)$ is not monotonic as it is in the Dirac relativistic equation, [10–13], and indeed for Schrödinger's non-relativistic equation. Consequently, comparison theorems for the Klein Gordon equation were restricted to positive energies [14–16], and some are only valid for the ground state. In the present study, we have established new comparison theorems valid for negative potentials and for both positive and negative eigen-energies, and not just for the ground state. Throughout this paper, V represents the time component of a four-vector; the scalar potential (a linear perturbation of the mass) is assumed to be zero.

The idea that had a profound effect on the present work and, in particular, eliminated an earlier positivity restriction for energies, was our thinking of v as a function of E. This enabled us to arrive at a *function* $v(E)$, whereas $E(v)$ is a two-valued expression. In sect. 2, we establish the principal features of the spectral curves $v(E)$ for the class of

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negative bounded potentials that vanish at infinity. In sect. 3 we solve the Klein-Gordon equation analytically for the square-well potential in $d \geq 1$ dimensions. In sect. 4 we prove some comparison theorems: the principal results claim that for any discrete eigenvalue $E \in (-m, m)$ and negative potential-shape functions $f_1(r)$ and $f_2(r)$ we have $f_1(r) \leq f_2(r) \implies v_1 \leq v_2$. In sect. 5 we exhibit a complete recipe for spectral bounds for this class of potentials based on comparisons with the exactly soluble square-well problem.

2 General features of the spectral curve $G(E) = v(E)$

2.1 One-dimensional case

The Klein-Gordon equation in one dimension is given by

$$\varphi''(x) = \left[m^2 - (E - V(x))^2\right]\varphi(x), \tag{1}$$

where φ'' denotes the second order derivative of φ with respect to x, natural units $\hbar = c = 1$ are used, and E is the energy of a spinless particle of mass m. We suppose that the potential function V is expressed as $V(x) = vf(x)$ with $v > 0$ and f satisfies the following conditions:

1) $V(x) = vf(x)$, $x \in \mathbb{R}$, where $v > 0$ is the coupling parameter and $f(x)$ is the potential shape;
2) f is even, that is $f(x) = f(-x)$;
3) f is not identically zero and non-positive;
4) f is attractive, that is f is monotone non-decreasing over $[0, \infty)$;
5) f vanishes at infinity, *i.e.* $\lim_{x\to\pm\infty} f(x) = 0$.

We also assume that $V(x) = vf(x)$ is in this class of potentials, for which the Klein-Gordon equation (1) has at least one discrete eigenvalue E, and that eq. (1) is the eigen-equation for the eigenstates. Because of condition 5, eq. (1) has the asymptotic form

$$\varphi'' = (m^2 - E^2)\varphi,$$

at infinity, with solutions $\varphi(x) = C_1 e^{\sqrt{k}|x|} + C_2 e^{-\sqrt{k}|x|}$, where C_1 and C_2 are constants of integration, and $k = m^2 - E^2$. The radial wave function of φ vanishes at infinity; thus, $C_1 = 0$. Since $\varphi \in L^2(\mathbb{R})$, then $k > 0$ which means that

$$|E| < m. \tag{2}$$

Suppose that $\varphi(x)$ is a solution of (1). Then by direct substitution we conclude that $\varphi(-x)$ is another solution of (1). Thus, by using linear combinations, we see that all the solutions of this equation may be assumed to be either even or odd. Hence, if φ is even then $\varphi'(0) = 0$, and if φ is odd then $\varphi(0) = 0$. Since $\varphi \in L^2(\mathbb{R})$ then $\int_{-\infty}^{+\infty} \varphi^2 \mathrm{d}x < \infty$. This means that the wave functions can be normalized and consequently we shall assume that φ satisfies the normalization condition

$$\|\varphi\|^2 = \int_{-\infty}^{\infty} \varphi^2(x)\mathrm{d}x = 1. \tag{3}$$

Definition 1. *We denote by $\langle f\rangle$ and $\langle f^2\rangle$ the mean values of f and f^2, respectively, where $\langle\varphi, \psi\rangle = \int_{-\infty}^{\infty} \varphi(x)\psi(x)\mathrm{d}x$ is the inner product on $L^2(\mathbb{R})$, that is $\langle f\rangle = \langle\varphi, f\varphi\rangle = \int_{-\infty}^{\infty} f(x)\varphi^2(x)\mathrm{d}x$ and $\langle f^2\rangle = \langle\varphi, f^2\varphi\rangle = \int_{-\infty}^{\infty} f^2(x)\varphi^2(x)\mathrm{d}x$.*

Lemma 1.

$$2E\langle f\rangle < v\langle f^2\rangle, \quad \forall |E| < m. \tag{4}$$

Proof. Expanding eq. (1) we get:

$$\varphi''(x) = (m^2 - E^2)\varphi(x) + 2Evf(x)\varphi(x) - v^2 f^2(x)\varphi(x).$$

Multiplying both sides by φ and integrating over $\mathbb{R}$ we obtain:

$$\int_{-\infty}^{\infty} \varphi''(x)\varphi(x)\mathrm{d}x = m^2 - E^2 + 2Ev\langle f\rangle - v^2\langle f^2\rangle.$$

After applying integration by parts and using the fact that φ vanishes at $\pm\infty$, the left-hand side of the last equation becomes $-\int_{-\infty}^{\infty}(\varphi'(x))^2\mathrm{d}x$. Thus, $-\int_{-\infty}^{\infty}(\varphi'(x))^2\mathrm{d}x + E^2 - m^2 = 2Ev\langle f\rangle - v^2\langle f^2\rangle$. Since the left-hand side is negative, we have the desired result. $\square$

We now define the operator K as

$$K = -\frac{\partial^2}{\partial x^2} + 2Evf - v^2 f^2. \tag{5}$$

If φ is solution of the Klein-Gordon equation (1), then we have

$$K\varphi = (E^2 - m^2)\varphi, \tag{6}$$

and it follows:

$$\langle \varphi, K\varphi \rangle = \langle \varphi, (E^2 - m^2)\varphi \rangle = E^2 - m^2. \tag{7}$$

We observe that the domain of K is $D_K = H^2(\mathbb{R})$, where $H^2(\mathbb{R})$ is the Sobolev space defined as follows:

$$H^2(\mathbb{R}) = \{\varphi \in L^2(\mathbb{R}) : \varphi', \varphi'' \in L^2(\mathbb{R})\}.$$

Since $\|K\varphi\| = |E^2 - m^2| \cdot \|\varphi\| \leq m^2\|\varphi\|$ for all $\varphi \in D_K$, then K is a bounded operator. This implies that K is continuous. We also observe that K is symmetric, that is to say: $\langle \varphi, K\psi \rangle = \langle K\varphi, \psi \rangle$.

We now consider a family of Klein-Gordon spectral problems where $v = v(E)$ is a function of E.

Let φ_E denote the partial derivative of φ with respect to E. If we differentiate the normalization integral (3) partially with respect to E, we obtain the orthogonality relation $\langle \varphi, \varphi_E \rangle = 0$. Furthermore, differentiating eq. (7) with respect to E we obtain:

$$\langle \varphi_E, K\varphi \rangle + \langle \varphi, K_E\varphi \rangle + \langle \varphi, K\varphi_E \rangle = 2E. \tag{8}$$

The symmetry of K and the orthogonality of φ and φ_E imply that

$$\langle \varphi, K\varphi_E \rangle = \langle \varphi_E, K\varphi \rangle = (E^2 - m^2)\langle \varphi_E, \varphi \rangle = 0.$$

Then by using the expression

$$K_E = 2vf + 2Evf - 2vv_E f^2 \tag{9}$$

in eq. (8), we obtain the key equation for our theorem in this section, namely,

$$v_E = \frac{E - v\langle f \rangle}{E\langle f \rangle - v\langle f^2 \rangle}. \tag{10}$$

Theorem 1. *If $E \geq v\langle f \rangle$, then $E_1 \leq E_2 \Rightarrow v(E_1) \geq v(E_2)$; and if $E < v\langle f \rangle$, then $E_1 < E_2 \Rightarrow v(E_1) < v(E_2)$.*

Proof. If $E \geq 0$, then $v_E \geq 0$, and the theorem holds immediately. On the other hand, if $E < 0$, then by (4), $E\langle f \rangle < 2E\langle f \rangle < v\langle f^2 \rangle$, which means that $E\langle f \rangle - v\langle f^2 \rangle < 0$. Thus $v\langle f \rangle \leq E < 0 \Rightarrow v_E \leq 0$, and $E < v\langle f \rangle \Rightarrow v_E > 0$. Therefore, the theorem has been proven. □

Theorem 2. *The spectral curve $G(E)$ is concave for all E, $|E| < m$.*

Proof. Suppose that for any $|E_i| < m$, φ_i is the corresponding wave function, $\langle f_i \rangle = \int_{-\infty}^{+\infty} f(x)(\varphi_i)^2 \mathrm{d}x$, and $\langle f_i^2 \rangle = \int_{-\infty}^{+\infty} f^2(x)(\varphi_i)^2 \mathrm{d}x$. Let the maximum value of $G(E)$ be equal to v_{cr}. By theorem 1, the corresponding value of E is $E_{cr} = v_{cr}\langle f_{cr} \rangle$. Consider the point $A(E_{cr}, v_{cr}\langle f_{cr} \rangle)$ and fix the point $B(E_n, v_n)$ on the spectral curve $G(E)$, where $v_n = G(E_n)$, such that $E_n \neq E_{cr}$ and $E_n \in (-m, m)$. Then

$$(AB) : G_c(E) = v_{cr} + \frac{v_{cr} - v_n}{v_{cr}\langle f_{cr} \rangle - E_n}\,(E - v_{cr}\langle f \rangle).$$

Assume, without loss of generality, that $E_{cr} < E_n$, and consider the function $t(E) = G(E) - G_c(E)$ where $E \in [E_{cr}, E_n]$. Then $t'(E) = \frac{\mathrm{d}t}{\mathrm{d}E} = \frac{E - v\langle f \rangle}{E\langle f \rangle - v\langle f^2 \rangle} + \frac{v_n - v_{cr}}{v_{cr}\langle f_{cr} \rangle - E_n}$, which vanishes at the point $(E_m, G(E_m))$ with

$$\begin{aligned} E_m &= \frac{v_m E_n \langle f_m \rangle - v_m v_{cr}\langle f_m \rangle\langle f_{cr} \rangle + v_m v_{cr}\langle f_m^2 \rangle - v_m v_n \langle f_m^2 \rangle}{E_n - v_{cr}\langle f_{cr} \rangle + \langle f_m \rangle (v_{cr} - v_n)} \\ &= \frac{v_m\langle f_m \rangle (E_n - v_{cr}\langle f_{cr} \rangle) + v_m\langle f_m \rangle^2 (v_{cr} - v_n) + v_m\langle f_m^2 \rangle (v_{cr} - v_n) - v_m\langle f_m \rangle^2 (v_{cr} - v_n)}{E_n - v_{cr}\langle f_{cr} \rangle + \langle f_m \rangle (v_{cr} - v_n)}. \end{aligned}$$

Hence

$$E_m = v\langle f_m \rangle + \frac{v_m(v_{cr} - v_n)\,(\langle f_m^2 \rangle - \langle f_m \rangle^2)}{E_n - v_{cr}\langle f_{cr} \rangle + \langle f_m \rangle (v_{cr} - v_n)}. \tag{11}$$

Since $t'(E_{cr}) > 0$ and $t(E_{cr}) = t(E_n) = 0$, then the point $(E_m, G(E_m))$ must be a maximum point of $t(E)$ over the interval $[E_{cr}, E_n]$ and $t(E) \geq 0$ over $[E_{cr}, E_n]$. This means that the chord $[AB]$ is always beneath the spectral curve $G(E)$ over $[E_{cr}, E_n]$ and the proof is complete. □

We observe that φ is not necessarily required to be a node-free state, this means that the previous theorem is valid for all states, ground state and any excited state. Spectral curves for the square-well and the Woods-Saxon potentials are exhibited in figs. 1 and 2.

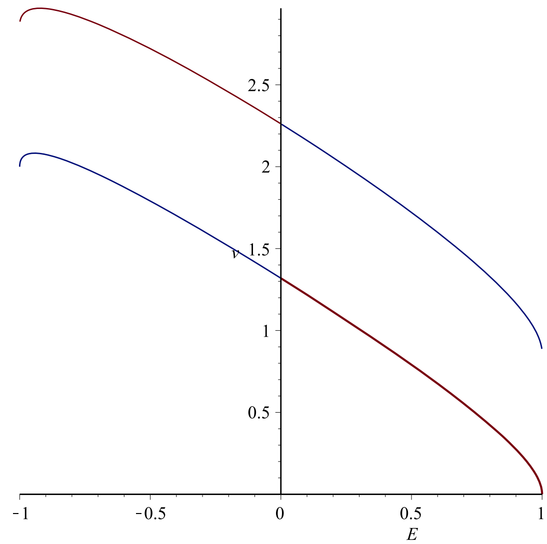

Fig. 1. Graphs of the function $v(E)$ in the square-well potential, for the ground state and the first excited state. We exhibit an explicit expression in sect. 5.

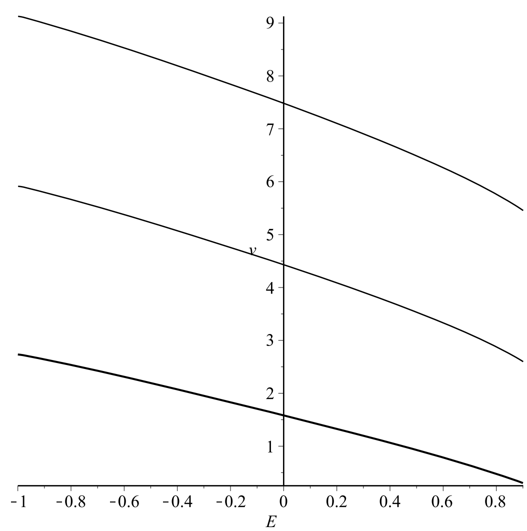

Fig. 2. Graphs of the function $v(E)$ in the Woods-Saxon potential shape $f(x) = -\frac{1}{1+e^{b(|x|-1)}}$ with $b = \frac{20}{7}$, for the ground state, the first excited state, and the second excited state. The graphs are plotted using a numerical shooting method of our own.

2.2 d-dimensional cases (d > 1)

The Klein-Gordon equation in d dimensions is given by

$$\Delta_d \Psi(r) = [m^2 - (E - V(r))^2]\Psi(r),$$

where natural units $\hbar = c = 1$ are used and E is the discrete energy eigenvalue of a spinless particle of mass m. We suppose here that the vector potential function $V(r)$, $r = \|\mathbf{r}\|$, is a radially symmetric Lorentz vector potential (the time component of a space-time vector), which satisfies the following conditions:

1) V is not identically zero and non-positive, that is $V \leq 0$;
2) V is attractive;
3) V vanishes at ∞.

The operator Δ_d is the d-dimensional Laplacian. Hence, the wave function for $d > 1$ can be expressed as $\Psi(r) = R(r)Y_{l_{d-1},\ldots,l_1}(\theta_1, \theta_2, \ldots, \theta_{d-1})$, where $R \in L^2(\mathbb{R}^d)$ is a radial function and $Y_{l_{d-1},\ldots,l_1}$ is a normalized hyper-spherical harmonic with eigenvalues $l(l+d-1)$, $l=0,1,2,\ldots$ [17] The radial part of the above Klein-Gordon equation can be written as

$$\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}R(r)\right)=\left[m^2-(E-V(r))^2+\frac{l(l+d-2)}{r^2}\right]R(r),$$

where R satisfies the second-order linear differential equation

$$R''(r)+\frac{d-1}{r}R'(r)=\left[m^2-(E-V(r))^2+\frac{l(l+d-2)}{r^2}\right]R(r).$$

Applying the change of variable $R(r)=r^{-\frac{d-1}{2}}\varphi(r)$, we obtain the following reduced second-order differential equation:

$$\varphi''(r)=\left[m^2-\big(E-V(r)\big)^2+\frac{Q}{r^2}\right]\varphi(r), \tag{12}$$

where

$$Q=\frac{1}{4}(2l+d-1)(2l+d-3),$$

with $l=0,1,2,\ldots$ and $d=2,3,4,\ldots$, which is the radial Klein-Gordon equation for $d>1$ dimensions. The reduced wave function φ satisfies $\varphi(0)=0$ and $\lim_{r\to\infty}\varphi=0$ [18]. For bound states, the normalization condition is

$$\int_0^\infty \varphi^2(r)\mathrm{d}r=1.$$

Since V vanishes at ∞, then eq. (12) becomes

$$\varphi''=(m^2-E^2)\varphi$$

near infinity, which means that $|E|<m$ by the same reasoning as used for eq. (2). Since the derivative of the term $\frac{Q}{r^2}$ in eq. (12) with respect to E is equal to zero, then by the same reasoning the relation (4) is also valid for all other $d>1$ dimensions. We define the operator

$$K=-\frac{\partial^2}{\partial r^2}+2Evf-v^2f^2+\frac{Q}{r^2}\,.$$

We have

$$\langle K\rangle=\langle(E^2-m^2)\varphi,\varphi\rangle=E^2-m^2.$$

As in the previous section, K is bounded and symmetric with $D_K=H^2(\mathbb{R}^d)$. We consider the same family of Klein-Gordon spectral problems with $v=v(E)$. Since $K_E=2vf+2Ev_Ef-2vv_Ef^2$, then we obtain the same relation as in the one-dimensional case,

$$v_E=\frac{E-v\langle f\rangle}{E\langle f\rangle-v\langle f^2\rangle}\,.$$

Theorem 3. *If $E\geq v\langle f\rangle$, then $E_1\leq E_2\Rightarrow v(E_1)\geq v(E_2)$, and if $E<v\langle f\rangle$, then $E_1<E_2\Rightarrow v(E_1)<v(E_2)$.*

Proof. Same as theorem 1. □

Theorem 4. *The spectral curve $G(E)$ is concave for all $|E|<m$.*

Proof. Same as theorem 2. □

We observe that as in the one-dimensional case, this theorem does not require the radial wave function to be node-free; it is valid for both ground and excited states.

3 Exact solution for the Klein-Gordon equation with the square-well potential

1) *One dimensional case*: Consider the Klein-Gordon equation in dimension $d=1$: $\varphi''(x)=[m^2-(E-g(x,t))^2]\varphi(x)$, and the square-well potential

$$g(r,t)=\begin{cases}-v_0, & |x|\leq t,\\ 0, & \text{elsewhere,}\end{cases}$$

where $v_0 > 0$. For $x < -t$, we get: $\varphi''(x) = (m^2 - E^2)\varphi(x)$. Thus, $\varphi(x) = Ae^{-kx} + Be^{kx}$ with $k^2 = m^2 - E^2$. Since φ vanishes at $-\infty$, then $A = 0$ and $\varphi(x) = Be^{kx}$. Similarly, for $x > t$ we obtain $\varphi(x) = Ce^{-kx}$. For $|x| \leq t$, $\varphi''(x) + w^2\varphi(x) = 0$ with $w = \sqrt{(E + v_0)^2 - m^2}$. Then $\varphi(x) = D\sin(wx) + E\cos(wx)$. Since, as shown in sect. 2.1, all the solutions are either even or odd, then the even solution is

$$\varphi(x) = \begin{cases} Be^{kx}, & x < -t, \\ E\cos(wx), & |x| \leq t, \\ Ce^{-kx}, & x > t, \end{cases}$$

and the odd solution is

$$\varphi(x) = \begin{cases} Be^{kx}, & x < -t, \\ D\sin(wx), & |x| \leq t, \\ Ce^{-kx}, & x > t. \end{cases}$$

Regarding the even solution, since φ is required to be continuously differentiable at t, then

$$E\cos(wt) = Ce^{-kt}, \tag{13}$$

and

$$-Ew\sin(wt) = -Cke^{-kt}. \tag{14}$$

Dividing eq. (14) by (13), we obtain the eigenvalue equation

$$w\tan wt = k. \tag{15}$$

Similarly, the eigenvalue equation for the odd states reads

$$w\cot(wt) = -k. \tag{16}$$

These equations allow us to compute the eigenvalue v_0 given the energy E.

2) $d > 1$ *dimensional cases*: The radial part of the Klein-Gordon equation reads [17]

$$R''(r) + \frac{d-1}{r}R'(r) = \left[m^2 - (E - g(r,t))^2 + \frac{l(l+d-2)}{r^2}\right]R(r), \tag{17}$$

where $l = 0, 1, 2, \ldots$ and

$$g(r,t) = \begin{cases} -v_0, & r \leq t, \\ 0, & \text{elsewhere}, \end{cases}$$

with $v_0 > 0$. For $d = 3$, the eigenvalue equation is [19]:

$$\frac{j_l'(k_i t)}{j_l(k_i t)} = \frac{h_l^{(1)\prime}(ikt)}{h_l^{(1)}(ikt)}, \tag{18}$$

where $k_i^2 = (E + v_0)^2 - m^2$, $k^2 = m^2 - E^2$, $i^2 = -1$, j_l is the spherical Bessel function of the first kind, and $h_l^{(1)}$ is the Hankel function of the first kind. In particular, the eigenvalue equation for the s-states ($l = 0$) is [19]:

$$k_i\cot(k_i t) = -k.$$

To generalize for any d-dimensional case, we consider the reduced form of the radial part of the Klein-Gordon equation (12). For $r < t$, we write it as

$$r^2\varphi'' + [k_i^2 r^2 - Q]\varphi(r) = 0.$$

Changing the variable r into $\sigma = k_i r$ we obtain the following differential equation:

$$\sigma^2\varphi''(\sigma) + [\sigma^2 - \nu(\nu+1)]\varphi(\sigma) = 0,$$

where $\nu = \frac{2l+d-3}{2}$. This is the Riccati-Bessel equation with solution $\varphi(\sigma) = C_1\sigma j_\nu(\sigma) + C_2\sigma y_\nu(\sigma)$ [20], where y_ν is the spherical Bessel function of the second kind. Since we have an irregular point at $\sigma = 0$, then $C_2 = 0$. For $r > t$ we obtain the differential equation

$$r^2\varphi''(r) + [-k^2 r^2 - Q]\varphi(r) = 0.$$

Using the change of variable $\sigma = ikr$ we obtain

$$\sigma^2\varphi''(\sigma) + [\sigma^2 - \nu(\nu+1)]\varphi(\sigma) = 0,$$

whose general solution is [20] $\varphi(\sigma) = W_1\sigma h^{(1)}(\sigma) + W_2\sigma h^{(2)}(\sigma)$, where $h^{(2)}$ is the Hankel function of the second kind. Since $\varphi \in L^2(\mathbb{R})$, then $W_2 = 0$. Since φ is continuously differentiable at $r = t$, then the corresponding eigenvalue equation is

$$\frac{[(k_i t)j_l(k_i t)]'}{(k_i t)j_l(k_i t)} = \frac{[(ikt)h_l^{(1)}(ikt)]'}{(ikt)h_l^{(1)}(ikt)}\,. \tag{19}$$

4 Comparison theorems for pairs of potential functions with different potential shapes

4.1 d = 1 dimensional case

Consider the Klein-Gordon equation in one dimension:

$$\varphi''(x) = [m^2 - (E - V(x))^2]\varphi(x), \tag{20}$$

where natural units $\hbar = c = 1$ are used, and E is the energy of a spinless particle of mass m. We assume that $V(x) = vf(x)$ with the same conditions in sect. 2.1, that is:

1) $V = vf$, where $v > 0$ is the coupling parameter and f is the potential shape of V;
2) V is an even function, that is $V(x) = V(-x)$;
3) V is not identically zero and a non-positive function, *i.e.* $V \leq 0$;
4) f is attractive, that is f is monotone non-decreasing over $[0,\infty)$;
5) f vanishes at infinity, *i.e.* $\lim_{x\to\pm\infty} f(x) = 0$.

By similar reasoning in sect. 2.1, we have $|E| < m$, and all the solutions of eq. (20) are either even or odd functions. We also assume that the wave function in this section satisfies the normalization condition, *i.e.*,

$$\|\varphi\|^2 = \int_{-\infty}^{\infty} \varphi^2(x)\mathrm{d}x = 1. \tag{21}$$

In this section, we consider the parameter $a \in [0,1]$ and the two potential shapes f_1 and f_2 with $f = f(a,x) = f_1(x) + a[f_2(x) - f_1(x)]$, where $f_1 \leq f_2 \leq 0$. Hence $f \leq 0$, attractive, even, vanishes at infinity, $f(0,x) = f_1(x)$ when $a = 0$, and $a = 1$ when $f(1,x) = f_2(x)$, and

$$\frac{\partial f}{\partial a} = f_2(x) - f_1(x) \geq 0. \tag{22}$$

Hence, f is monotone non-decreasing in the parameter a. The idea in this section is to study the variations of the coupling v with respect to a, provided $v = v(a)$ and the value of E is given as a constant, that is $\frac{\partial E}{\partial a} = 0$, and $-m < E < m$. We again consider the symmetric bounded operator K in (5), and we define φ_a to be the partial derivative of φ with respect to a. Differentiating equation (7) with respect to a we get:

$$\langle\varphi_a, K\varphi\rangle + \langle\varphi, K_a\varphi\rangle + \langle\varphi, K\varphi_a\rangle = 0. \tag{23}$$

Applying the partial derivative with respect to a to eq. (21) and using the symmetry of K, we obtain the new orthogonality relation

$$\langle\varphi_a, K\varphi\rangle = \langle\varphi, K\varphi_a\rangle = (E^2 - m^2)\langle\varphi_a, \varphi\rangle = 0.$$

We also have

$$K_a = 2Ev_a f + 2Ev(f_2 - f_1) - 2vv_a f^2 - 2v^2 f(f_2 - f_1),$$

with v_a defined as $\frac{\partial v}{\partial a}$. Equation (23) becomes:

$$Ev_a\langle f\rangle + Ev\int_{-\infty}^{\infty}(f_2(x) - f_1(x))\,\varphi^2(x)\mathrm{d}x - vv_a\langle f^2\rangle - v^2\int_{-\infty}^{\infty} f\,(f_2(x) - f_1(x))\,\varphi^2(x)\mathrm{d}x = 0.$$

This leads us to the following relation:

$$v_a = \frac{vI}{E\langle f\rangle - v\langle f^2\rangle}\,, \tag{24}$$

where

$$I = \int_{-\infty}^{\infty}(f_2(x) - f_1(x))\,(vf(x) - E)\,\varphi^2(x)\mathrm{d}x. \tag{25}$$

In the next two lemmas, we shall use the parity of φ and study the sign of φ'' on the interval $[0,\infty)$.

Lemma 2. *If φ is the node-free (ground) state, then φ'' changes its sign only once over* $[0,\infty)$.

Proof. Let $\varphi''(x)=0$. Then from eq. (20) we get $m^2-(E-V(x))^2=0$, which means that $V(x)=E-m$ or $V(x)=E+m$. Since $|E|<m$ and $V(x)\leq 0$, then $V\neq E+m$. Hence, $V(x)=E-m$ and $\varphi''(x)=0 \Longleftrightarrow x=V^{-1}(E-m)$, where V^{-1} is the inverse of the monotone function V.

1) *V is unbounded near 0:* Since V is unbounded near 0, then $\varphi''<0$ near 0, and since V vanishes at ∞, eq. (20) becomes $\varphi''=(m^2-E^2)\varphi>0$. Hence, φ is concave on $[0,V^{-1}(E-m))$ and convex on $(V^{-1}(E-m),\infty)$.
2) *V is bounded; that is $V_0\leq V\leq 0$:* Since φ is an even state, then $\varphi'(0)=0$, which means that $y=\varphi(0)$ is an equation of the tangent line to φ at $x=0$.
   If φ is convex near 0, then φ'' must change it sign at some $x_1\in[0,\infty)$ since we know that φ vanishes near ∞. However, eq. (20) becomes $\varphi''=(m^2-E^2)\varphi>0$ near ∞, which means that φ is convex near ∞. Thus φ'' should again change its sign at some $x_2\in[x_1,\infty)$. This means that φ has two inflection points on $[0,\infty)$, which is a contradiction. Hence, φ is concave on $[0,V^{-1}(E-m))$ and convex on $(V^{-1}(E-m),\infty)$. □

Lemma 3. *φ''changes its sign at least once over $[0,\infty)$, for any excited state φ.*

Proof. Using the parity of φ, it is sufficient to study the sign of φ'' on the interval $[0,\infty)$. If V is unbounded near 0, then $\varphi''<0$ near 0 and $\varphi''>0$ near ∞. If V is bounded; that is $V_0\leq V\leq 0$ where $V_0=V(0)$, then we divide the proof into the following two cases:

1) *φ has only one node:* Suppose that φ has one node α, then $\varphi''(x)=0\Longleftrightarrow x=\alpha$ or $x=V^{-1}(E-m)$. If $\varphi(x)>0$ for $x>\alpha$, then φ should attain a maximum value since it vanishes near ∞, and thus $\varphi''<0$. However, by the same condition that φ vanishes near ∞, φ'' should change its sign one more time. This means that $V^{-1}(E-m)\in(\alpha,\infty)$. Therefore
   A) if $\varphi(x)>0$ for $x>\alpha$, then $\varphi''(x)<0$, for $x\in(\alpha,V^{-1}(E-m))$, and $\varphi''(x)>0$ for $x\in(0,\alpha)\cup(V^{-1}(E-m),\infty)$;
   B) if $\varphi(x)<0$ for $x>\alpha$, then $\varphi''(x)>0$, for $x\in(\alpha,V^{-1}(E-m))$, and $\varphi''(x)<0$ for $x\in(0,\alpha)\cup(V^{-1}(E-m),\infty)$.
2) *φ has n nodes, $n\geq 2$:* Suppose that φ has n nodes, $x=\alpha_1,\alpha_2,\ldots,\alpha_n$, $n\geq 2$. Then

$$\varphi''(x)=0\Longleftrightarrow m^2-(E-V(x))^2=0 \quad \text{or} \quad \varphi(x)=0,$$

   which means that

$$x=\alpha_1,\alpha_2,\ldots,\alpha_n \quad \text{or} \quad V^{-1}(E-m).$$

   We shall now study the concavity of φ over the interval (α_{n-1},∞): If $\varphi(x)>0$ on (α_{n-1},α_n), then φ must attain a maximum value at some $x_0\in(\alpha_{n-1},\alpha_n)$ and φ is concave on (α_{n-1},α_n). For $x>\alpha_n$, φ changes both its sign and concavity. Thus φ becomes convex and negative for $x>\alpha_n$. However, since α vanishes near ∞, then φ'' vanishes and changes its sign one more time somewhere after its last node. This implies that $V^{-1}(E-m)\in(\alpha_n,\infty)$, and therefore $\varphi''(x)<0$ for $x\in(\alpha_{n-1},\alpha_n)\cup(V^{-1}(E-m),\infty)$, and $\varphi''(x)>0$ for $x\in(\alpha_n,V^{-1}(E-m))$. By the same reasoning, if $\varphi(x)<0$ on (α_{n-1},α_n), then $\varphi''(x)>0$ for $x\in(\alpha_{n-1},\alpha_n)\cup(V^{-1}(E-m),\infty)$, and $\varphi''(x)<0$ for $x\in(\alpha_n,V^{-1}(E-m))$. □

Lemma 4. *The integral I defined in relation* (25) *is non-positive for any state φ.*

Proof. We first write eq. (20) as

$$(\varphi(x))E^2 - \big(2vf(x)\varphi(x)\big)E + \big(\varphi''(x) - m^2\varphi(x) + v^2f^2(x)\varphi(x)\big) = 0.$$

This is a quadratic equation in E, and we have

$$E = vf(x) \pm \frac{\sqrt{v^2f^2(x)\varphi^2(x) - (\varphi(x)\varphi''(x) - m^2\varphi^2(x) + v^2f^2(x)\varphi^2(x))}}{\varphi(x)}.$$

Then

$$E = vf(x) - \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}\,, \tag{26}$$

or

$$E = vf(x) + \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}\,. \tag{27}$$

In solution (26), φ'' cannot change its sign because if $\varphi''(x) < 0$, then

$$vf(x) - \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}} \leq -\sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}} < -m,$$

and we already know that $|E| < m$. Hence, since we have shown in lemmas 2 and 3 that φ'' changes its sign, then E can only take the second solution (27). Therefore, the relation (25) becomes:

$$I = \int_{-\infty}^{\infty} -(f_2(x) - f_1(x))\sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}\varphi^2(x)\mathrm{d}x \leq 0.$$

□

Theorem 5.

$$f_1(x) \leq f_2(x) \Rightarrow v_1 \leq v_2,$$

for all $x \in [0, \infty)$.

Proof. Consider the relation (24). If $E \geq 0$, then $E\langle f\rangle - v\langle f^2\rangle < 0$, and if $E < 0$, then using the relation (4) we also get the same result. Thus, the denominator of eq. (24) is negative for all $|E| < m$. Since we also proved in lemma 4 that $I \leq 0$, then $v_a \geq 0$ for all $a \in [0, 1]$ and $E \in (-m, m)$. This result completes the proof of the theorem. □

4.2 d-dimensional cases (d > 1)

In this section, we use the same reduced Klein-Gordon equation stated in (12), with φ satisfying $\varphi(0) = 0$ and the same normalization condition $\int_0^\infty \varphi^2(r)\mathrm{d}r = 1$. We assume the same conditions for the potential shape f as in sect. 2.2. This proof is not valid for the s-states of the 2-dimensional case, that is to say for $d = 2$ and $l = 0$. We shall prove this in the next section.

Lemma 5. *φ'' changes its sign at least once, for any state φ.*

Proof.

1) *φ is a node-free state:* $\varphi''(r) = 0 \iff m^2 - (E - V(r))^2 + \frac{Q}{r^2} = 0$, and near ∞, $\varphi'' = (m^2 - E^2)\varphi > 0$, which means that φ is convex near ∞. If φ is concave near 0, then the theorem is proved. If φ is convex near 0, then φ'' should change its sign at least at some solutions $\{r_1, r_2\}$, of the equation $m^2 - (E - V(r))^2 + \frac{Q}{r^2} = 0$, in order to be positive near ∞.
2) *φ has one node:* Suppose that φ has one node α, then $\varphi''(r) = 0 \iff r = \alpha$ or $r = r_1, r_2, \ldots, r_n$, where the $r_i's$ are roots of the equation $m^2 - (E - V(r))^2 + \frac{Q}{r^2} = 0$, $i = 1, \ldots, n$. We now study the sign of φ'' for $r > \alpha$: If $\varphi(r) > 0$, then, owing to the fact that φ vanishes at ∞, it should attain a maximum value over the interval (α, ∞) becoming concave near α^+. Similarly, we deduce that $\varphi''(r)$ should change its sign at least once over (α, ∞), implying that there exists $r_i \in (\alpha, \infty)$. If $\varphi(r) < 0$, then we can also prove this lemma by the same reasoning.

3) *φ has n nodes, $n \geq 2$:* Suppose that φ has n nodes, $\alpha_1, \alpha_2, \ldots, \alpha_n$ with $n \geq 2$.
Then $\varphi''(r) = 0 \Longleftrightarrow m^2 - (E - V(r))^2 + \frac{Q}{r^2} = 0$ or $\varphi = 0$, which means: $r = \alpha_1, \alpha_2, \ldots, \alpha_n, r_1, r_2, \ldots, r_n$, where the $r_i's$ are the solutions of the equation

$$m^2 - (E - V(r))^2 + \frac{Q}{r^2} = 0, \quad i = 1, 2, \ldots, n.$$

We study the concavity of φ over the interval (α_{n-1}, α_n):
If there exists some $r_i \in (\alpha_{n-1}, \alpha_n)$, then φ'' changes its sign at least once over (α_{n-1}, α_n).
If there is not any inflection point of α between α_{n-1} and α_n, then φ'' does not change its sign on (α_{n-1}, α_n); however, since φ vanishes at ∞, then there must be at least one inflection point $r_i \in (\alpha_{n-1}, \alpha_n)$, which means that φ changes its concavity at least once over (φ_{n-1}, ∞). □

Lemma 6. *The integral I defined in relation* (25) *is non-positive for any state φ and for all $d > 1$, except for the s-states of $d = 2$, that is: when $d = 2$ and $l = 0$.*

Proof. The expression (20), written as

$$(\varphi(r))E^2 - (2vf(r)\varphi(r))E + \left(\varphi''(r) - m^2\varphi(r) + v^2 f^2(r)\varphi(r) - \frac{Q}{r^2}\varphi(r)\right) = 0,$$

is a quadratic equation in E.

Thus,

$$E = vf(r) \pm \sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}\,.$$

If $\varphi''(r) < 0$, then $vf(r) - \sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}} < -m$, which means that E cannot take this value since $|E| < m$. Hence,

$$E = vf(r) + \sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}\,. \tag{28}$$

Using relation (28) in (25) we get:

$$I = -\int_0^\infty (f_2(r) - f_1(r))\sqrt{m^2 + \frac{Q}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}\varphi^2(r)\mathrm{d}r \leq 0.$$

□

Theorem 6.

$$f_1(r) \leq f_2(r) \Longrightarrow v_1 \leq v_2,$$

for all $r \in [0, \infty)$ and $d > 1$, except for the s-states for $d = 2$, that is, when $d = 2$ and $l = 0$.

Proof. Same proof as theorem 5. □

4.3 S-states for the 2-dimensional case

The reduced Klein-Gordon equation in this case reads

$$\varphi''(r) = \left[m^2 - (E - V(r)^2) - \frac{1}{r^2}\right]\varphi(r).$$

Thus $E = vf(r) \pm \sqrt{m^2 - \frac{1}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}$. Eliminating the solution $E = vf(r) - \sqrt{m^2 - \frac{1}{r^2} - \frac{\varphi''(r)}{\varphi(r)}}$ fails because of the existence of the term $-\frac{1}{r^2}$, and consequently, the proof of theorem 0.3.1 is not valid. Thus, we use the non-reduced form of the Klein-Gordon radial equation, namely

$$R''(r) + \frac{d-1}{r}R'(r) = \left[m^2 - (E - V(r))^2 + \frac{l(l+d-2)}{r^2}\right]R(r),$$

where $d = 2$, $l = 0$, and $\int_0^\infty R^2(r)\mathrm{d}r = 1$. Hence,

$$R''(r) + \frac{1}{r}R'(r) = \left[m^2 - (E - V(r))^2\right] R(r). \tag{29}$$

We assume that $V = vf$, with f satisfying the same conditions of sect. 0.3.1.

Define the symmetric operator

$$K = -\frac{\partial^2}{\partial r^2} - \frac{\partial}{\partial r} + 2Evf - v^2 f^2.$$

Then

$$\langle K \rangle = E^2 - m^2. \tag{30}$$

Differentiating (30) with respect to the parameter a we get

$$\langle R_a, KR\rangle + \langle R, K_a R\rangle + \langle R, KR_a\rangle = 0, \tag{31}$$

where $K_a = \frac{\partial K}{\partial a}$.

But

$$\frac{\partial}{\partial a}\left[\int_0^\infty R^2(r)\mathrm{d}r\right] = 2\int_0^\infty R(r)\frac{\partial R(r)}{\partial a} = 0.$$

Then we obtain the orthogonality relation $\langle R, R_a\rangle = \langle R_a, R\rangle = 0$.

Therefore, $\langle R_a, KR\rangle = \langle R, KR_a\rangle = (E^2 - m^2)\langle R, R_a\rangle = 0$, with $R_a = \frac{\partial R}{\partial a}$. We also have $K_a = 2Ev_a f + 2Ev(f_2 - f_1) - 2vv_a f^2 - 2v^2 f(f_2 - f_1)$, where $v_a = \frac{\partial v}{\partial a}$.

Thus, using K_a in eq. (31) we obtain

$$v_a = \frac{v\left[\int_0^\infty (f_2(r) - f_1(r))\,(vf(r) - E)R^2(r)\right]}{E\langle f\rangle - v\langle f^2\rangle}. \tag{32}$$

Writing eq. (29) as

$$(R(r))E^2 - 2(vf(r)R(r))E + \left(R''(r) + \frac{1}{r}R'(r) + v^2 f^2(r)R(r) - m^2 R(r)\right) = 0,$$

we obtain a quadratic equation of E. Thus

$$E = vf(r) \pm \sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}. \tag{33}$$

Lemma 7. *There exists an interval $J \subset [0,\infty)$ such that* $-\frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)} > 0$.

Proof.

1) *R is a node-free state:*

$$R''(r) = 0 \iff m^2 - (E - V(r))^2 - \frac{R'(r)}{rR(r)} = 0 \iff V(r) = E \pm \sqrt{m^2 - \frac{R'}{rR(r)}}.$$

If R is decreasing near 0, then $-\frac{R'(r)}{rR(r)} > 0$ near 0.

If R is increasing near 0, then it must attain a maximum value at some $r_0 \in [0,\infty)$ and end up decreasing since $\lim_{r\to\infty} R(r) = 0$. Thus, $-\frac{R'}{rR(r)} > 0$ on (r_0,∞).

Hence, in both cases R must be decreasing on a subset (r_0,∞) of $[0,\infty)$, and $\sqrt{m^2 - \frac{R'(r)}{rR(r)}} > m$ on this subset interval.

Therefore, V cannot take the value $E + \sqrt{m^2 - \frac{R'(r)}{rR(r)}}$ since V is non-positive and

$$R''(r) = 0 \iff V(r) = E - \sqrt{m^2 - \frac{R'(r)}{rR(r)}}. \tag{34}$$

Let r_i be a root of eq. (34).

If $r_i \in (r_0,\infty)$, then $J = (r_0, r_i)$.

If $r_i \notin (r_0,\infty)$, then there must exist at least another inflection point $r_j \in (r_0,\infty)$ because R vanishes at infinity, which also implies that $R > 0, R' < 0$, and $R'' < 0$ on (r_0, r_j). Therefore, $J = (r_0, r_j)$.

2) *R is an excited state:* Suppose that R has n nodes $\alpha_1, \alpha_2, \ldots, \alpha_n$ and consider the interval (α_n, ∞). Then

$$R'' = 0 \iff m^2 - (E - V(r))^2 - \frac{R'(r)}{rR(r)} = 0. \tag{35}$$

If R is increasing near α^+, then it should attain a maximum value at some $r_0 \in (\alpha_n, \infty)$, become decreasing, and change its concavity at $r_i \in (r_0, \infty)$, where r_i is a root of eq. (35), since $\lim_{x\to\infty} R(r) = 0$. Hence, $R > 0$, $R' < 0$, and $R'' < 0$ on (r_0, r_i) and therefore $J = (r_0, r_i)$.
If R is decreasing near α^+, then by the same reasoning we conclude that $R < 0$, $R' > 0$, and $R'' > 0$ on (r_0, r_i) and $J = (r_0, r_i)$. □

Since we have proven the existence of an interval J such that $-\frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)} > 0$, and since $|E| < m$, then the option $E = vf(r) - \sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}$ in expression (33) is falsified.

Therefore

$$E = vf(r) + \sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}. \tag{36}$$

Theorem 7.

$$f_1(r) \le f_2(r) \Longrightarrow v_1 \le v_2,$$

for all $r \in [0, \infty)$.

Proof. Using expression (36) in eq. (32) we get

$$v_a = \frac{-v\int_0^\infty \left[(f_2(r) - f_1(r))\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}R^2(r)\right] \mathrm{d}r}{\int_0^\infty f(r)\left[\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}R^2(r)\right] \mathrm{d}r} > 0.$$

Hence, the proof is complete. □

5 Square-well spectral bounds for general bounded potential shapes

In this section we exhibit a complete recipe for finding square-well potential bounds for any *bounded* potential shape f in the class considered in the previous sections, and consequently, spectral bounds for the coupling v, provided the energy is fixed. We have chosen the square-well potential because we know the analytical solution for the Klein-Gordon problem with this potential. Before showing this solution, we state the following lemma.

Lemma 8. *Consider the d-dimensional Klein-Gordon equation ($d \ge 1$)*

$$\varphi''(r) = \left[m^2 - (E - V(r))^2 + \frac{Q}{r^2}\right]\varphi(r), \tag{37}$$

where $V(r) = vf(r)$ and f belongs to the class of potential shapes defined in the previous sections. We define $s > 0$ and E_1 to be the new energy corresponding to the potential $V_1(r) = v(f(r) - s)$. Then $|E + vs| < m$ and $E_1 = E - vs$.

Proof. For $r \to +\infty$, the Klein-Gordon equation becomes $\varphi''(r) = [m^2 - (E + vs)^2]\varphi(r)$; thus, $\varphi(r) = C_1 e^{kr} + C_2 e^{-kr}$ with $k = \sqrt{m^2 - (E + vs)^2}$. Since φ vanishes at ∞, then $C_1 = 0$, and since $\varphi \in L^2(\mathbb{R})$, then $|E + vs| < m$. Moreover, we can write (37) as $\varphi''(r) = [m^2 - (E - vs - V(r) + vs)^2 + \frac{Q}{r^2}]\varphi(r) = [m^2 - (E - vs - v(f(r) - vs))^2 + \frac{Q}{r^2}]\varphi(r) = [m^2 - ((E - vs) - V_1(r))^2 + \frac{Q}{r^2}]\varphi(r)$. Therefore, $E_1 = E - vs$. □

5.1 A compact recipe for general spectral bounds

Consider an attractive potential $V(r) = vf(r)$, where f is a bounded potential shape in the class defined in the previous sections. We want to find the best square-well spectral bounds for the graph $v = G(E)$. We define the downward vertically-shifted square-well potential

$$g(r, t_1) = \begin{cases} f(0), & r \le t_1, \\ f(t_1), & \text{elsewhere}, \end{cases}$$

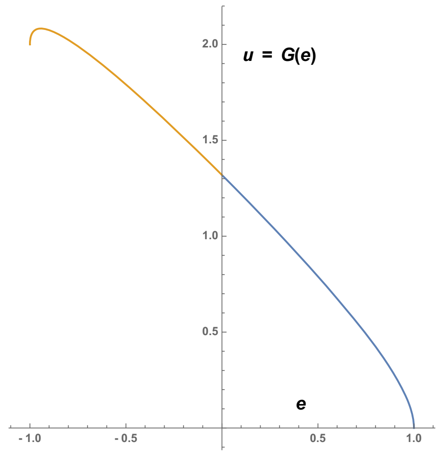

Fig. 3. *u versus e*.

with $s > 0$, and the square-well potential

$$g(r,t_2) = \begin{cases} f(t_2), & r \leq t_2, \\ 0, & \text{elsewhere.} \end{cases}$$

Thus, $g(r,t_1) \leq f(r) \leq g(r,t_2)$ for all $r \geq 0$, and for each pair of contact points $\{t_1, t_2\}$. We observe that $f(r)$ has infinite families of lower and upper bounds $G_L^{(t_1)}(E) \leq G(E) \leq G_U^{(t_2)}(E)$, where $G_L^{(t_1)}(E)$ and $G_U^{(t_2)}(E)$ are the respective spectral functions $v_L(E)$ and $v_U(E)$. The final step is to optimize over the parameter t in order to obtain the best square-well spectral bounds for $G(E)$, that is

$$G_L(E) = \max_{t_1>0} G_L^{(t_1)}(E) \leq G(E) \leq G_U(E) = \min_{t_2>0} G_U^{(t_2)}(E). \tag{38}$$

These functions are extracted from the eigenvalue equations (15) and (16) for the one-dimensional case, and from (18) and (19) in the higher dimensional cases. For example, we consider a square-well potential with depth A and semi-width b in dimension $d = 1$. Define the new variables $e = Eb$, $u = Ab$, $\mu = mb$, and $t = b[(E+A)^2 - m^2]^{\frac{1}{2}}$. Then from eq. (15) the ground state solution becomes:

$$e(t) = \pm\big[\mu^2 - (t \cdot \tan(t))^2\big]^{\frac{1}{2}} \quad \text{and} \quad u(t) = (t^2 + \mu^2)^{\frac{1}{2}} - e(t).$$

For definiteness, we now assume $\mu = 1$. We observe that $e = 0$ when $t = t_0 \approx 0.860334$. The graph depicting $u = G(e)$ is shown in fig. 3.

5.2 The Woods-Saxon potential in 1 dimension

We consider the Woods-Saxon potential $V(x) = vf(x)$, where $f(x) = -1(1 + e^{\frac{(|x|-1)}{q}})^{-1}$, and $q > 0$ is a range parameter. We are interested in finding an upper bound and a lower bound for the coupling constant v, for any given value of $|E| < m$ and for $q = 0.005$. Since the Klein-Gordon equation with the square-well potential had been solved analytically, we use a square-well potential as an upper bound for f, and another downward vertically-shifted square-well as a lower bound. We define the functions

$$g_u(x, 0.9675) = \begin{cases} -0.9984, & |x| \leq 0.9675, \\ 0, & \text{elsewhere,} \end{cases}$$

and

$$g_l(x, 1.03) = \begin{cases} -1.001, & |x| \leq 1.03, \\ -0.0025, & \text{elsewhere.} \end{cases}$$

Since $f_l(x) \leq f(x) \leq f_u(x)$ for all $x \in (-\infty, +\infty)$, then according to theorem 5, we conclude that $G_L(E) = v_l \leq v \leq G_U(E) = v_u$, where v_l and v_u are the respective couplings for f_l and f_u. For example, if we fix $E = -0.512574196$, we get $v_u = 1.81478$ and $v_l = 1.79017$. Hence we conclude that $1.79017 \leq v \leq 1.81478$. This result has been verified numerically, using our own shooting method realized in Maple, and with which we find $v = 1.80494$. In figs. 4 to 6 we exhibit spectral curves for the Woods-Saxon potential in vertical sequence, square-well lower bound, numerical approximation, square-well upper bound.

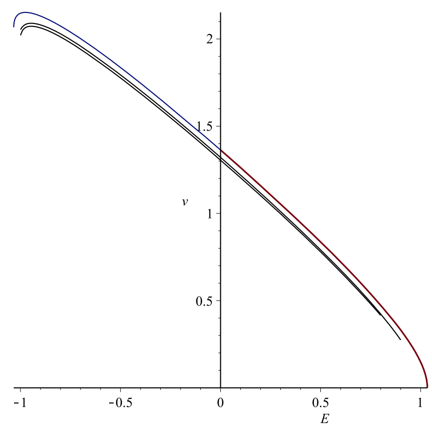

Fig. 4. Graphs for v_l, v, and v_u *versus* E for $-1 < E < 1$.

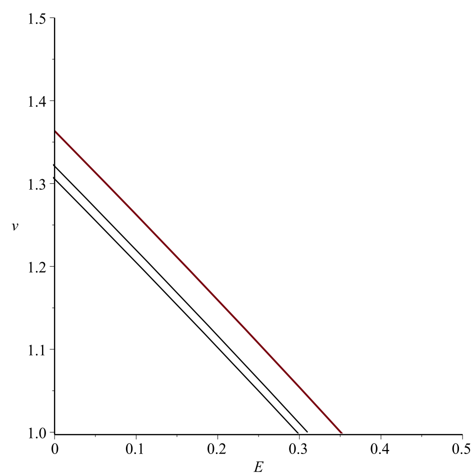

Fig. 5. Graphs for v_l, v, and v_u *versus* E for $0 < E < 0.5$.

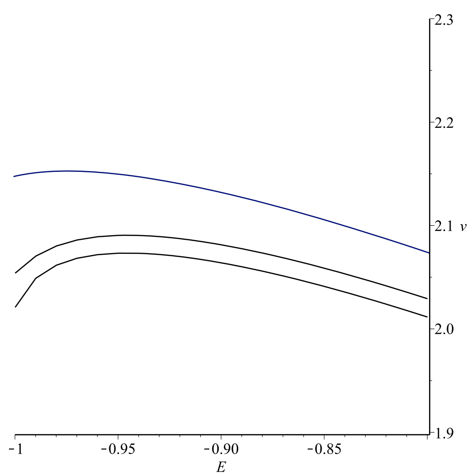

Fig. 6. Graphs for v_l, v, and v_u *versus* E for $-1 < E < -0.8$.

6 Conclusion

The radial reduced eigenequations for a one-particle potential model might in suitable units be written, for the non-relativistic and Klein-Gordon cases, respectively, as

– (NR)
$$\varphi''(r) = \left[(2m)(v\, f(r) - E) + \frac{Q}{r^2}\right]\varphi(r);$$
– (KG)
$$\varphi''(r) = \left[m^2 - (E - v\, f(r))^2 + \frac{Q}{r^2}\right]\varphi(r),$$

where $Q = \frac{1}{4}(2l + d - 1)(2l + d - 3)$, the potential has shape $f(r) < 0$ and coupling parameter $v > 0$. We note that a slightly different formulation of the Klein-Gordon equation is required if $d = 2$ and $\ell = 0$. By familiarity with well-known Schrödinger examples, or by a variational analysis of them we expect, for suitable $v > v_0 > 0$, to find bound states with nonrelativistic energies $E(v)$ having monotonic behaviour $E'(v) < 0$ if the potential shape $f(r)$ is negative. However, these assumptions are not correct for the corresponding Klein-Gordon eigenvalues. This makes it difficult to design physically realistic potential models for relativistic problems.

In this paper, we first represent the relation between the coupling v and a discrete Klein-Gordon eigenvalue E by writing v as a function $v = G(E)$ of E for $-m < E < m$. We show generally that the spectral curve $v = G(E)$ is concave, and at most unimodal with a maximum close to $E = -m$. For the purpose of comparing the spectral implications of a change in the potential shape, a bridging parameter $a \in [0, 1]$ is introduced such that $f = f_1 + a(f_2 - f_1)$. By studying the dependence of v on a for each fixed value of E, we establish the comparison theorem $f_1 \le f_2 \Longrightarrow G_1(v) \le G_2(v)$. These results are valid for all negative and positive eigenenergies, and for both ground and excited states. They allow us to devise spectral approximations in much the same way as is possible for the corresponding Schrödinger problem where the discrete spectrum can be defined variationally and the concomitant comparison theorems follow almost automatically by means of variational arguments. As an illustration, we are able to use the exact solution of the square-well problem to construct upper and lower bounds for the discrete Klein-Gordon spectrum generated by any given member of the class of bounded negative potentials that we have considered in the present study.

Partial financial support of his research under Grant No. GP3438 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

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Appendix B

Submitted Paper

Refining the General comparison theorem for the Klein–Gordon equation

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We exhibit a simpler condition for our Klein–Gordon comparison theorem $f_1 \leq f_2 \implies G_1(E) \leq G_2(E)$, where f_1 and f_2, defined as two monotone non-decreasing functions on $[0, \infty)$, are the shapes of two symmetric central potentials V_1 and V_2, and $v_1 = G_1(E)$ and $v_2 = G_2(E)$ are their corresponding coupling parameters that are functions of the eigen-energy $E \in (-m, m)$. We weaken the condition for the ground states by proving that if $\int_0^x \left[f_2(t) - f_1(t)\right]\varphi_i(t)dt \geq 0$, the corresponding coupling parameters remain ordered, where $\varphi_i = 1, \varphi_1$, or φ_2, φ_1 and φ_2 being the bound state solutions of the Klein–Gordon equation with potentials V_1 and V_2 respectively. These results are valid for any energy $E \in (-m, m)$, but they are restricted to the ground state.

Keywords: Klein–Gordon equation, potential function, refined comparison theorem.

I. INTRODUCTION

The elementary comparison theorem of non-relativistic quantum mechanics states that if two potentials are ordered, then the respective discrete energies are correspondingly ordered. This theorem is valid in the Schrödinger case since it is a direct result of the min-max variational principle, as the Hamiltonian $H = -\Delta + V$ is bounded from below [1]. It is important because it provides lower and upper bounds for the energy-eigenvalues in other unsolved Klein–Gordon equations.
However, this principle is no more valid in the simple form in the relativistic case because the energy operators are not bounded from below [2], [3], [4]. Counter examples in the square well and the exponential potentials are found in Greiner [5], as well as the cut off Coulomb potential [6]. Thus several comparison theorems were established [7], [8], [9], [10], but those related to the Klein–Gordon equation were all restricted to positive energies.

In our previous paper we were able to generalize these comparison theorems by studying the eigen-values in the coupling parameter, which are single-valued in the Klein–Gordon equation, in order to avoid two-valued spectral functions $E(v)$.

We consider the Klein–Gordon relativistic equation with a central attractive potential $V(x) = vf(x)$, for which a single potential moves in. We proved in our previous paper [11] that if two potential shapes are ordered, $f_1(x) \leq f_2(x)$, then the corresponding spectral curves are similarly ordered. We were able to establish this theorem after presenting $v = G(E)$ to be dependent on the eigen-energy $E \in (-m, m)$, so that we obtain a function $v(E)$, rather than a two-valued expression $E(v)$. In this paper we refine the condition for this theorem for ground states by proving that the ordering of the coupling parameters is still preserved for the ground state, even if the potential shapes cross over, as long as $\int_0^x \left[f_2(t) - f_1(t)\right]dt \geq 0$. Moreover, if one of the wave functions φ_1 or φ_2 is known, we prove that $\int_0^x \left[f_2(t) - f_1(t)\right]\varphi_i(t)dt \geq 0 \implies G_1(E) \leq G_2(E)$, $i = 1, 2$. This is a stronger version of the latter theorem because since the ground state is non-increasing on $[0, \infty)$, this allows the potential

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shapes to cross over even more with the ordering of couplings is still preserved. The idea of refining the comparison theorems of non-relativistic and relativistic quantum mechanics has been first presented by Hall [12], and was applied for the Dirac equation [13], [14], and the Klein–Gordon equation [15], but the latter case was restricted to non-negative energies. The corresponding results are obtained for all dimensions $d \geq 1$.

II. REFINED THEOREMS.

A. One dimensional case

The Klein–Gordon equation in one dimension is given by:

$$\varphi''(x) = \left[m^2 - \left(E - V(x)\right)^2\right]\varphi(x), \quad x \in \mathbb{R}. \tag{1}$$

where φ'' denotes the second order derivative of φ with respect to x, natural units $\hbar = c = 1$ are used, and E is the energy of a spinless particle of mass m. We suppose that the potential function V is expressed as $V(x) = vf(x)$ with $v > 0$ and f satisfies the following conditions:

1. $V(x) = vf(x), x \in \mathbb{R}$, where $v > 0$ is the coupling parameter and $f(x)$ is the potential shape;
2. f is even $f(x) = f(-x)$;
3. f is not identically zero, and is non-positive, that is $f(x) \leq 0$;
4. f is attractive, that is f is monotone non-decreasing over $[0, \infty)$;
5. f vanishes at infinity, i.e $\lim\limits_{x\to\pm\infty} f(x) = 0$.

We also assume that $V(x) = vf(x)$ is in this class $\mathcal{P}$ of potentials, for which the Klein–Gordon equation (1) has at least one discrete eigenvalue E, and that equation (1) is the eigen-equation for the eigenstates. Because of condition 5, equation (1) has the asymptotic form

$$\varphi'' = (m^2 - E^2)\varphi,$$

at infinity, with solutions $\varphi(x) = C_1 e^{\sqrt{k}|x|} + C_2 e^{-\sqrt{k}|x|}$, where C_1 and C_2 are constants of integration, and $k = m^2 - E^2$. The radial wave function of φ vanishes at infinity; thus, $C_1 = 0$. Since $\varphi \in L^2(\mathbb{R})$, then $k > 0$ which means that

$$|E| < m. \tag{2}$$

Suppose that $\varphi(x)$ is a solution of (1). Then by direct substitution we conclude that $\varphi(-x)$ is another solution of (1). Thus, by using linear combinations, we see that all the solutions of this equation may be assumed to be either even or odd. Hence, if φ is even then $\varphi'(0) = 0$, and if φ is odd then $\varphi(0) = 0$. Since $\varphi \in L^2(\mathbb{R})$ then $\int_{-\infty}^{+\infty} \varphi^2 dx < \infty$. This means that the wave functions can be normalized and consequently we shall assume that φ satisfies the normalization condition

$$||\varphi||^2 = \int_{-\infty}^{\infty} \varphi^2(x)dx = 1. \tag{3}$$

Lemma II.1.

$$E\int_0^\infty f(x)\varphi^2(x)dx \, < \, v\int_0^\infty f^2\varphi^2(x)dx, \quad \forall\, |E| \, < m. \tag{4}$$

Proof. Expanding equation (1) we get:

$$\varphi''(x) = (m^2 - E^2)\varphi(x) + 2Evf(x)\varphi(x) - v^2 f^2(x)\varphi(x).$$

Multiplying both sides by φ and integrating over $[0,+\infty)$ we obtain:

$$\int_0^\infty \varphi''(x)\varphi(x)dx = m^2 - E^2 + 2Ev\int_0^\infty f\varphi^2(x)dx - v^2\int_0^\infty f^2\varphi^2(x)dx.$$

After applying integration by parts and using the fact that $(\varphi\varphi')\Big|_0^\infty = 0$ for any φ, the left-hand side of the last equation becomes $-\displaystyle\int_0^\infty \big(\varphi'(x)\big)^2 dx$. Thus

$$2E\int_0^\infty f(x)\varphi^2(x)dx - v\int_0^\infty f^2\varphi^2(x)dx = -\int_0^\infty \big(\varphi'(x)\big)^2 dx + E^2 - m^2 < 0.$$

1. If $E \geq 0$, then the result follows immediately;
2. If $E < 0$, then

$$E\int_0^\infty f(x)\varphi^2(x)dx < 2E\int_0^\infty f(x)\varphi^2(x)dx,$$

and we get the desired result.

□

We now define the operator K as:

$$K = -\frac{\partial^2}{\partial x^2} + 2Evf - v^2 f^2. \tag{5}$$

If φ is solution of the Klein–Gordon equation (1), then we have:

$$K\varphi = (E^2 - m^2)\varphi, \tag{6}$$

and it follows

$$\langle K\rangle = \langle \varphi, K\varphi\rangle = \langle \varphi, (E^2 - m^2)\varphi\rangle = E^2 - m^2. \tag{7}$$

We observe that the domain of K is $D_K = H^2(\mathbb{R})$, where $H^2(\mathbb{R})$ is the Sobolev space defined as follows:

$$H^2(\mathbb{R}) = \{\varphi \in L^2(\mathbb{R}) : \varphi', \varphi'' \in L^2(\mathbb{R})\}.$$

Since $||K\varphi|| = |E^2 - m^2| \cdot ||\varphi|| \leq m^2||\varphi||$ for all $\varphi \in D_K$, then K is a bounded operator. This implies that K is continuous. We also observe that K is symmetric, that is to say: $\langle \varphi, K\psi\rangle = \langle K\varphi, \psi\rangle$.

We now consider the parameter $a \in [0,1]$ and the two potential shapes f_1 and f_2 with $f = f(a,x) = f_1(x) + a\big[f_2(x) - f_1(x)\big]$, where $f_1 \leq f_2 \leq 0$. Hence f is non-positive, attractive, even, and vanishes at infinity. We note that $f(0,x) = f_1(x)$ when $a = 0$, and $a = 1$ when $f(1,x) = f_2(x)$, and

$$\frac{\partial f}{\partial a} = f_2(x) - f_1(x) \geq 0. \tag{8}$$

Hence, f is monotone non-decreasing in the parameter a. Let v depend on a and E is be a constant, that is $v = v(a)$ and $\frac{\partial E}{\partial a} = 0$, and $-m < E < m$. We again consider the symmetric bounded operator K in (5), and we define φ_a to be the partial derivative of φ with respect to a. Differentiating equation (7) with respect to a we get:

$$\langle \varphi_a, K\varphi\rangle + \langle \varphi, K_a\varphi\rangle + \langle \varphi, K\varphi_a\rangle = 0 \tag{9}$$

Applying the partial derivative with respect to a to equation (3) and using the symmetry of K, we obtain the new orthogonality relation

$$\langle \varphi_a, K\varphi\rangle = \langle \varphi, K\varphi_a\rangle = (E^2 - m^2)\langle \varphi_a, \varphi\rangle = 0.$$

We also have:

$$K_a = 2Ev_a f + 2Ev(f_2 - f_1) - 2vv_a f^2 - 2v^2 f(f_2 - f_1), \tag{10}$$

with v_a defined as $\frac{\partial v}{\partial a}$. Equation (9) becomes:

$$Ev_a \int_0^\infty f\varphi^2(x)dx + Ev \int_0^\infty \Big(f_2(x) - f_1(x)\Big)\varphi^2(x)dx - vv_a \int_0^\infty f^2\varphi^2(x)dx$$
$$-v^2 \int_0^\infty f\Big(f_2(x) - f_1(x)\Big)\varphi^2(x)dx = 0.$$

This leads us to the following relation:

$$v_a = \frac{vI}{E\displaystyle\int_0^\infty f(x)\varphi^2(x)dx - v\int_0^\infty f^2\varphi^2(x)dx}, \tag{11}$$

where

$$I = \int_0^\infty \Big(f_2(x) - f_1(x)\Big)\Big(vf(x) - E\Big)\varphi^2(x)dx. \tag{12}$$

Lemma II.2. *The ground state eigenfunction φ of the Klein–Gordon equation is a non-increasing function for $x \in [0, \infty)$, and for any energy E such that $|E| < m$.*

Proof. Since φ is an even state, then $\varphi'(0) = 0$, and since [11] φ is concave on $\big[0, V^{-1}(E - m)\big)$ and convex on $\big[V^{-1}(E - m), \infty\big)$, then $\varphi'(x) \le 0, \quad x \in [0, \infty)$. □

Theorem II.1. *For any two potentials f_1, $f_2 \in \mathcal{P}$ we have:*

$$\mu(x) = \int_0^x [f_2(t) - f_1(t)]dt \ge 0 \quad x \in [0, \infty) \implies G_1(E) \le G_2(E), \tag{13}$$

for any ground state energy E.

Proof. Applying integration by parts to (12) we get

$$I = (vf(x) - E)\varphi^2(x)\mu(x)\Big|_0^\infty - \int_0^\infty \big[vf'(x)\varphi^2(x) + 2(vf(x) - E)\varphi(x)\varphi'(x)\big]\mu(x)dx.$$

Regarding that $\lim_{x\to\infty} \varphi(x) = 0$ and $\mu(0) = 0$, we get

$$I = -\int_0^\infty \big[vf'(x)\varphi^2(x) + 2(vf(x) - E)\varphi(x)\varphi'(x)\big]\mu(x)dx.$$

Since [11]

$$E = vf(x) + \sqrt{m^2 - \frac{\varphi''(x)}{\varphi(x)}}, \tag{14}$$

$\varphi'(x) \le 0$, and

$$f'(x) = \frac{\partial f}{\partial x} = (1 - a)f_1'(x) + af_2'(x) \ge 0,$$

then, $I \le 0$.
Therefore, following **Lemma I.1.** $v_a \ge 0$, and the theorem is proven. □

This theorem allows us to say that graphs of f_1 and f_2 cross over in such a way that preserves the positivity of $\mu(x)$, then the corresponding coupling constants are ordered as $v_1 \le v_2$ for each $E \in (-m, m)$.

We now state a stronger version of the above theorem, which can be applied in case we know one of the ground states φ_1 or φ_2:

Theorem II.2. *For any potentials $f_1,\ f_2 \in \mathcal{P}$ we have:*

$$\rho(x) = \int_0^x [f_2(t) - f_1(t)]\varphi_j(t)dt \ge 0 \quad x \in [0, \infty) \implies G_1(E) \le G_2(E),$$

for $j = 1, 2$ and for any ground state energy E.

Proof. Suppose, *w.l.g*, that $j = 1$. Applying the operator $\frac{\partial}{\partial a}$ to the expression

$$K\varphi = (E^2 - m^2)\varphi \tag{15}$$

we get

$$K_a\varphi + K\varphi_a = (E^2 - m^2)\varphi_a, \tag{16}$$

where $\varphi_a = \dfrac{\partial \varphi}{\partial a}$.
We then multiply (16) by φ_1 and apply the inner product to get

$$\langle \varphi_1, K_a\varphi\rangle = -\langle \varphi_1, K\varphi_a\rangle + \langle (E^2 - m^2)\varphi_1, \varphi_a\rangle,$$

which implies that

$$\langle \varphi_1, K_a\varphi\rangle = -\langle \varphi_1, K\varphi_a\rangle + \langle K\varphi_1, \varphi_a\rangle. \tag{17}$$

Since K is symmetric, then $\langle \varphi_1, K\varphi_a\rangle = \langle K\varphi_1, \varphi_a\rangle$. Then relation (17) becomes

$$\langle \varphi_1, K_a\varphi\rangle = 0. \tag{18}$$

Using (10) we obtain

$$v_a = \frac{v\,\langle \varphi_1, (f_2 - f_1)(vf - E)\varphi\rangle}{\langle \varphi_1, f(E - vf)\varphi\rangle}. \tag{19}$$

Using (14) we observe that the denominator of (19) is negative. Applying integration by parts to the numerator changes it into

$$\big(vf(x) - E\big)\varphi(x)\rho(x)\Big|_0^\infty - \int_0^\infty \big[vf'(x)\varphi(x) + \big(vf(x) - E\big)\varphi'(x)\big]\rho(x)dx. \tag{20}$$

Since $\lim_{x\to\infty}(x) = 0$ and $\rho(0) = 0$ then (20) becomes

$$-\int_0^\infty \Big[vf'(x)\varphi(x) + \big(vf(x) - E\big)\varphi'(x)\Big]\rho(x)dx \le 0.$$

Therefore $v_a \ge 0$ and the proof is complete. $\square$

B. d - dimensional cases ($d \ge 2$)

The Klein–Gordon equation in d dimensions is given by

$$\Delta_d\Psi(r) = [m^2 - (E - V(r))^2]\Psi(r),$$

where natural units $\hbar = c = 1$ are used and E is the discrete energy eigenvalue of a spinless particle of mass m. We suppose here that the vector potential function $V(r)$, $r = ||\mathbf{r}||$, is a radially-symmetric Lorentz vector potential (the time component of a space-time vector), which belongs to the class $\mathcal{P}_d$ with the following properties:

1. $V(r) = vf(r), r \in [0,\infty)$, where $v > 0$ is the coupling parameter and $f(r)$ is the potential shape;
2. f is not identically zero and non-positive;
3. f is attractive, that is f is monotone non-decreasing over $[0,\infty)$;
4. f is not more singular than $r^{-(d-1)}$, $r \in [0,\infty)$, that is $\lim_{r\to 0} r^{(d-2)} f(r) = A, \quad -\infty < A \leq 0$;
5. f vanishes at infinity, i.e $\lim_{r\to\infty} f(r) = 0$.

This is a wider potential class than $\mathcal{P}$, since it contains Coulomb and Coulomb - like potentials, such as the Yukawa and the Hulthén potentials. The operator Δ_d is the d-dimensional Laplacian. Hence, the wave function for $d > 1$ can be expressed as $\Psi(r) = R(r)Y_{l_{d-1},\ldots,l_1}(\theta_1, \theta_2, ..., \theta_{d-1})$, where $R \in L^2(\mathbb{R}^d)$ is a radial function and $Y_{l_{d-1},\ldots,l_1}$ is a normalized hyper-spherical harmonic with eigenvalues $l(l+d-1)$, $l = 0, 1, 2, ...$ [16] The radial part of the above Klein–Gordon equation can be written as:

$$\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}R(r)\right) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{l(l+d-2)}{r^2}\right]R(r),$$

where R satisfies the second-order linear differential equation

$$R''(r) + \frac{d-1}{r}R'(r) = \left[m^2 - \big(E - V(r)\big)^2 + \frac{l(l+d-2)}{r^2}\right]R(r). \tag{21}$$

Since V vanishes at ∞, then equation (21) becomes

$$\varphi'' = (m^2 - E^2)\varphi$$

near infinity, which means that $|E| < m$. The normalization condition for bound states is

$$\int_0^\infty R^2(r) r^{d-1} dr = 1. \tag{22}$$

Differentiating (22) with respect to a we obtain the orthogonality relation $\langle R_a, R\rangle = \langle R, R_a\rangle = 0$. We also define $f(r,a) = af_1(r) + (1-a)f_2(r)$, $f_1, f_2 \in \mathcal{P}_d$, and we consider the operator

$$K = -\frac{\partial^2}{\partial r^2} - \frac{\partial}{\partial r} + 2Evf - v^2 f^2. \tag{23}$$

By the same reasoning for the one-dimensional case we obtain the relation

$$v_a = \frac{vI}{E\langle f\rangle - v\langle f^2\rangle},$$

where

$$I = \int_0^\infty \Big(f_2(r) - f_1(r)\Big)\Big(vf(r) - E\Big) r^{(d-1)} R^2(r) dr, \tag{24}$$

$\langle f\rangle = \int_0^\infty f(r)R^2(r)r^{d-1}dr$, and $\langle f^2\rangle = \int_0^\infty f^2(r)R^2(r)r^{d-1}dr$.
Using [11]

$$E = vf(r) + \sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}, \tag{25}$$

we get

$$v_a = \frac{vI}{\displaystyle\int_0^\infty \left[\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}R^2(r)\right] r^{d-1} f(r) dr}. \tag{26}$$

Lemma II.3. *The ground state eigenfunction of the Klein–Gordon equation is non-increasing for $r \in [0, \infty)$ and $|E| < m$.*

Proof. For $l = 0$, equation (21) can be written as

$$R'(r) = r^{-(d-1)} \int_0^r F(t)R(t)t^{d-1}dt \tag{27}$$

where

$$F(t) = m^2 - \big(E - vf(t)\big)^2.$$

Replacing E by the expression (25) and using this in $F'(t) = \frac{dG}{dt}$ we find

$$F'(t) = 2vf'(t)\big(E - vf(t)\big) = 2\left[\sqrt{m^2 - \frac{R''(t)}{R(t)} - \frac{R'(t)}{tR(t)}}\right] vf'(t) \geq 0.$$

Thus we have reached the same result as in [17], but extended to $|E| < m$. Hence, $R'(r) \leq 0$ for all $r \in [0, \infty)$ and $|E| < m$. □

Theorem II.3. *If f_1, $f_2 \in \mathcal{P}_d$ such that $(f_2 - f_1)$ has t^{d-1}-weighted area, then:*

$$\eta(r) = \int_0^r [f_2(t) - f_1(t)]t^{d-1}dt \geq 0 \quad r \in [0, \infty) \implies G_1(E) \leq G_2(E), \tag{28}$$

where E is the ground state energy.

Proof. Integrating (24) by parts we get

$$I = (vf(r) - E)R^2(r)\eta(r)\Big|_0^\infty - \int_0^\infty \Big[vf'(r)R^2(r) + 2\big(vf(r) - E\big)R(r)R'(r)\Big]\eta(r)dr.$$

Using $\lim_{x\to\infty} R(r) = 0$ and $\eta(0) = 0$ we obtain

$$I = -\int_0^\infty \Big[vf'(r)R^2(r) + 2\big(vf(r) - E\big)R(r)R'(r)\Big]\eta(r)dr.$$

Hence, relation (26) is non-negative and the theorem is proved. □

As in the one-dimensional case, we state a stronger version of the previous refining theorem:

Theorem II.4. *For any two potentials $f_1, f_2 \in \mathcal{P}_d$ we have:*

$$\sigma(r) = \int_0^r [f_2(t) - f_1(t)]t^{d-1}R_j(t)dt \geq 0 \quad r \in [0, \infty) \implies G_1(E) \leq G_2(E), \tag{29}$$

for $j = 1, 2$, where E is the ground state energy E.

Proof. In the same manner of the proof of the one-dimensional theorem we arrive to the following formula

$$v_a = \frac{v\langle R_1, (f_2 - f_1)(vf - E)R\rangle}{\langle R_1, f(E - vf)R\rangle}, \tag{30}$$

which is equal to

$$\frac{-\displaystyle\int_0^\infty \Big[vf'(r)R(r) + \big(vf(r) - E\big)R'(r)\Big]\sigma(r)dr}{\displaystyle\int_0^\infty R_1(r)\left[\sqrt{m^2 - \frac{R''(r)}{R(r)} - \frac{R'(r)}{rR(r)}}\right]R(r)r^{d-1}f(r)dr} \geq 0. \tag{31}$$

Hence we have reached our desired result. □

C. Sign of Coulomb-like energy eigenvalues in dimension $d \geq 3$

In this section we study the sign of the energy eigenvalues of a certain class of Coulomb-like potentials. We first apply the change of variable to $R(r) = r^{-\frac{d-1}{2}}\varphi(r)$ to (21), to obtain the following reduced second-order differential equation:

$$\varphi''(r) = \left[m^2 - \big(E - vf(r)\big)^2 + \frac{Q}{r^2}\right]\varphi(r), \tag{32}$$

where

$$Q = \frac{1}{4}(2l + d - 1)(2l + d - 3),$$

with $l = 0, 1, 2, \ldots$. The reduced wave function φ satisfies $\varphi(0) = 0$ and $\lim_{r\to\infty} \varphi = 0$ [18]. For bound states, the normalization condition is:

$$\int_0^\infty \varphi^2(r)dr = 1.$$

Theorem II.5. *Let $f \in \mathcal{P}_d$ such that $f(r) = -\frac{w(r)}{r}$ with $w(r)$ non-increasing, $w(0) \leq 1$, and $\lim_{r\to\infty} w(r) = 0$. Then the corresponding ground state energy E of equation (32) is positive for $v < \frac{d-2}{2}$.*

Proof. Multiplying equation (32) by φ and integrating over $[0, \infty)$ we get

$$-2Ev\left\langle f\right\rangle = \left\langle -\Delta\right\rangle + m^2 - E^2 + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle - v^2\left\langle f^2\right\rangle. \tag{33}$$

Using Hardy's inequality $\left(\langle -\Delta\rangle \geq \left\langle \frac{(d-2)^2}{4r^2}\right\rangle\right)$ ([19]), equation (33) becomes

$$-2Ev\left\langle f\right\rangle \geq \left\langle \frac{(d-2)^2}{4r^2}\right\rangle + m^2 - E^2 + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle - v^2\left\langle f^2\right\rangle.$$

Since $m^2 - E^2 > 0$ for all $E \in (-m, m)$ and $v < \frac{d-2}{2}$ then

$$-2Ev\left\langle f\right\rangle > \frac{(d-2)^2}{4}\left\langle \frac{1}{r^2} - f^2\right\rangle + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle \tag{34}$$

Replacing $f(r)$ by $\frac{w(r)}{r}$ and using $d \geq 3$ in (34) we conclude that

$$-2Ev\left\langle f\right\rangle > \frac{1}{4}\left\langle \frac{1 - w^2(r)}{r^2}\right\rangle + \left\langle \frac{(d-1)(d-3)}{r^2}\right\rangle \geq 0.$$

Hence, $E > 0$. $\square$

III. SPECTRAL BOUNDS FOR POTENTIAL SHAPES

A. Square-Well and Exponential for General Spectral Bounds for Potential Shapes

In this section we provide a method for finding the best lower and upper spectral bounds for any bounded potential shape f. We use the square-well potential and the exponential potential as a lower bound and an upper bound respectively. We have mentioned a similar idea in our previous paper [11] using square-well spectral bounds, but we were confined by the condition that the graphs cannot cross over. Since we have been able to refine our previous comparison theorem, we can find better bounds now. We have chosen the square-well and the exponential potentials because we know the exact solutions of the Klein–Gordon equation with each of these potentials [20],[21], [11].

Consider an attractive potential $V \in \mathcal{P}$ such that $V(r) = vf(r)$. Let $V_1(r) = v_1 f_1(r)$ be the square-well potential such that

$$f_1(x) = \begin{cases} f(0), & |x| \le t \\ 0, & \text{elsewhere} \end{cases},$$

with

$$\int_0^t \big(f(r) - f_1(r)\big)dr > 0,$$

and

$$\int_0^\infty \big(f(r) - f_1(r)\big)dr = 0.$$

We also consider the exponential potential $V_2(r) = v_2 f_2(r)$ with $f_2(r) = -e^{-qr}$, $q > 0$, which intersects with f at $r = \alpha$ such that

$$\int_0^\alpha \big(f_2(r) - f(r)\big)dr > 0,$$

and

$$\int_0^\infty \big(f_2(r) - f(r)\big)dr = 0.$$

Hence, for any eigenenergy $E \in (-m, m)$ we have $G_L(E) \le G(E) \le G_U(E)$ where G_L, G, and G_U are the respective graphs of the spectral functions $v_1(E), v(E)$, and $v_U(E)$ respectively.

Applications

1. Let $V(x) = vf(x)$ be the Gaussian potential where $f(x) = -e^{-qx^2}$, and $q > 0$ is a range parameter. We want to find a lower and an upper bound for the coupling constant v, for any given eigenenergy $E \in (-m, m)$ and $q = -0.8$. We choose the square-well potential $V_1(x) = v_1 f_1(x)$ and the exponential potential $V_2(x) = v_2 f_2(x)$ with

$$f_1(x) = \begin{cases} -1, & |x| \le \frac{\sqrt{5\pi}}{4} \\ 0, & \text{elsewhere} \end{cases},$$

and

$$f_2(x) = -e^{-\frac{4}{\sqrt{5\pi}}x}.$$

We have $\int_0^{\frac{\sqrt{5\pi}}{4}} \big(f(x) - f_1(x)\big)dx \approx 0.20816$ and $\int_0^\infty \big(f(x) - f_1(x)\big)dx = 0$(**fig.**1). On the other hand, f and f_2 cross over at $x_0 \approx 0.8$ (**fig.**2) with $\int_0^{x_0} \big(f_2(x) - f(x)\big)dx \approx 0.15253$ and $\int_0^\infty \big(f_2(x) - f(x)\big)dx = 0$. We fix $E = -0.0377$ and we deduce that $v_1 \le v \le v_2$ where $v_1 = 1.36$ and $v_2 = 1.9$. We have numerically verified this result by using our own shooting method realized in Maple, and with which we find $v = 1.581$. The graphs of $v_1(E), v(E)$, and $v_2(E)$ are shown in figure (3).

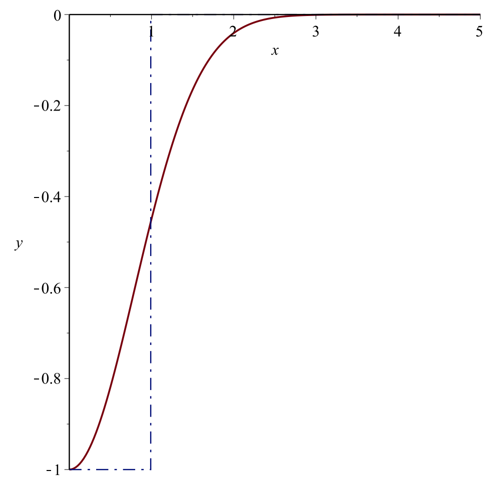

Figure 1: Potential Shapes $f_1(x) = -1$ if $|x| \leq \frac{\sqrt{5\pi}}{4}$ and 0 elsewhere, dashed lines and $f(x) = -Ae^{-qx^2}$ full line, where $A = 1$ and $q = 0.8$ were applied.

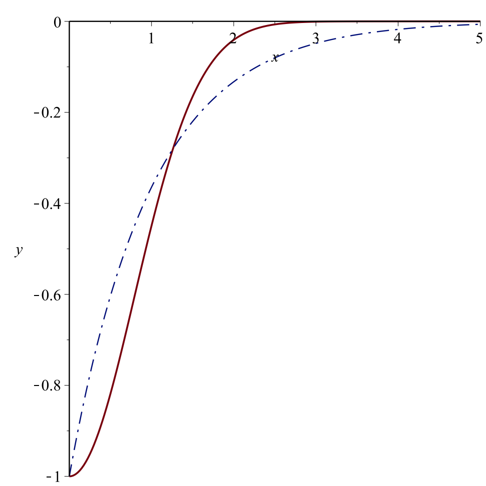

Figure 2: Potential Shapes $f(x) = -Ae^{-qx^2}$ dashed lines and $f_2(x) = -Be^{-ax}$ full line, where $q = 0.8$, $a = \frac{4}{\sqrt{5\pi}}$, and $A = B = 1$ were applied.

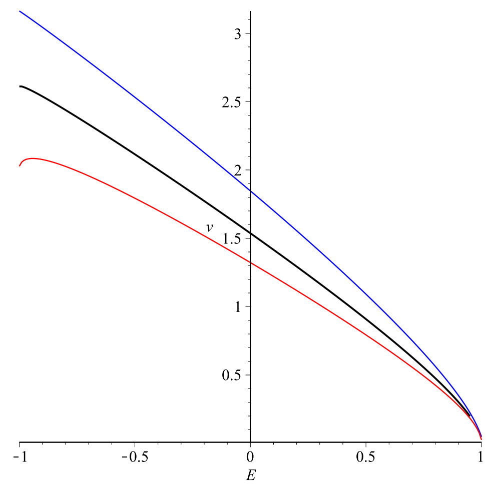

Figure 3: Graphs for $v_1(E), v(E)$, and $v_2(E)$ corresponding to $f_1(x) = -1$ if $|x| \leq \frac{\sqrt{5\pi}}{4}$ and 0 elsewhere, $f(x) = -e^{-0.8x^2}$, and $f_2(x) = -e^{-\frac{4x}{\sqrt{5\pi}}}$ respectively, for $-1 < E < 1$.

2. In this example we consider the potential $V(x) = vf(x)$ where $f(x) = -\dfrac{\beta}{(e^{-qx} + e^{qx})^2}$. We find the spectral bounds for $\beta = 3$. We choose the exponential potentials $V_1(x) = v_1 f_1(x)$ and $V_2(x) = v_2 f_2(x)$ such that

$$f_1(x) = -e^{-0.46666x},$$

and

$$f_2(x) = -0.75e^{-0.35x}.$$

This example shows that the refinement theorem is still valid even if the corresponding potential shapes cross over more than once, as long as the integral of their difference is convergent. Figures (4) and (5) show how the relative graphs of f_1, f, and f, f_2 cross over, with

$$\int_0^{\infty} \big(f(x) - f_1(x)\big)dx = \int_0^{\infty} \big(f_2(x) - f(x)\big)dx = 0.$$

We fix $E = -0.314$ and we get $v_1 = 1.9 \leq v \leq v_2 = 2.39$. We verify this result numerically and find that $v = 2.0943$. The graphs of v_1, v, and v_2 are shown in figure (6).

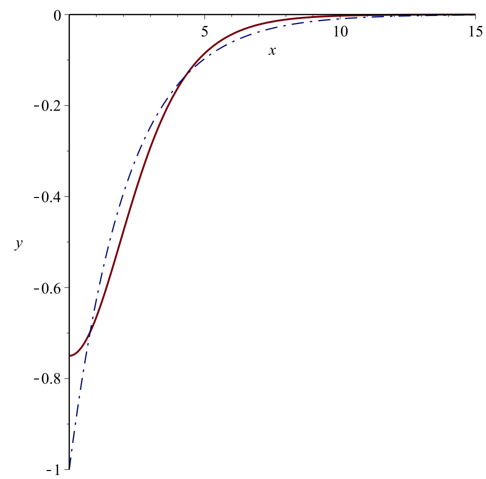

Figure 4: Potential Shapes $f_1(x) = -Ae^{-qx}$ dashed lines and $f(x) = -\dfrac{\beta}{(e^{-0.35x} + e^{0.35x})^2}$ full line, where $q = 0.35$, $C = b = 1$, and $A = 1$ were applied.

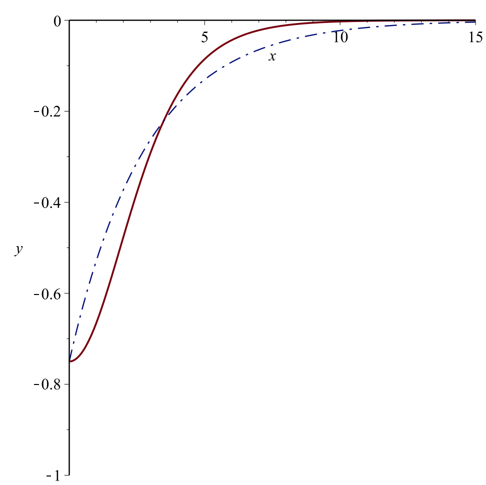

Figure 5: Potential Shapes $f_2(x) = -Ae^{-qx}$ dashed lines and $f(x) = -\dfrac{\beta}{(e^{-0.35x} + e^{0.35x})^2}$ full line, where $q = 0.35$ and $A = 0.75$ were applied.

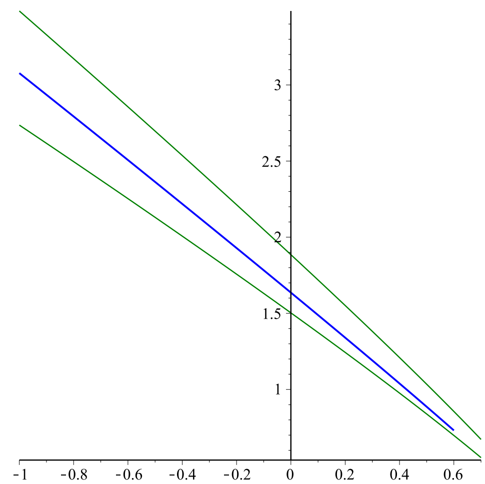

Figure 6: Graphs for $v_1(E), v(E)$, and $v_2(E)$ corresponding to $f_1(x) = -e^{-0.46666x}$, $f(x) = -\dfrac{\beta}{(e^{-0.35x} + e^{0.35x})^2}$, and $f_2(x) = -0.75e^{-0.35x}$ respectively, for $-1 < E < 1$.

B. Hulthén and Coulomb Spectral Bounds for Singular Potentials

Since we know the exact solutions of the Klein–Gordon equation with the Coulomb and Hlthén potentials [22] [23], we can find spectral bounds for any singular potential in $\mathcal{P}_d$.

The Yukawa Potential in dimension $d = 3$

Consider the Yukawa potential $V(r) = vf(r)$ with $f(r) = -\dfrac{e^{-ar}}{r}$ [24] , where $a > 0$ is a range parameter. We shall find a lower and an upper bound for the coupling constant v, for any $E \in (-m, m)$, for $a = 0.5$. We choose the Hulthén potentials $V_1(r) = v_1 f_1(r)$ and $V_2(r) = v_2 f_2(r)$ where

$$f_1(r) = -\frac{1}{e^{1.001r} - 1},$$

and

$$f_2(r) = -\frac{1}{e^{0.966} - 1}.$$

We fix $E = 0.96$ and obtain $v_1 = 0.4895$ and $v_2 = 0.4799$. Since $f_1(r) > f(r)$ for $r \in [0, \infty)$ as shown in figure (7), then according to our simple general comparison theorem [11], we find that $v_1 > v$. On the other hand, f and f_2 cross over at $r_0 \approx 1.2$ as shown in the right graph of figure (8), with $\displaystyle\int_0^{r_0} \big(f_2(r) - f(r)\big) r^2 dx = 0.0108 > 0$. Hence, applying our refined version of the general comparison theorem, we obtain $v > v_2$. We have numerically verified this result by finding that $v = 0.4834$. The graphs of $v_1(E), v(E)$, and $v_2(E)$ are shown in figure (9).

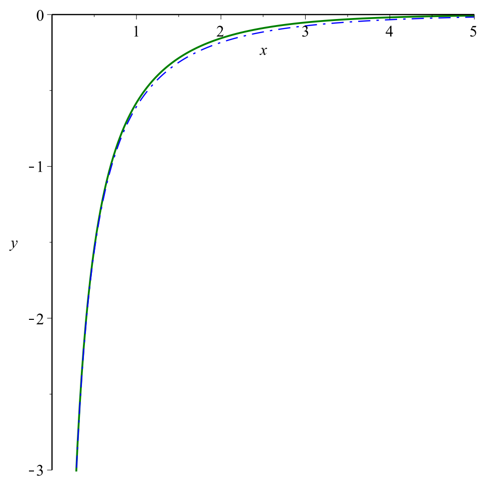

Figure 7: Potential Shapes $f_1(r) = -\dfrac{1}{e^{1.001r} - 1}$ full line and $f(r) = -\dfrac{e^{-ar}}{r}$ dashed lines, where $a = 0.5$ was applied.

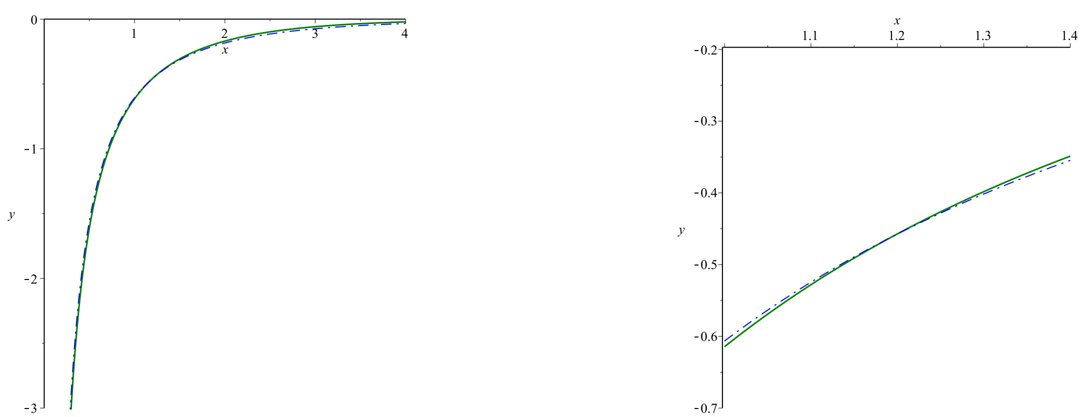

Figure 8: Left graph: potential shape $f_2(r) = -\dfrac{1}{e^{0.966} - 1}$ solid line and $f(r) = -\dfrac{e^{-ar}}{r}$ dashed lines. They intersect at $r_0 \approx 1.2$ as shown in the right graph. $a = 0.5$ was applied.

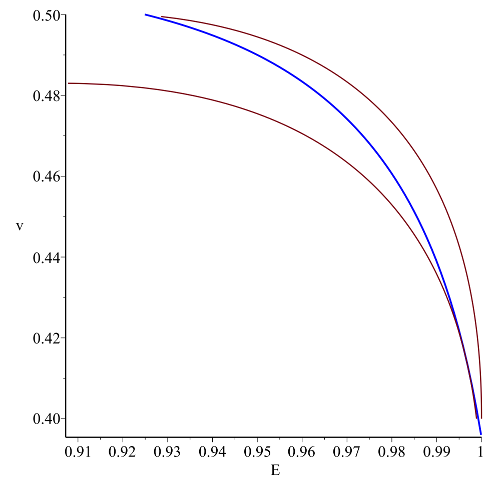

Figure 9: Graphs for $v_1(E), v(E)$, and $v_2(E)$ corresponding to $f_1(x) = -\dfrac{1}{e^{1.001r}-1}$, $f(r) = -\dfrac{e^{-0.5r}}{r}$, and $f_2(r) = -\dfrac{1}{e^{0.966r}-1}$ respectively, for $-1 < E < 1$.

IV. CONCLUSION

We have shown in this paper that our general comparison theorem for the Klein–Gordon equation, $f_1 \leq f_2 \implies v_1 \leq v_2$, still holds for the nodeless states, even if the condition is weakened to $\displaystyle\int_0^x \big[f_2(t) - f_1(t)\big]dt \geq 0$ for $d = 1$, and $\displaystyle\int_0^r \big[f_2(t) - f_1(t)\big]t^{d-2}dt \geq 0$ for $d \geq 3$, on $[0, \infty)$. We have also proven that if we know one of the wave functions φ_1 or φ_2, we can replace the new condition by $\displaystyle\int_0^x \big[f_2(t) - f_1(t)\big]\varphi_i(t)dt \geq 0$ for $d = 1$, and $\displaystyle\int_0^r \big[f_2(t) - f_1(t)\big]t^{d-2}\varphi_i(t)dt \geq 0$ for $d \geq 3$, with $i = 1, 2$. The latter conditions provide us with a stronger theorem because since the ground state is non-increasing on $[0, \infty)$, the potential shapes are even allowed to cross over more with preserving the ordering of the coupling parameters $v_1 = v_1(E)$ and $v_2 = v_2(E)$, for any eigen-energy $E \in (-m, m)$. We have also proven that for any potential whose shape $f(r)$ is no more singular than $r^{-(d-2)}$, $(d \geq 3)$, with $f(r) = -\dfrac{w(r)}{r}$, where $w(r)$ is non-increasing on $[0, \infty)$ and $w(0) \leq 1$, the lowest eigen-energy is always positive for $v < \dfrac{1}{2}$. As an application to our refined theorem, we have constructed upper and lower bounds for the discrete spectrum generated by any given central negative bounded potential, using the exact solutions of the Klein–Gordon equation with the square-well and the exponential potentials.

Acknowledgments

Partial financial support of his research under Grant No. GP3438 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

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