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Analysis and Numerical Solution of Eigenvalue Problems in Radial Schrödinger Equations

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unter der Anleitung von
Ao. Univ. Prof. Dr. Ewa B. Weinmüller

durch
Albert Fandl, BSc.

Marktplatz 32
3470 Kirchberg am Wagram

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Abstract

We investigate the numerical approximation of eigenvalues and eigenfunctions of the radial Schrödinger Equation

$$-u''(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right) u(r) = \lambda u(r), \quad r \in (0, \infty)$$

with Hydrogen Atom potential, Yukawa potential and Hulthén potential via a finite difference scheme. To apply the scheme we introduce a class of functions $t : (0, \infty) \rightarrow (0, 1)$ to transform the infinite domain of the eigenfunctions to a finite interval. We analyze the spectrum of the transformed radial Schrödinger Equation and discuss the results of the numerical experiments for two specific transformations.

1 Introduction

An important mathematical issue, which is raised in quantum physics, is the calculation of eigenvalues and eigenfunctions in context of the radial Schrödinger equation

$$-u''(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right) u(r) = \lambda u(r), \quad 0 < r < \infty \quad (1)$$

with boundary conditions

$$u(0) = u(\infty) = 0, \quad (2)$$

where $\ell \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$ denotes the *azimuthal quantum number*, $V(r)$ the *potential*, λ an eigenvalue and $u(r)$ an associated eigenfunction. There are only a few potentials V and values of ℓ , where explicit formulas for eigenvalues and eigenfunctions are known. This is the case for the *Hydrogen Atom* potential $V(r) = -Z/r$ and arbitrary $\ell \geq 0$, and for the *Hulthén* potential $V(r) = -\frac{2\alpha}{1-e^{-\alpha r}}$, if $\ell = 0$. In general, however, eigenvalues and eigenfunctions of the equation need to be computed numerically.

One way to solve this problem numerically is as follows. First we compress the infinite interval $(0, \infty)$ of the independent variable r in Equation (1) to the finite interval $(0, 1)$. We express the transformation by a function $t : (0, \infty) \rightarrow (0, 1)$. With the change of variable $r \mapsto t(r) = s$ we then transform Equation (1) to

$$-A_2(s)z''(s) + A_1(s)z'(s) + A_0(s)z(s) = \lambda z(s), \quad 0 < s < 1, \quad (3)$$

with boundary conditions

$$z(0) = z(1) = 0, \quad (4)$$

where the coefficient functions $A_i(s)$, $i = 0, 1, 2$ have singularities at $s = 0$ and $s = 1$. Eventually we want to numerically calculate the eigenfunctions and eigenvalues of the new Equation (3) with boundary conditions (4) via a finite difference scheme, resulting in the so-called matrix methods. However, we still have to investigate, whether the eigenvalue problem given by (3)-(4) is well-posed and has eigenfunctions which are smooth on the interval $(0, 1)$.

The case of a single singularity at the endpoints of equations of the form (3) is a widely discussed subject in the literature ([5], [6], [18]). In our case, when we have singularities at both endpoints of the equation, we establish a unitary mapping L to connect the Sturm Liouville expression of the new Equation (3) to the Sturm Liouville expression of the radial Schrödinger Equation (1). Such unitary mappings can be seen as generalizations of *Liouville's* transformation, they are also suggested by [12] and [7]. It turns out that the Sturm Liouville expressions of the two equations are equivalent. A detailed discussion of the original radial Schrödinger equation then reveals that it in fact only admits boundary conditions of the type (2) and has a non-empty set of eigenvalues. Also, local analysis shows that the eigenfunctions are smooth functions on $(0, \infty)$. These results can be carried over to the new Equation (3) via the unitary mapping L , which moreover links eigenfunctions of (3)-(4) to eigenfunctions of (1)-(2) in a one-to-one correspondence.

This thesis is organized as follows:

Section 2, Preliminaries, is subdivided in the two subsections, 2.1 Local analysis and 2.2 Sturm Liouville theory. Subsection 2.1 deals with the local analysis of solutions of 2nd order ordinary differential equations, where we split the domain of the independent variable x in ordinary, regular singular and irregular singular points. In Subsection 2.2, on the other hand, we want to give a brief overview on Sturm Liouville theory and self-adjoint operators, which we will use to analyze eigenfunctions and eigenvalues of the radial Schrödinger equation as well as the unitary mapping L .

In Section 3 we deal with the existence of eigenvalues and eigenfunctions of the original radial Schrödinger Equation (1) with boundary conditions (2), where we consider the *hydrogen atom* potential, the *Hulthén* potential and the *Yukawa* potential.

In Section 4 we introduce the unitary mapping L as well as specify the set of transformations t , which we will consider in this thesis. We describe the above results and show how the radial Schrödinger Equation (1) is linked to the new Equation (3). Finally we discuss the transformed Equation (3) for two specific transformations TCII and ATCII.

In Section 5 we deal with the numerical solution of the transformed equation via a finite difference scheme. We present the numerical method and discuss the results of the numerical experiments for the two specific transformations TCII and ATCII. The `matlab` code can be found at the end of this section.

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2 Preliminaries

2.1 Local analysis

In this section we will study the local behaviour of the solutions of the 2nd order ordinary differential equation

$$y''(x) + p(x)y'(x) + q(x)y(x) = 0 \quad (5)$$

with arbitrary coefficient functions $p, q : \mathbb{C} \rightarrow \mathbb{C}$. At this point we need to point out that from now on all the analysis and calculations (i.e. analyticity of functions, roots of polynomials) are supposed to take place in the complex plane, although we eventually are applying the developed theory to a differential equation with real valued coefficient functions.

There is a common classification for the points x_0 of the domain of (5):

1. The point x_0 is called **ordinary** point, if $p(x)$ and $q(x)$ are analytic at x_0 .
2. The point x_0 is called **singular** point, if $p(x)$ and/or $q(x)$ have a singular point at x_0 . Singular points can be divided in the following two subcases:
 - (a) The singular point x_0 is called **regular singular** point, if the order of the poles does not exceed 1 for $p(x)$, or 2 for $q(x)$.
 - (b) A singular point x_0 , which is not regular singular, is called **irregular singular** point.

To classify the point $x_0 = \infty$, we apply the involution transformation $t = \frac{1}{x}$ on Equation (5). The point $x_0 = \infty$ then corresponds to the point $t_0 = 0$ in the transformed equation and is called ordinary, regular singular or irregular singular, if t_0 in the transformed equation is called likewise.

Remark 2.1. The above classification of singular points is in fact equivalent to an alternative classification, which is widely used in the literature [5],[6],[18].

Suppose the differential equation is given by

$$\frac{d}{dx}Y(x) = (x - x_0)^{-\alpha} A(x) Y(x), \quad (6)$$

where $Y : \mathcal{D}(\subset \mathbb{C}) \rightarrow \mathbb{R}^n, \alpha \geq 1$ and the coefficient matrix $A : \mathcal{D} \rightarrow \mathbb{R}^{n \times n}$ is analytic at x_0 . Then in this setting we call the point x_0

1. **singularity of the first kind**, if $\alpha = 1$, or
2. **singularity of the second kind**, if $\alpha > 1$.

In what follows we want to show that the two classifications are indeed equivalent. Let x_0 be singular point of (5), and without loss of generality assume $x_0 = 0$. Let $\alpha \geq 1$ so that $x^\alpha p(x) =: p_0(x)$ and $x^{2\alpha} q(x) =: q_0(x)$ are analytic functions at x_0 . If x_0 is a regular singular point, then $\alpha = 1$, and if x_0 is a irregular singular point, then $\alpha > 1$. We are going to rewrite (5) to take form (6).

We start by setting

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} = \begin{pmatrix} y(x) \\ x^\alpha y'(x) \end{pmatrix}. \quad (7)$$

The derivative of the first component is

$$\frac{d}{dx} Y_1 = y' = x^{-\alpha} Y_2 \quad (8)$$

For the second component, we observe that (15) is in fact equivalent to

$$x^\alpha y'' = -x^\alpha qy - x^\alpha p y', \quad (9)$$

and therefore the derivation of the second component yields

$$\frac{d}{dx} Y_2 = (x^\alpha)' y' + x^\alpha y'' = -x^\alpha qy + ((x^\alpha)' - x^\alpha p) y' \quad (10)$$

$$= x^{-\alpha} \cdot (-x^{2\alpha} qy + [(x^\alpha)' - x^\alpha p] x^\alpha y') \quad (11)$$

$$= x^{-\alpha} \cdot (-q_0 Y_1 + [(x^\alpha)' - p_0] Y_2). \quad (12)$$

Overall this yields for Y the first order system of equations

$$\frac{d}{dx} Y = x^{-\alpha} \begin{pmatrix} 0 & 1 \\ -q_0 & (x^\alpha)' - p_0 \end{pmatrix} Y. \quad (13)$$

Here we can see that regular singular points with $\alpha = 1$ correspond to the singularities of the first kind and irregular singular points with $\alpha > 1$ to the singularities of the second kind. (See also [5], [6])

2.1.1 Ordinary points

At ordinary points the solutions are locally analytic functions. This is due to a result by [15] (Theorem 4.2), a variation of Picard-Lindelöf's theorem.

Theorem 2.1. *Let $\Omega \subset \mathbb{C}^{n+1}$ be an open set and suppose $f(z, w)$, $f : \Omega \rightarrow \mathbb{C}$ is analytic and bounded in Ω . Then there exists a unique solution for the initial value problem*

$$\frac{d}{dz}w = f(z, w), \quad w(z_0) = w_0 \quad (14)$$

which itself is analytic at z_0 .

As a result of this theorem we also obtain that solutions at ordinary points are analytic functions. Suppose we have

$$y''(x) + p(x)y'(x) + q(x)y(x) = 0. \quad (15)$$

Rewriting (15) into a first order system we obtain

$$\frac{d}{dx}Y = \begin{pmatrix} 0 & 1 \\ -q(x) & -p(x) \end{pmatrix} Y, \quad Y = \begin{pmatrix} y(x) \\ y'(x) \end{pmatrix}. \quad (16)$$

With the initial conditions $(1 \ 0)^T, (0 \ 1)^T$ we have two linearly independent analytic functions. Since this is a complete set of solutions at x_0 , any solution at x_0 is locally analytic.

2.1.2 Regular singular points

The discussion of regular singular points goes back to Fuchs and Frobenius. [10] Fuchs observed that at an regular singular point the solution multiplied by an appropriate power of $(x - x_0)^{-\alpha}$, $\alpha \in \mathbb{R}$, becomes finite. This leads to the definition of the Frobenius series

$$y(x) = (x - x_0)^\alpha \sum_{n=0}^{\infty} a_n (x - x_0)^n. \quad (17)$$

The exponent α in the Frobenius series is called *indicial exponent*. Moreover, it can be shown that the Frobenius series solution has nonvanishing radius of convergence.

This leads to the following theorem:

Theorem 2.2. *Let x_0 be a regular singular point of Equation (15). Then there exists a solution in form of a Frobenius series at x_0 .*

Proof. Without loss of generality we assume $x_0 = 0$. Following the definition of a regular singular point we obtain

$$p(x) = \sum_{n=-1}^{\infty} p_n x^n, \quad q(x) = \sum_{n=-2}^{\infty} q_n x^n. \quad (18)$$

Thus, the functions $p_0(x) = x \cdot p(x)$ and $q_0(x) = x^2 \cdot q(x)$ are analytic at $x = 0$ and we define the differential operator

$$L = x^2 \frac{d^2}{dx^2} + p_0(x) \cdot x \frac{d}{dx} + q_0(x), \quad (19)$$

so that the differential equation becomes $Ly = 0$.

We have a solution of the differential equation in Frobenius form

$$y(x, \alpha) = \sum_{n=0}^{\infty} a_n x^{\alpha+n}. \quad (20)$$

if and only if $Ly(x, \alpha) = 0$, or, changing the order of summation and differentiation,

$$Ly(x, \alpha) = \sum_{n=0}^{\infty} a_n Lx^{\alpha+n}. \quad (21)$$

We further compute

$$\begin{aligned} Lx^{\alpha+n} &= (\alpha+n)(\alpha+n-1)x^{\alpha+n} + p_0(x)(\alpha+n)x^{\alpha+n} + q_0(x)x^{\alpha+n} \\ &= [(\alpha+n)(\alpha+n-1) + p_0(x)(\alpha+n) + q_0(x)]x^{\alpha+n} = P(x, \alpha+n)x^{\alpha+n}, \end{aligned} \quad (22)$$

where the function $P(x, \alpha+n)$ is defined in an appropriate way.

For $n = 0$ we have

$$P(x, \alpha) = \alpha(\alpha-1) + p_0(x)\alpha + q_0(x) \quad (23)$$

$$= \alpha^2 + (p_0(x) - 1)\alpha + q_0(x), \quad (24)$$

which is analytic at $x = 0$ and a polynomial of second degree in α . Therefore, it can be expanded into the power series

$$P(x, \alpha) = \sum_{n=0}^{\infty} P_n(\alpha)x^n. \quad (25)$$

(We could also have done this by expanding p_0 and q_0 into power series in (24) and computing the coefficients manually.) For the first term the expansion yields

$$P_0(\alpha) = \alpha^2 + (p_0(0) - 1)\alpha + q_0(0), \quad (26)$$

the so-called *indicial polynomial*.

Using the above, we compute the right hand side of (21) and obtain

$$\sum_{n=0}^{\infty} a_n P(x, \alpha+n)x^{\alpha+n} = \sum_{n=0}^{\infty} \left[\sum_{k=0}^n a_k P_{n-k}(\alpha+k) \right] x^{\alpha+n}. \quad (27)$$

Thus, the series (20) solves equation $Ly(x, \alpha) = 0$, if and only if

$$\sum_{k=0}^n a_k P_{n-k}(\alpha+k) = 0. \quad (28)$$

In other words, it is a solution to the differential equation if and only if the coefficients a_k are computed according to the recursion relation

$$a_0 P_0(\alpha) = 0, \quad (29)$$

$$a_n = -\frac{1}{P_0(\alpha+n)} \sum_{k=0}^{n-1} a_k P_{n-k}(\alpha+k). \quad (30)$$

Suppose that $a_0 = 0$ in (29). If (20) is not the null-polynomial, there exists $N > 0$ such that $a_N \neq 0$. Suppose that N is the first integer of this kind. Hence, the choice of $\tilde{\alpha} = \alpha + N$ as indicial exponent and $(a_{N+n})_{n \in \mathbb{N}}$ as coefficients results in the same Frobenius series. Therefore we can assume that $a_0 \neq 0$ and that the indicial exponent α has to be a root of the indicial polynomial $P_0(\alpha)$.

Let α_1, α_2 be the roots of (24), $\operatorname{Re}\alpha_1 > \operatorname{Re}\alpha_2$. Then we have that the recursion for $a_n, n > 0$ in (30) is well-defined for $\alpha = \alpha_1$, since P_0 does not have roots at $\alpha_1 + n$ for $n > 0$. Thus, we have found a solution of the differential equation, which is in form of a Frobenius series. \square

Solutions of homogeneous linear differential equation form a linear space. Hence we can also interpret the arbitrary coefficient a_0 in (29) as an arbitrary multiplicative constant of the Frobenius series solution.

Theorem 2.3. *The Frobenius series (20) has a radius of convergence at least as large as the distance to the nearest singularity of the coefficient functions $p(x), q(x)$.*

Proof. We are going to show the result via a ratio test for a_n . Therefore we take the absolute values in the n th recursion

$$a_n = -\frac{1}{P_0(\alpha + n)} \sum_{k=0}^{n-1} a_k P_{n-k}(\alpha + k), \quad (31)$$

and use the triangle inequality to conclude

$$|a_n| \leq \frac{1}{|P_0(\alpha + n)|} \sum_{k=0}^{n-1} |a_k| |P_{n-k}(\alpha + k)|. \quad (32)$$

In order to find an upper bound for $|P_{n-k}(\alpha + k)|$, we recall that $P(x, \alpha) = \sum_{n=0}^{\infty} P_n(\alpha)x^n$, which yields

$$\frac{\partial}{\partial x} P(x, \alpha) = \sum_{n=0}^{\infty} (n+1)P_{n+1}(\alpha)x^n. \quad (33)$$

Like $P(x, \alpha)$, the derivative $\frac{\partial}{\partial x} P(x, \alpha)$ is a real valued and analytic function. It also has the same radius of convergence R_{\max} as (25). This implies that it assumes its maximal value on the boundary of a circle with radius R , if $R < R_{\max}$, according to the maximum principle. Thus, we have

$$(n+1)P_{n+1}(\alpha)R^n \leq M(\alpha), \quad (34)$$

for all $n > N$ for a $N > 0$. It follows that

$$P_{n+1}(\alpha) \leq \frac{1}{n+1} M(\alpha) R^{-n} < M(\alpha) R^{-n}, \quad (35)$$

and

$$|a_n| < \frac{1}{|P_0(\alpha + n)|} \sum_{k=0}^{n-1} |a_k| M(\alpha + k) R^{-(n-k)-1}. \quad (36)$$

We define the right hand side as b_n and observe that

$$\begin{aligned} b_{n+1} &= \frac{1}{|P_0(\alpha + n + 1)|} \left(M(\alpha + n)|a_n| + \sum_{k=0}^{n-1} |a_k| M(\alpha + k) R^{-(n-k)} \right) \\ &= \frac{M(\alpha + n)}{|P_0(\alpha + n + 1)|} |a_n| + \frac{b_n}{R} \frac{|P_0(\alpha + n)|}{|P_0(\alpha + n + 1)|} \\ &< b_n \left(\frac{M(\alpha + n)}{|P_0(\alpha + n + 1)|} + \frac{1}{R} \frac{|P_0(\alpha + n)|}{|P_0(\alpha + n + 1)|} \right). \end{aligned} \quad (37)$$

If we replace the inequality in (37) by an equality, we are able to introduce yet another sequence c_n via the recursion relation

$$c_{n+1} = c_n \left(\frac{M(\alpha + n)}{|P_0(\alpha + n + 1)|} + \frac{1}{R} \frac{|P_0(\alpha + n)|}{|P_0(\alpha + n + 1)|} \right), \quad c_0 = 1. \quad (38)$$

Obviously, $a_n < b_n < c_n$. The first fraction in brackets in (38) tends to zero; we postpone the proof to the Lemma 2.1 in the appendix. The second fraction

$$\frac{|P_0(\alpha + n)|}{|P_0(\alpha + n + 1)|} \quad (39)$$

tends to 1 as $n \rightarrow \infty$, because for arbitrary polynomials of second degree

$$\lim_{x \rightarrow \infty} \frac{x^2 + ax + b}{(x+1)^2 + a(x+1) + b} = \lim_{x \rightarrow \infty} \frac{x^2 + ax + b}{x^2 + (2+a)x + (1+a+b)} = \lim_{x \rightarrow \infty} \frac{1}{1} = 1 \quad (40)$$

by the L'Hôpital's rule. It follows that

$$\lim_{n \rightarrow \infty} \frac{c_{n+1}}{c_n} = \frac{1}{R}. \quad (41)$$

The power series with coefficients c_n has radius of convergence R . Recall that $R < R_{\max}$ is arbitrary. We see that the radius of convergence of (20) is at least as large as the smaller radius of convergence of $p_0(x), q_0(x)$. \square

At regular singular points it is not only possible to obtain a solution in Frobenius form, but also to find the second linearly independent solution. The structure of the second solution depends on the difference of the indicial exponents α_1, α_2 . This is the subject of the next theorem. For the proof and further discussion of the solutions we refer to the appendix of this section.

Theorem 2.4. *Let x_0 be a regular singular point of the equation and α_1, α_2 ($\alpha_1 > \alpha_2$) be the roots of the indicial polynomial. Then there exists a solution in Frobenius form*

$$y_1 = x^{\alpha_1} \Phi_1(x) \quad (42)$$

where Φ_1 is analytic at x_0 . A second linearly independent solution is given by

$$y_2 = x^{\alpha_2} \Phi_2(x) \quad (43)$$

for $\alpha_1 - \alpha_2 \notin \mathbb{N}_0$, where Φ_2 is analytic at x_0 , or

$$y_2 = x^{\alpha_2} \Phi_2(x) + x^{\alpha_1} \Phi_1(x) \log(x) \quad (44)$$

for $\alpha_1 - \alpha_2 = N$, $N \in \mathbb{N}$, or

$$y_2 = x^{\alpha_1} \Phi_1(x) \log(x) \quad (45)$$

for $\alpha_1 = \alpha_2$.

2.1.3 Irregular singular points

At an irregular singular point it is not possible to produce a general formula for the local behaviour. In fact at an irregular singular point there is always at least one solution which is not of Frobenius form [3]. However it is still possible to retrieve the *leading local behaviour* of the solutions as proposed in [3].

For this reason, we introduce the notation

$$f(x) \ll g(x), \quad \text{as } x \rightarrow x_0. \quad (46)$$

This is a shorthand for

$$\lim_{x \rightarrow x_0} \frac{f(x)}{g(x)} = 0 \quad (47)$$

and we say that f is *asymptotically small* compared to g . Similarly we write

$$f(x) \sim g(x), \quad \text{as } x \rightarrow x_0 \quad (48)$$

instead of

$$\lim_{x \rightarrow x_0} \frac{f(x)}{g(x)} = 1. \quad (49)$$

Note that \sim constitutes an equivalence relation.

Now [3] suggests the following steps for finding the leading behaviour of the solutions at an irregular singular point, called *method of dominant balance*:

1. Replace equality with asymptotic equality and drop terms that appear small. The remaining terms will produce the leading behaviour.
2. Solve the asymptotic relation as if it was a equation.
3. Peel off the leading behaviour by inserting a factorized ansatz into the original equation and restart the method with the unknown factor. The solution to the new asymptotic relation will be asymptotically small compared to the previously found factor.

2.1.4 Appendix to regular singular points

In Lemma 2.1 we give the proof for the statement in (38) in Theorem 2.3. In the Appendix we also derive the second solution at the regular singular point x_0 , as stated in Theorem 2.4.

Lemma 2.1. *The term*

$$\frac{M(\alpha + n)}{P_0(\alpha + n + 1)} \quad (50)$$

in (38) in Theorem 2.3 tends to 0 as $n \rightarrow \infty$.

Proof. For the numerator we recall that we have defined $M(\alpha)$ in (34) as the maximal value of $\frac{\partial}{\partial x}P(x, \alpha)$ for $|x| \leq R$. A direct derivation of the indicial polynomial (24) yields

$$\frac{\partial}{\partial x}P(x, \alpha) = \alpha p'_0(x) + q'_0(x). \quad (51)$$

Thus, we conclude that

$$M(\alpha) = \max_{|x|=R} |\alpha p'_0(x) + q'_0(x)| \leq \sigma \max_{|x|=R} |p'_0(x)| + \max_{|x|=R} |q'_0(x)| \quad (52)$$

is bounded by a linear function of $\sigma = |\alpha|$.

For the denominator we rewrite $P_0(\alpha) = \alpha^2 + (P_0(\alpha) - \alpha^2)$ and use the lower triangle inequality to obtain

$$|P_0(\alpha)| \geq |\alpha|^2 - |P_0(\alpha) - \alpha^2|. \quad (53)$$

Here, the definition of the indicial polynomial yields

$$|P_0(\alpha) - \alpha^2| = |(p_0(0) - 1)\alpha + q_0(0)| \leq |p_0(0) - 1|\sigma + |q_0(0)|. \quad (54)$$

Thus, we have

$$|P_0(\alpha)| \geq \sigma^2 - |p_0(0) - 1|\sigma - |q_0(0)|. \quad (55)$$

We denote the right hand side of (52) by $\phi_1(\sigma)$ and the right hand side of (55) by $\phi_2(\sigma)$ and note that ϕ_1, ϕ_2 are strictly increasing. Moreover, $|\alpha + n| \leq \sigma + n$ and $|\alpha + n + 1| \geq n + 1 - \sigma > n - \sigma$. Hence, we conclude

$$\frac{M(\alpha + n)}{P_0(\alpha + n + 1)} \leq \frac{\phi_1(|\alpha + n|)}{\phi_2(|\alpha + n + 1|)} < \frac{\phi_1(n + \sigma)}{\phi_2(n - \sigma)} \rightarrow 0 \quad \text{as } n \rightarrow \infty, \quad (56)$$

since the numerator is of a lower grade than the denominator. \square

Next we are going to prove two rather technical lemmas for the Frobenius series $y(x, \alpha)$, which we will need in the proof of Theorem 2.4. From now on, we let the coefficients a_n depend on α as well, so that the Frobenius series becomes

$$y(x, \alpha) = \sum_{n=0}^{\infty} a_n(\alpha)x^{n+\alpha}. \quad (57)$$

Lemma 2.2. *The series $\sum_{n=0}^{\infty} a_n(\alpha)x^n$ with coefficients $a_n(\alpha)$ defined by (29)-(30) converges uniformly in x in a common α -neighborhood of the roots α_1, α_2 of the indicial polynomial.*

Proof. We start with the result of the proof of Theorem 2.3. There we have found a sequence of coefficients c_n in (38), such that $a_n < c_n$ and

$$c_{n+1} = c_n \left(\frac{M(\alpha + n)}{|P_0(\alpha + n + 1)|} + \frac{1}{R} \frac{|P_0(\alpha + n)|}{|P_0(\alpha + n + 1)|} \right), \quad c_0 = 1. \quad (58)$$

To prove uniform convergence of the series $\sum_{n=0}^{\infty} a_n(\alpha)x^n$ we are going to construct a sequence of coefficients d_n , which is independent of α , such that $a_n(\alpha) < d_n$.

Therefore we find the upper bound

$$|P_0(\alpha)| = |\alpha^2 + (p_0(0) - 1)\alpha + q_0(0)| \leq \sigma^2 + |p_0(0) - 1|\sigma + |q_0(0)|, \quad (59)$$

and denote the right hand side by $\phi_3(\sigma)$. Let $\tau > |\alpha_1|, |\alpha_2|$. With the definition of ϕ_1, ϕ_2 in the previous lemma, we define a sequence d_n via

$$d_{n+1} = d_n \left(\frac{\phi_1(n + \tau)}{\phi_2(n - \tau)} + \frac{1}{R} \frac{\phi_3(n + \tau)}{\phi_2(n - \tau)} \right), \quad d_0 = 1, \quad (60)$$

such that $c_n(\alpha) < d_n$. Furthermore,

$$\frac{|P_0(\alpha + n)|}{|P_0(\alpha + n + 1)|} \leq \frac{\phi_3(|\alpha + n|)}{\phi_2(|\alpha + n + 1|)} < \frac{\phi_3(n + \tau)}{\phi_2(n - \tau)} \rightarrow 1, \quad \text{as } n \rightarrow \infty \quad (61)$$

and by the previous lemma

$$\frac{\phi_1(n + \tau)}{\phi_2(n - \tau)} \rightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (62)$$

This shows that the radius of convergence for the power series $\sum_{n=0}^{\infty} d_n x^n$ is at least R by the ratio test.

Thus, with $a_n(\alpha) < d_n$, we have that the series $\sum_{n=0}^{\infty} a_n(\alpha)x^n$ converges uniformly in x for all α in a common neighborhood of α_1, α_2 (cf. [10]). \square

Lemma 2.3. *The condition (30) for the coefficients $a_n(\alpha)$ of the Frobenius series $y(x, \alpha)$ is equivalent to*

$$a_n(\alpha) = a_0(\alpha) \cdot \left[\prod_{k=1}^n P_0(\alpha + k) \right]^{-1} \cdot h_n(\alpha) \quad (63)$$

for a particular $h_n(\alpha)$

Proof. We prove (63) by induction. The initial step $n = 1$

$$a_1(\alpha) = -\frac{1}{P_0(\alpha + 1)} a_0(\alpha) P_1(\alpha) \quad (64)$$

holds if we set $h_1(\alpha) = -P_1(\alpha)$.

The step $n - 1 \rightarrow n$ holds because of

$$a_n(\alpha) = -\frac{1}{P_0(\alpha + n)} \sum_{k=0}^{n-1} a_k(\alpha) P_{n-k}(\alpha + k) \quad (65)$$

$$= -\frac{1}{P_0(\alpha + n)} \sum_{k=0}^{n-1} \left(\frac{a_0(\alpha) \cdot h_k(\alpha)}{\prod_{l=1}^k P_0(\alpha + l)} \right) P_{n-k}(\alpha + k) \quad (66)$$

$$= -\frac{a_0(\alpha)}{\prod_{k=1}^n P_0(\alpha + k)} \sum_{k=0}^{n-1} \left(\prod_{l=k+1}^{n-1} P_0(\alpha + l) \right) \cdot h_k(\alpha) \cdot P_{n-k}(\alpha + k) \quad (67)$$

$$= a_0(\alpha) \cdot \left[\prod_{k=1}^n P_0(\alpha + k) \right]^{-1} \cdot h_n(\alpha), \quad (68)$$

if we set

$$h_n(\alpha) = -\sum_{k=0}^{n-1} \left(\prod_{l=k+1}^{n-1} P_0(\alpha + l) \right) \cdot h_k(\alpha) \cdot P_{n-k}(\alpha + k). \quad (69)$$

Note that $h_n(\alpha)$ is an entire function of α . \square

Proof of Theorem 2.4. Without loss of generality we set $x_0 = 0$.

1. First, let $\alpha_1 - \alpha_2 \notin \mathbb{N}_0$. Then none of the numbers $\alpha_1 + n, n \in \mathbb{N}$ nor $\alpha_2 + n, n \in \mathbb{N}$ is a root of P_0 . Therefore the recursion relation (29)-(30) not only yields a Frobenius solution for α_1 , but also a Frobenius solution for α_2 , since the coefficients of $y(x, \alpha_2)$ are well defined. The solution $y(x, \alpha_2)$ has the same radius of convergence.
2. Next, let $\alpha_1 - \alpha_2 = N \in \mathbb{N}$. This means the indicial polynomial has roots at α_2 and $\alpha_2 + N = \alpha_1$. Clearly it is not possible to calculate the coefficients for α_2 according to (30), since the computation of the N th coefficient a_N is not well defined.

However, it is possible to circumvent this problem if we let a_n depend on α and switch to the alternative recursion (63). There we set the first coefficient to

$$a_0(\alpha) := \prod_{k=1}^N P_0(\alpha + k) \cdot C(\alpha) \quad (70)$$

for some arbitrary function $C(\alpha)$, so that (63) becomes

$$a_n(\alpha) = C(\alpha) \cdot \begin{cases} \prod_{k=n+1}^N P_0(\alpha + k) \cdot h_n(\alpha) & \text{if } n \leq N, \\ \left[\prod_{k=N+1}^n P_0(\alpha + k) \right]^{-1} \cdot h_n(\alpha) & \text{if } n > N. \end{cases} \quad (71)$$

Hence $a_n(\alpha_2)$ is well defined for all $n \in \mathbb{N}$. To find the second solution of the differential equation we recall from the proof of Theorem 2.2

$$L \sum_{n=0}^{\infty} a_n(\alpha) x^{n+\alpha} = a_0(\alpha) P_0(\alpha) x^\alpha. \quad (72)$$

Here it holds that

$$\begin{aligned} P_0(\alpha + N) &= (\alpha + N - \alpha_1)(\alpha + N - \alpha_2) \\ &= (\alpha - \alpha_2)(\alpha + \alpha_1 - 2\alpha_2), \end{aligned} \quad (73)$$

and therefore the right hand side of (72) reads:

$$\begin{aligned} &a_0(\alpha)P_0(\alpha)x^\alpha \\ &= \left(\prod_{k=1}^N P_0(\alpha + k) \right) \cdot C(\alpha) \cdot (\alpha - \alpha_1)(\alpha - \alpha_2) \cdot x^\alpha \end{aligned} \quad (74)$$

$$= \left(\prod_{k=1}^{N-1} P_0(\alpha + k) \right) C(\alpha) \cdot (\alpha - \alpha_1)(\alpha - \alpha_2)^2(\alpha + \alpha_1 - 2\alpha_2)x^\alpha. \quad (75)$$

The right hand side has a double root at α_2 and hence

$$\left[\frac{d}{d\alpha} a_0(\alpha)P_0(\alpha)x^\alpha \right]_{\alpha=\alpha_2} = 0 \quad (76)$$

holds. Taking the derivative with respect to α on the left hand side of (72) yields

$$\frac{\partial}{\partial \alpha} L \left(x^\alpha \sum_{n=0}^{\infty} a_n(\alpha)x^n \right) = L \left(\frac{\partial}{\partial \alpha} x^\alpha \sum_{n=0}^{\infty} a_n(\alpha)x^n \right) \quad (77)$$

$$= L \left(\log(x)x^\alpha \sum_{n=0}^{\infty} a_n(\alpha)x^n + x^\alpha \sum_{n=0}^{\infty} a'_n(\alpha)x^n \right). \quad (78)$$

Here we used the uniform convergence from Lemma 2.2. When we set $\alpha = \alpha_2$ we obtain the second solution of $Ly = 0$,

$$v(x, \alpha_2) \log(x) + w(x, \alpha_2), \quad (79)$$

with

$$v(x, \alpha_2) = \sum_{n=0}^{\infty} a_n(\alpha_2)x^{n+\alpha_2}, \quad w(x, \alpha_2) = \sum_{n=0}^{\infty} a'_n(\alpha_2)x^{n+\alpha_2}. \quad (80)$$

For more details on the coefficients and the solution in this case as well as the role of the arbitrary function $C(\alpha)$ we refer to [10] and [3].

3. Finally, let $\alpha_1 = \alpha_2$. Then the indicial polynomial is $P_0(\alpha) = (\alpha - \alpha_1)^2$. To find the second solution in this case we use the same trick as before. From the proof of Theorem 2.2 we have that

$$L \sum_{n=0}^{\infty} a_n x^{n+\alpha} = a_0 P_0(\alpha) x^\alpha = a_0 (\alpha - \alpha_1)^2 x^\alpha. \quad (81)$$

We derive both sides with respect to α and set $\alpha = \alpha_1$. The right hand side vanishes because it has a double root at α_1 . The derivation of the right hand side yields

$$\frac{\partial}{\partial \alpha} L \left(x^\alpha \sum_{n=0}^{\infty} a_n x^{n+\alpha} \right) = L \left(\log(x)x^\alpha \sum_{n=0}^{\infty} a_n x^n \right). \quad (82)$$

Thus, $\log(x)y(x, \alpha_1)$ with

$$y(x, \alpha_1) = \sum_{n=0}^{\infty} a_n x^{n+\alpha_1} \quad (83)$$

is a second, linear independent solution of the differential equation.

□

2.2 Sturm Liouville theory

Another way to discuss linear homogeneous ordinary differential equations of 2nd order is within the framework of the Sturm Liouville (SL) theory. Here we view the differential equation as differential expression of an operator, albeit we are particularly interested in the self-adjoint versions. This proves to be especially helpful for eigenvalue problems like the radial Schrödinger equation. The set of eigenvalues of the eigenvalue problem then can be described by the discrete spectrum of a specific self-adjoint operator A .

In this section we want to give a brief introduction into the Sturm Liouville theory. In particular we will deal with Sturm Liouville expressions τ , the maximal and minimal operators T and T_0 , self-adjoint extensions A of the minimal operator, singular SL expressions and the discrete spectrum $\sigma_d(A)$ of self-adjoint extensions.

The core element of Sturm Liouville theory is the *SL expression* τ , which is used to describe differential equations of the form

$$-\frac{d}{dr} \left(p(r) \frac{d}{dr} u(r) \right) + q(r)u(r) = \lambda w(r)u(r), \quad r \in I = (a, b), \quad (84)$$

where $p, q, w : I \rightarrow \mathbb{R}$ are arbitrary coefficient functions and λ is an (unknown) eigenvalue. With the SL expression τ , Equation (84) can be written as

$$\tau u = \lambda u, \quad (85)$$

where τ is given by the expression

$$\tau = \frac{1}{w(r)} \left(-\frac{d}{dr} p(r) \frac{d}{dr} + q(r) \right), \quad r \in I = (a, b). \quad (86)$$

Example 2.1. *The radial Schrödinger equation is given by*

$$-u''(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right) u(r) = \lambda u(r), \quad r \in (0, \infty). \quad (87)$$

Using τ , we can rewrite it as

$$\tau u = \lambda u, \quad (88)$$

when the Sturm Liouville expression τ is given by

$$\tau = -\frac{d^2}{dr^2} + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right), \quad r \in (0, \infty). \quad (89)$$

Alternatively, τ is given by (86) and the coefficient functions

$$p(r) = 1, \quad q(r) = \frac{\ell(\ell+1)}{r^2} + V(r), \quad w(r) = 1 \quad (90)$$

on $I = (0, \infty)$.

We study SL expressions τ for functions u in the Hilbert space $\mathcal{L}^2(I, w)$, that is the space of all measurable functions u , such that

$$\int_a^b |u(r)|^2 w(r) dr < \infty.$$

This space can be equipped with the scalar product

$$(u, v) := \int_a^b \bar{u} \cdot v w dr, \quad u, v \in \mathcal{L}^2(I, w).$$

As in [17], we require that the coefficient functions p, q, w in (86) satisfy the following conditions:

1. p, q, w are measurable functions with $1/p, q, w \in \mathcal{L}^1_{loc}(I)$ (integrable on every compactum $[\alpha, \beta] \subset I$).
2. $p(r) \neq 0, w(r) > 0$ for almost every $r \in I$.

The maximal domain of functions u , on which the differential expression τ makes sense, is the set

$$\mathcal{D}_{max} = \{u : I \rightarrow \mathbb{C} \mid u, pu' \in AC_{loc}(I), u, \tau u \in \mathcal{L}^2(I, w)\}. \quad (91)$$

The operator

$$T_{max} : \begin{cases} \mathcal{D}_{max} & \rightarrow \mathcal{L}^2(I, w) \\ u & \mapsto \tau u \end{cases}$$

is called the maximal operator.

The adjoint operator T_{max}^* of the maximal operator, that is the operator defined as

$$(u, T_{max} v) = (T_{max}^* u, v), \quad u \in \mathcal{D}(T_{max}^*), v \in \mathcal{D}(T_{max}),$$

is called the minimal operator T_0 . Formally it is defined as the closure of the preminimal operator [19]

$$T'_{min} : \begin{cases} \mathcal{D}_0 & \rightarrow \mathcal{L}^2(I, w) \\ u & \mapsto \tau u \end{cases}$$

defined on the set

$$\mathcal{D}_0 = \{u \in \mathcal{D}_{max} \mid u \text{ has compact support in } I\}. \quad (92)$$

When the operators T_0, T are viewed as subsets of $\mathcal{L}^2(I, w) \times \mathcal{L}^2(I, w)$, it holds that $T_0 \subset T$ [17].

Furthermore T_0 is a *symmetric* operator

$$(u, T_0 v) = (T_0 u, v), \quad u, v \in \mathcal{D}_0, \quad (93)$$

because for $u, v \in \mathcal{D}_0$ we have $u(a) = v(a) = u(b) = v(b)$ and therefore

$$\begin{aligned}
(u, T_0 v) &= \int_a^b u(r) \cdot (\tau v)(r) \cdot w(r) dr = \int_a^b u \frac{1}{w} (-(pv)') + qv) w dr \\
&= \int_a^b -u(pv)' dr + \int_a^b uqv dr = -[u pv']_a^b + \int_a^b u' pv' dr + \int_a^b uqv dr \\
&= \int_a^b u' pv' dr + \int_a^b uqv dr.
\end{aligned} \tag{94}$$

For $(T_0 u, v)$ a similar calculation yields

$$(T_0 u, v) = \int_a^b pu'v' dr + \int_a^b uqv dr, \tag{95}$$

which completes the proof.

Finally, we say that an operator A is a symmetric extension of T_0 , if

$$T_0 \subset A \subset A^* \subset T. \tag{96}$$

A symmetric extension, which satisfies $A = A^*$, is called self-adjoint realization of τ . [17]

This is how far we can get before looking closer at the coefficient functions of τ . The SL expression τ is called

- **regular at a** , if $-\infty < a$ and $1/p, q, w \in \mathcal{L}^1([a, c])$ for one/any $c \in I$, and similarly
- **regular at b** , if $b < \infty$ and $1/p, q, w \in \mathcal{L}^1([d, b])$ for one/any $d \in I$.

If τ is regular at a and b , it is called **regular**.

If τ is not regular at a (resp. b), it is called **singular at a** (resp. b). Expressions, which are singular at least at one endpoint, are called **singular** SL expressions. ([17], pp.38-39)

One reason for this classification is that for regular τ the self-adjoint realizations A have purely discrete spectrum (see also Definition 2.2). ([17], 13.14c)

For singular problems we cite Weyl's famous alternative (cf. [17], 13.18):

Theorem 2.5 (Weyl's Alternative). *Let τ be Sturm-Liouville differential expression on $I = (a, b)$, and, without loss of generality, fix one endpoint, say a . Then either holds*

1. *for all $z \in \mathbb{C}$ every solution u of $(\tau - z)u = 0$ is in $\mathcal{L}^2([a, c], w)$ (LIMIT-CIRCLE case; LC), for one/any $c \in I$, or*
2. *for all $z \in \mathbb{C}$ exists at least one solution of $(\tau - z)u = 0$, which is not in $\mathcal{L}^2([a, c], w)$ (LIMIT-POINT case; LP), for one/any $c \in I$.*

In this framework regular endpoints are classified as LC endpoints.

For the next two theorems we need the definition of the deficiency indices of a SL expression τ . The pair of deficiency indices for τ is defined as

$$N_+ = \dim(T_0 + i), \quad (97)$$

$$N_- = \dim(T_0 - i). \quad (98)$$

Theorem 2.6 ([17], 13.19). *Let τ be SL expression on $I = (a, b)$. The deficiency indices (N_+, N_-) for τ are*

1. $(2, 2)$, if LC at both endpoints,
2. $(1, 1)$, if LP on one endpoint and LC on the other,
3. $(0, 0)$, if LP at both endpoints.

Theorem 2.7 ([16], 10.10). *Let S be a closed symmetric operator in complex Hilbert space with finite and equal deficiency indices (m, m) . Then it holds that*

1. *The symmetric extension T of S is self-adjoint, if and only if T is m -dimensional extension of S .*
2. *The symmetric restriction T of S^* is self-adjoint, if and only if T is m -dimensional restriction of S^* .*

This means, according to 2.6 and 2.7, that when we have LP at both endpoints and consider the maximal and minimal operators of the problem T_0, T , any self-adjoint realization A of τ is a 0-dimensional extension of T_0 , and a 0-dimensional restriction of T . In other words, $T_0 = A$ and $A = T$. Also, the maximal and the minimal operator then collapse into the single operator $T_0 = T$ ([17], proof of 13.19). Therefore, in the case of LP at both endpoints, there exists only one self-adjoint realization A of τ , which equals to

$$A = T_0 = T. \quad (99)$$

This result will become especially useful in Section 3, when we discuss self-adjoint operators of the radial Schrödinger equation, which is LP at both endpoints.

The reason we look for self-adjoint realizations A of τ is of course the spectral theorem for self-adjoint operators, which essentially states that all the information of a self-adjoint operator A can be stored in its associated spectral measure.

Theorem 2.8 ([14], 3.7, Spectral Theorem). *To every self-adjoint operator A there corresponds a unique projection-valued measure P_A such that*

$$A = \int_{\mathbb{R}} \lambda dP_A(\lambda). \quad (100)$$

Another way to store the spectral information of a self-adjoint operator A is via its spectrum and the associated subspaces of the Hilbert space $\mathcal{L}^2(I, w)$. The spectrum is usually defined through its complementary set, the resolvent set of A .

Here we want to cite the Definition (2.4) from [14],

Definition 2.1. *Let A be a (densely defined) closed operator. The resolvent set of A is defined by*

$$\rho(A) = \{z \in \mathbb{C} \mid (A - z)^{-1} \text{ is a bounded linear operator on the Hilbert space } \mathcal{L}^2(I, r)\}. \quad (101)$$

More precisely, $z \in \rho(A)$ if and only if $(A - z) : \mathcal{D}(A) \rightarrow \mathfrak{H}$ is bijective and its inverse is bounded. The complement of the resolvent set is called the spectrum of A ,

$$\sigma(A) = \rho(A)^c. \quad (102)$$

In particular, $z \in \sigma(A)$ if $A - z$ has a nontrivial kernel. A function $\psi \in \ker(A - z)$ is called an eigenfunction and z is called an eigenvalue in this case.

In this thesis we are mainly interested in the discrete part of the spectrum $\sigma(A)$, the so-called *discrete spectrum* of A , which is the set of eigenvalues. Again we cite [14], (6.4)

Definition 2.2 ([14]). *The discrete spectrum $\sigma_d(A)$ is the set of all eigenvalues which are discrete points of the spectrum and whose corresponding eigenspaces are finite dimensional.*

Remark 2.2. It should be noted that the complement of the discrete spectrum is called the essential spectrum $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A)$. For more information on the essential spectrum we refer to [14], (6.4), respectively [16], (9.2).

3 The radial Schrödinger equation

In this section we prove the existence of eigenvalues and eigenfunctions for the radial Schrödinger equation

$$-\frac{d^2}{dr^2}u(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r)\right)u(r) = \lambda u(r), \quad 0 < r < \infty, \quad (103)$$

with some potential $V(r)$. We are particularly interested in three different potentials:

- the Coulomb or Hydrogen potential for a charge $Z > 0$,

$$V(r) = -\frac{Z}{r} \quad (104)$$

(Equation (103) then is also a model for the Hydrogen Atom),

- the Yukawa potential with parameter $\alpha > 0$,

$$V(r) = -\frac{2e^{-\alpha r}}{r}, \quad (105)$$

- and the Hulthén potential with parameter $\alpha > 0$,

$$V(r) = -\frac{2\alpha e^{-\alpha r}}{e^{-\alpha r} - 1}. \quad (106)$$

In the literature the free parameter α in the Yukawa and the Hulthén potential is also referred to as the *screening parameter* and is usually further restricted to $\alpha_c > \alpha > 0$. Here, α_c stands for the *critical value* of the screening parameter. The critical value is the greatest value of α for which Equation (103) still has at least one eigenvalue.

In Subsection 3.1, we see that the eigenfunctions u satisfy the boundary conditions $u(0) = u(\infty) = 0$ in a natural way. Also the eigenfunctions turn out to be smooth functions on $I = (0, \infty)$.

In Subsection 3.2, we derive the exact eigenfunctions and eigenvalues for Equation (103) in the Hydrogen Atom model.

In Subsection 3.3, we discuss the set of eigenvalues for the Yukawa and Hulthén potential. These potentials can be written as perturbations of the Coulomb potential, and we discuss the spectral properties of Equation (103), following mainly the extensive literature in [16],[17] and [14]. The main focus of course lies on the discrete spectrum, which is the set of eigenvalues here. Additionally we consider the role of the critical value of the parameter α . In this case we mainly cite the results from [13] and [4]. Finally, we would like to point out that in the special case of the Hulthén potential with $\ell = 0$, formulas of the exact eigenfunctions and eigenvalues are known and can be found in [9].

3.1 Local behaviour of the eigenfunctions

In this section we study the local behaviour of the eigenfunctions of Equation (103), which we write in more convenient form as

$$\frac{d^2}{dr^2}u(r) = \left(-\lambda + V(r) + \frac{\ell(\ell+1)}{r^2}\right)u(r). \quad (107)$$

In particular we will see, that the eigenfunctions satisfy $u(0) = u(\infty) = 0$ and are smooth functions on $I = (0, \infty)$.

To carry out the analysis, we classify the points of the domain according to Section 2.1 as ordinary, regular singular or irregular singular points. For this reason, we first need to find the full behaviour of the coefficient function in Equation (107).

The Coulomb, Yukawa and Hulthén potential have a first order pole at the origin, vanish at infinity and are analytic throughout the interval $(0, \infty)$. For the eigenvalue λ , we assume for now that $\lambda < 0$.¹ Thus the coefficient function in Equation (107) has a singularity at $r = 0$, tends to λ for $r \rightarrow \infty$ and is analytic throughout the interval $(0, \infty)$. The singularity at $r = 0$ is a first order pole, if $\ell = 0$, and a second order pole, if $\ell > 0$.

According to Section 2.1, this means that $r = 0$ is a regular singular point, $0 < r < \infty$ are ordinary points and $r = \infty$ is an irregular singular point.

We first treat the singularity at $r = 0$. The indicial polynomial at this point is

$$f(\rho) = -\rho(\rho - 1) + \ell(\ell + 1) = -(\rho - (\ell + 1))(\rho + \ell), \quad (108)$$

which yields that the indicial exponents are $\rho_1 = \ell + 1$ and $\rho_2 = -\ell$. According to the results of Section 2.1, the set of solutions of Equation (107) at $r = 0$ behaves like

$$u_1^{\leftarrow}(r) = r^{\ell+1} v_1(r), \quad \text{for } r \rightarrow 0, \quad (109)$$

$$u_2^{\leftarrow}(r) = r^{-\ell} v_2(r) + r^{\ell+1} v_1(r) \log(r), \quad \text{for } r \rightarrow 0, \quad (110)$$

where v_1, v_2 are analytic functions at $r = 0$ with $v_1(0) \neq 0$ and $v_2(0) \neq 0$. The notation here means that $u_i^{\leftarrow}(r) = f(r)$ if and only if $\lim_{r \rightarrow 0} u_i(r) = O(f(r))$ for some function $f(r)$. From the set of solutions only u_1^{\leftarrow} satisfies the boundary condition $u(0) = 0$.

On the other hand, at the irregular singular point $r = \infty$, we drop the terms in Equation (107) which are asymptotically small for $r \rightarrow \infty$ and obtain

$$\frac{d^2}{dr^2}u(r) = -\lambda u(r). \quad (111)$$

Since $\lambda < 0$, we write $|\lambda|$ instead of $-\lambda$ from now on and set $\lambda_1 := \sqrt{|\lambda|}$. According to Section 2.1, we now expect the leading behaviour of the solutions of Equation (107) to be

$$u_1^{\rightarrow}(r) = e^{-\lambda_1 r}, \quad \text{for } r \rightarrow \infty, \quad (112)$$

$$u_2^{\rightarrow}(r) = e^{\lambda_1 r}, \quad \text{for } r \rightarrow \infty. \quad (113)$$

¹In Section 3.3 we will see that this is indeed the case.

Similar to above, the notation here means that $u_i^\rightarrow(r) = f(r)$ if and only if $\lim_{r \rightarrow \infty} u_i(r) = O(f(r))$ for some function $f(r)$. From the set of solutions only u_1^\rightarrow satisfies the boundary condition $\lim_{r \rightarrow \infty} u(r) = 0$.

Additionally, only u_1^\leftarrow and u_1^\rightarrow are square integrable at the respective endpoints in general. This is particularly the case for $\ell > 0$. On the other hand, we demand in Section 2.2 that eigenfunctions are square integrable functions on the whole interval $(0, \infty)$, and thus in particular at the endpoints. Therefore the eigenfunctions of Equation (107) satisfy the boundary conditions $u(0) = u(\infty) = 0$ for $\ell > 0$, since the behaviour of the eigenfunctions at the endpoints can be described by the functions u_1^\leftarrow and u_1^\rightarrow .

When $\ell = 0$, the function u_2^\leftarrow is square integrable at $r = 0$ too. However, eigenfunctions associated with u_2^\leftarrow are commonly excluded in physics via the boundary condition $u(0) = 0$ (see also the proof of Theorem 10.8 in [14]).

Furthermore, the above yields that according to Theorem 2.5 the endpoint $r = 0$ is LIMIT-CIRCLE and $r = \infty$ LIMIT-POINT for $\ell = 0$, and both endpoints are LIMIT-POINT, when $\ell > 0$.

Finally, the smoothness of the eigenfunctions on $I = (0, \infty)$ follows, if we recall from Section 2.1 that at ordinary points there exists a (locally) analytic solution to every initial value problem. Since this implies that the fundamental system of solutions is analytic as well, this carries over to arbitrary solutions at this point. Thus, for any solution u of Equation (107), we obtain that $u \in C^\infty(I)$, since analyticity is a local property.

3.2 The Hydrogen Atom

The radial Schrödinger equation of the Hydrogen Atom is probably among the most famous equations in quantum mechanics. Formulas for the eigenfunctions and eigenvalues can be derived explicitly. They can be found in many textbooks on quantum mechanics, e.g. [11], [14]. The derivation here mainly follows the methods and notation that were used in [11].

The radial Schrödinger equation for the Hydrogen Atom is given by

$$\frac{d^2}{dr^2}u(r) = \left(-\lambda - \frac{Z}{r} + \frac{\ell(\ell+1)}{r^2}\right)u(r), \quad r \in (0, \infty). \quad (114)$$

First, division by λ_1^2 and the scale transformation $\rho = \lambda_1 r$ simplifies it to

$$\frac{d^2}{d\rho^2}u(\rho) = \left(1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right)u(\rho), \quad \rho \in (0, \infty), \quad (115)$$

where we have set

$$\rho_0 = \frac{Z}{\lambda_1}. \quad (116)$$

From the discussion in Subsection 3.1 we can conclude that the overall solution looks like

$$u(\rho) = \rho^{\ell+1} v(\rho) e^{-\rho}, \quad (117)$$

where v is an analytic function on $(0, \infty)$. The computation of the second order derivative of the right hand side in (115) yields (the primes denote derivatives with respect to ρ)

$$\left[\left(\frac{\ell(\ell+1)}{\rho^2} + 1 + \frac{v''}{v}\right) + 2\left(-\frac{\ell+1}{\rho} + \frac{\ell+1}{\rho}\frac{v'}{v} - \frac{v'}{v}\right)\right]u. \quad (118)$$

Thus, the proposed solution reduces the entire Equation (115) to

$$\left[\frac{v''}{v} + 2\left(-\frac{\ell+1}{\rho} + \frac{\ell+1}{\rho}\frac{v'}{v} - \frac{v'}{v}\right)\right]u = -\frac{\rho_0}{\rho}u. \quad (119)$$

Factoring off $u \neq 0$ this is equivalent to a differential equation for v given as

$$\rho \frac{d^2}{d\rho^2}v + (2(\ell+1) - 2\rho) \frac{d}{d\rho}v + (\rho_0 - 2(\ell+1))v = 0. \quad (120)$$

With yet another scale transformation $x = 2\rho$ this becomes

$$x \frac{d^2}{dx^2}v + (2(\ell+1) - x) \frac{d}{dx}v + \left(\frac{\rho_0}{2} - (\ell+1)\right)v = 0. \quad (121)$$

Fortunately, for specific values of ρ_0 , this differential equation is known as the differential equation for the *associated Laguerre polynomial* L_n^k .

Laguerre's differential equation itself is given by

$$x \frac{d^2}{dx^2}y(x) + (1-x) \frac{d}{dx}y(x) + ny(x) = 0, \quad (122)$$

where $n \in \mathbb{N}_0$. Its solution are the so-called *Laguerre polynomials*, which are given by the Rodrigues formula

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n}(x^n e^{-x}). \quad (123)$$

The n th Laguerre polynomial $L_n(x)$ is a polynomial of n th grade.

Still, this does not suffice to reproduce the solutions for (121). The k th associated Laguerre polynomial is defined as

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x). \quad (124)$$

It is a solution for the differential equation

$$xy''(x) + (k+1-x)y'(x) + ny(x) = 0, \quad n = 0, 1, \dots \quad k \leq n. \quad (125)$$

Thus, the solution for (121) can be expressed in terms of associated Laguerre polynomials if $\frac{\rho_0}{2} - (\ell + 1) = n \in \mathbb{N}_0$, or

$$\rho_0 = 2(n + \ell + 1), \quad n \in \mathbb{N}_0. \quad (126)$$

With (116) and $\lambda_1 = \sqrt{|\lambda|}$ this becomes the formula for the eigenvalues

$$\lambda_n = - \left(\frac{Z}{2(n + \ell + 1)} \right)^2, \quad n \in \mathbb{N}_0, \quad (127)$$

known as *Bohr's* formula. [11]

To see that these are indeed all eigenvalues, let us assume the factor v in (117) to be a power series $\sum_{n=0}^{\infty} a_n \rho^n$. (From Section 3.1 we know that $v_1 = ve^{-\rho}$ is analytic at $\rho = 0$). It solves (120) or, equivalently,

$$\rho v'' + 2(\ell + 1)v' = 2\rho v' + (2(\ell + 1) - \rho_0)v. \quad (128)$$

Inserting the related power series the left hand side becomes

$$\begin{aligned} & \sum_{n=0}^{\infty} n(n-1)a_n \rho^{n-1} + \sum_{n=0}^{\infty} 2(\ell+1)na_n \rho^{n-1} \\ &= \sum_{n=0}^{\infty} a_{n+1}(n+1)(n+2(\ell+1))\rho^n. \end{aligned} \quad (129)$$

The right hand side is

$$\begin{aligned} & \sum_{n=0}^{\infty} 2na_n \rho^n + \sum_{n=0}^{\infty} (2(\ell+1) - \rho_0)a_n \rho^n \\ &= \sum_{n=0}^{\infty} a_n (2(n + \ell + 1) - \rho_0) \rho^n. \end{aligned} \quad (130)$$

Comparing powers of ρ yields

$$a_{n+1}(n+1)(n+2(\ell+1)) = a_n(2(n + \ell + 1) - \rho_0). \quad (131)$$

The fraction

$$\frac{a_{n+1}}{a_n} = \frac{2(n + \ell + 1) - \rho_0}{(n+1)(n+2(\ell+1))} \quad (132)$$

shows that the series becomes finite (and is the associated Laguerre polynomial) if and only if ρ_0 is chosen as above. Suppose $\rho_0 \neq 2(n + \ell + 1)$. Since

$$\frac{a_{n+1}}{a_n} = \frac{2}{n+1} - \frac{\rho_0 + 2(\ell+1)}{(n+1)(n+2(\ell+1))} \quad (133)$$

behaves like $\frac{2}{n+1}$ for large n , this means that

$$v(\rho) \sim e^{2\rho}, \quad \text{for } \rho \rightarrow \infty. \quad (134)$$

But this would imply that the overall solution in (117) behaves like

$$u(\rho) \sim \rho^{\ell+1} \cdot e^\rho \quad \text{for } \rho \rightarrow \infty, \quad (135)$$

which clearly violates the boundary condition

$$\lim_{r \rightarrow \infty} u(r) = 0. \quad (136)$$

Therefore, $\rho_0 = 2(n + \ell + 1)$ and all eigenvalues of (114) are given by (127).

3.3 Eigenvalues of the Yukawa and Hulthén potential

In the case of hydrogen atom (Coulomb potential), we were able to compute the eigenvalues and corresponding eigenfunctions explicitly. In this section however, we look at the radial Schrödinger equation from a Sturm Liouville point of view. This will enable us to discuss the radial Schrödinger equation with Yukawa and Hulthén potentials, where, in general, no explicit formulas for the eigenvalues and corresponding eigenfunctions are known.

With the Sturm Liouville terminology of Section 2.2 the right hand side of the radial Schrödinger Equation (103) on the interval $I = (0, \infty)$ becomes the Sturm-Liouville expression

$$\tau_\ell = -\Delta + \frac{\ell(\ell+1)}{r^2} + V(r). \quad (137)$$

Here we denote $\frac{d^2}{dr^2}$ by the *Laplacian* Δ . In Section 3.1 we have seen that this SL expression has LP endpoints at $r = 0$, $r = \infty$, when $\ell > 0$, and a LC endpoint at $r = 0$ and LP endpoint at $r = \infty$, when $\ell = 0$, where we additionally set the boundary condition $u(0) = 0$. According to the Theorems 2.6 and 2.7 we now have that there exists only one self-adjoint realization of τ_ℓ , which we will denote by A_ℓ .

For a start, we discuss the self-adjoint operator A_ℓ with the Coulomb potential $V(r) = -Z/r$. In the previous section, we already have found the discrete part of the spectrum of A_ℓ , the set of eigenvalues $\sigma_d(A_\ell)$, which are given by (127). In Theorem 3.5 we cite a result from [14], which will give us a complete picture of the spectrum of A_ℓ with the Coulomb potential. On the basis of the operator A_ℓ with the Coulomb potential, we now embark on a discussion of A_ℓ with the Yukawa and Hulthén potential.

Rewriting the Yukawa potential

$$-\frac{2e^{-\alpha r}}{r} = -\frac{2}{r} + \frac{2(1 - e^{-\alpha r})}{r}, \quad (138)$$

as well as the Hulthén potential

$$-\frac{2\alpha}{e^{\alpha r} - 1} = -\frac{2}{r} \cdot \frac{\alpha r}{e^{\alpha r} - 1} = -\frac{2}{r} + \frac{2}{r} \left(1 - \frac{\alpha r}{e^{\alpha r} - 1}\right) \quad (139)$$

reveals that the potentials can be seen as *perturbations* of the Coulomb potential.

For $\alpha \rightarrow 0^+$ the perturbations vanish and the potentials descend into the Coulomb potential, as can be easily seen for the Yukawa potential in (138). For the Hulthén potential this can be seen from

$$\lim_{\alpha \rightarrow 0^+} -\frac{2\alpha}{e^{\alpha r} - 1} = \lim_{\alpha \rightarrow 0^+} -\frac{2}{re^{\alpha r}} = -\frac{2}{r}. \quad (140)$$

We denote the perturbations by

$$W_1 = \frac{2(1 - e^{-\alpha r})}{r}, \quad (141)$$

and

$$W_2 = \frac{2}{r} \left(1 - \frac{\alpha r}{e^{\alpha r} - 1}\right). \quad (142)$$

The perturbations are almost everywhere bounded functions, $W_1, W_2 \in \mathcal{L}^\infty(I)$, as can be seen from

$$\lim_{r \rightarrow 0} W_1(r) = \lim_{r \rightarrow 0} \frac{2\alpha e^{-\alpha r}}{1} = 2\alpha \quad (143)$$

$$\lim_{r \rightarrow 0} W_2(r) = \lim_{r \rightarrow 0} \frac{2(e^{\alpha r} - 1 - \alpha r)}{r(e^{\alpha r} - 1)} = \lim_{r \rightarrow 0} \frac{2\alpha^2 e^{\alpha r}}{2\alpha e^{\alpha r} + r\alpha^2 e^{\alpha r}} = \alpha \quad (144)$$

Furthermore, they also tend to 0 as $r \rightarrow \infty$ and hence $W_1, W_2 \in \mathcal{L}_0^\infty(I)$, since

$$\lim_{r \rightarrow \infty} W_1(r) = \lim_{r \rightarrow \infty} \frac{2(1 - e^{-\alpha r})}{r} = 0 \quad (145)$$

for W_1 ; for W_2 consider

$$\lim_{r \rightarrow \infty} \frac{\alpha r}{e^{\alpha r} - 1} = \lim_{r \rightarrow \infty} \frac{\alpha}{\alpha e^{\alpha r}} = 0, \quad (146)$$

therefore we have

$$\lim_{r \rightarrow \infty} W_2(r) = \left(\lim_{r \rightarrow \infty} \frac{2}{r} \right) \cdot \left(1 - \lim_{r \rightarrow \infty} \frac{\alpha r}{e^{\alpha r} - 1} \right) = 0. \quad (147)$$

To study the influence of perturbations in more detail, we define the *multiplication operator* for $\mathcal{L}^\infty(I)$ perturbations on $\mathcal{L}^2(I)$ as

$$M_W : \begin{cases} \mathcal{L}^2(I) & \rightarrow \mathcal{L}^2(I), \\ u & \mapsto W \cdot u. \end{cases} \quad (148)$$

As a shorthand notation, we will also write W instead of M_W , even though we really mean the multiplication operator with W on $\mathcal{L}^2(I)$. Because of

$$\|M_W u\|_{\mathcal{L}^2(I)} = \|W \cdot u\|_{\mathcal{L}^2(I)} \leq \|W\|_{\mathcal{L}^\infty(I)} \cdot \|u\|_{\mathcal{L}^2(I)} \quad (149)$$

the multiplication operator with perturbation $W \in \mathcal{L}^\infty(I)$ is not only well-defined, but also a bounded operator. For real-valued perturbations it is also symmetric

$$(u, Wv) = \int_0^\infty \overline{u(r)} W(r)v(r) dr = \int_0^\infty \overline{W(r)u(r)} v(r) dr = (Wu, v). \quad (150)$$

Before we get to our first result on perturbations of self-adjoint operators, we need the following definition.

Definition 3.1 (Teschl, [14], 6.1). *An operator V is called T -bounded or relatively bounded with respect to T , if $\mathcal{D}(T) \subseteq \mathcal{D}(V)$ and if there are constants $a, b \geq 0$ such that*

$$\|Vu\| \leq a\|u\| + b\|Tu\|, \quad u \in \mathcal{D}(T). \quad (151)$$

The infimum of all b for which a corresponding a exists such that the above equation holds is called the T -bound of V .

Also, we define the sum $T + V$ of two operators $T : \mathcal{D}(T) \rightarrow \mathcal{L}^2(I), V : \mathcal{D}(V) \rightarrow \mathcal{L}^2(I)$ as the pointwise sum of the operators on the domain $\mathcal{D}(T+V) = \mathcal{D}(T) \cap \mathcal{D}(V)$.

Theorem 3.1 (KATO-RELLICH, [16], 9.2).

1. Let T be self-adjoint and V be symmetric and T -bounded with T -bound less than 1. Then $T + V$ is self-adjoint.
2. Let T be essentially self-adjoint and V be symmetric and T -bounded with T -bound less than 1. Then $T + V$ is essentially self-adjoint, $\overline{T + V} = \overline{T} + \overline{V}$.

So, by Kato-Rellich we know that the above perturbed Coulomb potentials correspond to self-adjoint operators on the same domain as the self-adjoint operator of the unperturbed Coulomb potential.

The perturbations also preserve another important feature of the Coulomb-potential, the boundedness from below, which implies that the spectrum of the self-adjoint operators is bounded from below as well (cf. [16], 8.26). This also implies the existence of a lowest eigenvalue λ_0 , which is referred to as the *ground state* of the Schrödinger operator (cf. [14], 10.5). Before we get to our result on the stability of the half-boundedness, we cite the following definition of half-bounded operators.

Definition 3.2 ([14], before 2.12). *A symmetric operator T is called bounded from below, if*

$$(u, Tu) \geq \gamma \|u\|^2, \quad u \in \mathcal{D}(T) \quad (152)$$

for some $\gamma \in \mathbb{R}$.

Theorem 3.2 (STABILITY OF HALF-BOUNDEDNESS, [16], 9.7). *Let T be self-adjoint and bounded from below with lower bound γ_T . Let V be symmetric and T -bounded with T -bound less than 1. Then $T + V$ is bounded from below as well.*

More exactly, let

$$\|Vu\| \leq a\|u\| + b\|Tu\|, \quad u \in \mathcal{D}(T) \quad (153)$$

with $b < 1$, then

$$\gamma := \gamma_T - \max \left\{ \frac{a}{1-b}, a + b|\gamma_T| \right\}$$

is a lower bound of $T + V$ (this lower bound is by no means optimal).

The lower bound γ_T of the self-adjoint operator with Coulomb potential has already been found. It is the lowest eigenvalue λ_0 .

The third of our main results will show that the discrete spectrum of the considered operators is indeed contained in $[\gamma, 0]$ (where γ is the lower bound), since the essential spectrum for the above perturbations will always stay the same, namely $[0, \infty)$. Recall that the spectrum of self-adjoint operators is real-valued and $\sigma(T) = \sigma_d(T) \dot{\cup} \sigma_{ess}(T)$. Before we formulate the result, we cite the following definition of T -compact operators.

Definition 3.3 ([16], before 9.12). *Let T, V with $\mathcal{D}(T) \subseteq \mathcal{D}(V)$. The operator V is called T -compact or relatively compact with respect to T , if*

$$V|_{\mathcal{D}(T)} : (\mathcal{D}(T), \|\cdot\|_T) \rightarrow \mathcal{L}^2(I) \quad (154)$$

is a compact operator². Equivalently, V is called T -compact, if for any sequence

²Here $\|\cdot\|_T$ is the restriction of $\|\cdot\|$ to $\mathcal{D}(T)$

$x_n \in \mathcal{D}(V)$, where $\|x_n\|_T$ is bounded, there exists a subsequence x_{n_k} such that Vx_{n_k} converges.

Theorem 3.3 (STABILITY OF THE ESSENTIAL SPECTRUM, [16], 9.14). *Let T be self-adjoint, V symmetric and T -compact, then $T + V$ is self-adjoint and it holds that $\sigma_{ess}(T + V) = \sigma_{ess}(T)$.*

Theorem 3.3 states that as long as the perturbations are symmetric and T -compact, the essential spectrum of the operators T and $T + V$ is the same. To see that W_1 and W_2 are relatively compact with respect to the self-adjoint operator T for the Coulomb potential, we will cite a result given in [14]. However, this result is stated for the *Schrödinger equation in three dimensions*. This equation is actually the origin of the radial Schrödinger equation. A detailed description, how the radial Schrödinger equation is derived from the Schrödinger equation in 3D, can be found in chapter 4 of [11] and in chapter 10.4 of [14].

As the name already suggests, the Schrödinger equation in 3D is defined for functions $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$, instead of $u : I = (0, \infty) \rightarrow \mathbb{R}$ for the radial equation. Similarly, in the 3D case we consider SL expressions of the form

$$\tau = -\Delta + V(x), \quad x \in \mathbb{R}^3 \quad (155)$$

instead of

$$\tau = -\Delta + \frac{\ell(\ell + 1)}{r^2} + V(r), \quad r \in I. \quad (156)$$

In [14] the operator with SL expression (155) and the 3D-version of the Coulomb potential

$$V(x) = -\frac{Z}{|x|}, \quad x \in \mathbb{R}^3 \quad (157)$$

is itself viewed as a perturbation of the *free Schrödinger operator* with SL expression $\tau = -\Delta$. For this operator the following theorem holds:

Theorem 3.4 ([14], 7.8). *The free Schrödinger operator $T = -\Delta$ with core $C_c^\infty(\mathbb{R}^3)$, the set of smooth, compactly supported functions on \mathbb{R}^3 , is self-adjoint and its spectrum is characterized by*

$$\sigma_d(T) = \emptyset, \quad \sigma_{ess}(T) = [0, \infty). \quad (158)$$

Now we can give the result by [14], which states that the operators with SL expression (155) and the 3D versions of the potentials considered in this thesis are relatively compact with respect to the free Schrödinger operator, and hence inherit its essential spectrum.

Theorem 3.5 ([14], 10.2). *Let $V = V_1 + V_2$ be real-valued with $V_1 \in \mathcal{L}^2(\mathbb{R}^3)$ and $V_2 \in \mathcal{L}_0^\infty(\mathbb{R}^3)$. Then V is relatively compact with respect to $T = -\Delta$. In particular $T + V$ is self-adjoint, bounded from below and $\sigma_{ess}(T + V) = \sigma_{ess}(T)$.*

Formally, of course, we need to make a distinction between the potential V in Equation (137) and the corresponding 3D version of V in Equation (155). However, following the convention from [17] on page 224 in Chapter 18.3, we refer to both by the same symbol V .

The condition in Theorem 3.5 can be rewritten for radial potentials. In [14] it is claimed that for *spherically symmetric* potentials (just as the ones considered above) the condition becomes $V(r) = V_1(r) + V_2(r)$, where

$$V_1(r) \in \mathcal{L}^2(I, w), \quad V_2(r) \in \mathcal{L}^\infty(I). \quad (159)$$

Here, w denotes the weight function $w(r) = r^2$. The Coulomb potential for instance can be partitioned like

$$V_1(r) = \begin{cases} -\frac{Z}{r} & r \leq c \\ 0 & c < r, \end{cases} \quad V_2(r) = \begin{cases} 0 & r \leq c \\ -\frac{Z}{r} & c < r, \end{cases} \quad (160)$$

where $c \in I$ is arbitrary. Since the Hulthén and the Yukawa potential differ from the Coulomb potential only by the $\mathcal{L}^\infty(I)$ -functions W_1 and W_2 , the result follows.

Next, we cite a result from [17], which says that for $\alpha \neq 0$ the perturbed Coulomb potentials only have finitely many eigenvalues.

Theorem 3.6 (Weidmann [17],18.15). *Let the function $V : I \rightarrow \mathbb{R}$ be locally bounded with*

- (i) $V(r) \geq -c/r^2$ with $c < 1/4$ for large r ,
- (ii) $r^{3/2}V(r) \rightarrow 0$ for $r \rightarrow 0$,
- (iii) $V(r) \in \mathcal{L}^2([0, c], w(r))$, where $w(r) = r^2$ and $c \in I$.

Then the preminimal operator T'_{min} , produced by $\tau = -\Delta + V(|x|)$ on $C_0^\infty(\mathbb{R}^3)$, is essentially self-adjoint, and $T_0 = \overline{T'_{min}}$ has at most finitely many negative eigenvalues, with finite geometric multiplicity.

The conditions in Theorem 3.6 hold for the Hulthén and Yukawa potential, but not for the Coulomb potential, which has an infinite number of eigenvalues, as we see in Equation (127). Just as the Coulomb potential, the Hulthén and the Yukawa potential have a first order pole at $r = 0$. Therefore, (ii) and (iii) are clearly satisfied. To see that (i) holds, consider in the Yukawa case

$$-\frac{2e^{-\alpha r}}{r} \geq -\frac{c}{r^2} \Leftrightarrow \frac{2}{\alpha}x \leq ce^x, \quad x = \alpha r \rightarrow \infty, \quad (161)$$

and in the Hulthén case

$$-\frac{2\alpha}{e^{\alpha r} - 1} \geq -\frac{c}{r^2} \Leftrightarrow \frac{2}{\alpha}x^2 \leq c(e^x - 1), \quad x = \alpha r \rightarrow \infty. \quad (162)$$

Finally, we deal with the question, whether the discrete spectrum of the perturbed Coulomb potentials contains any eigenvalues at all. In general, the Hulthén and the Yukawa potential lie above the Coulomb potential, because the perturbations W_1, W_2 are positive functions. For $\alpha \rightarrow \infty$, the potentials tend

to 0 and the operators converge to the free Schrödinger operator. Therefore the critical value α_c of the parameter α , which guarantees that there is at least one eigenvalue, is of special interest.

The critical value for the Hulthén respectively Yukawa potential has been calculated by Lassaut and Lombard in [13]. The relevant values ($2/\alpha_c = \gamma_c$) are

$$\gamma_c = \pi^2/6, \quad (\text{Hulthén}, \ell = 0), \quad (163)$$

$$\gamma_c \approx 1.6798, \quad (\text{Yukawa}, \ell = 0). \quad (164)$$

In particular, Lassaut and Lombard made the transformation $x = \alpha r$ in

$$-\frac{d^2}{dr^2}u(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right) u(r) = \lambda u(r) \quad (165)$$

to obtain

$$-\frac{d^2}{dx^2}u(x) + \left(\frac{\ell(\ell+1)}{x^2} + \frac{2}{\alpha} \tilde{V}(x) \right) u(x) = \tilde{\lambda} u(x), \quad (166)$$

where $\tilde{\lambda} = \lambda/\alpha$ and

$$\tilde{V}(x) = -\frac{e^{-x}}{x} \quad (167)$$

in the Yukawa case and

$$\tilde{V}(x) = -\frac{1}{e^x - 1} \quad (168)$$

for the Hulthén potential, and calculated the critical value of the parameter $\gamma = 2/\alpha$.

Another way to find an upper bound for α_c in the Yukawa case can be found in [4] by Bylicki, Stachów, Karwowski and Mukherjee. They propose that as a necessary condition for the potential to hold bound states, the effective potential

$$V_{\text{eff}}(r) = \frac{\ell(\ell+1)}{r^2} + V(r) \quad (169)$$

needs to have roots in the positive real numbers and take negative values in between.³ For the Yukawa potential the effective potential is

$$V_{\text{eff}}(r) = \frac{\ell(\ell+1)}{r^2} - \frac{e^{-\alpha r}}{r}. \quad (170)$$

Making the transformation $x = \alpha r$ yields

$$V_{\text{eff}}(x) = \frac{p}{x^2} - \frac{e^{-x}}{x}, \quad (171)$$

where $p = \ell(\ell+1)/\alpha$. The above function has a minimum at x when

$$\begin{aligned} -2px^{-3} + e^{-x}x^{-1} + e^{-x}x^{-2} &= 0 \\ \Leftrightarrow 2p &= (x^2 + x)e^{-x} = g(x). \end{aligned} \quad (172)$$

³In WKB theory, the roots of the effective potential are called *turning points* of the equation.

This means that $\tilde{V}_{\text{eff}}(x)$ has a minimum at x_{\min} when $2p$ is chosen not larger than the maximum of $g(x)$, which becomes zero for $x = 0$ and $x \rightarrow \infty$ and is positive in between. Substituting (172) into (171) yields

$$\tilde{V}_{\text{eff}}(x_{\min}) = (x_{\min} - 1) \frac{e^{-x_{\min}}}{2x_{\min}}, \quad (173)$$

which means that $\tilde{V}_{\text{eff}}(x)$ has negative values if $x_{\min} < 1$ or

$$p < g(1)/2 = e^{-1} \approx 0.367879. \quad (174)$$

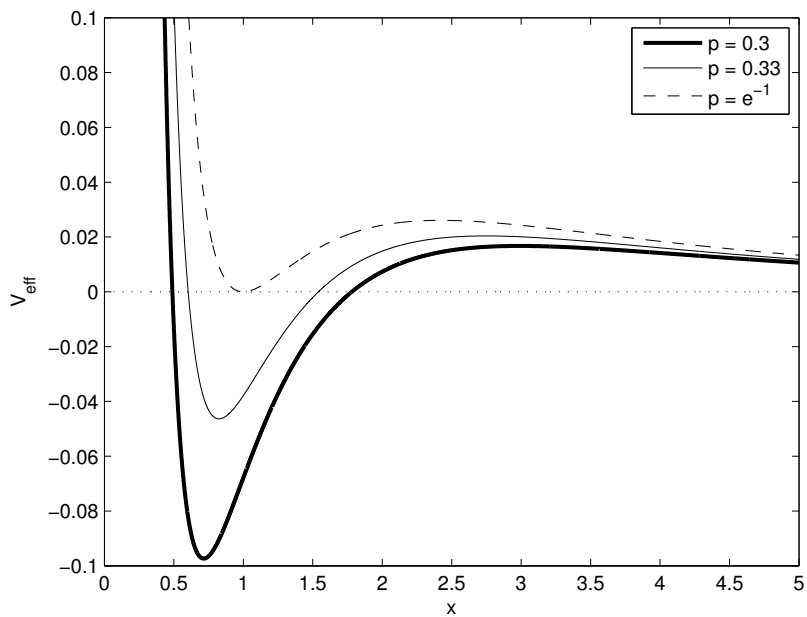


Figure 1: Plot of the effective potential $\tilde{V}_{\text{eff}}(x)$ (Yukawa) given in (171) for different values of $p = \ell(\ell + 1)/\alpha$. Here, we see that the effective potential has negative values as long as $p \leq e^{-1} \approx 0.367879$, which is a necessary condition for the potential to allow eigenvalues for the radial Schrödinger equation. (See also [4])

4 The transformed radial Schrödinger equation

In the last section we proved the existence of eigenvalues and eigenfunctions of the radial Schrödinger equation

$$-u''(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right) u(r) = \lambda u(r) \quad (175)$$

on the domain $r \in (0, \infty)$. In this section we are going to apply a change of the independent variable $r \mapsto s$ that transforms the infinite interval $(0, \infty)$ to the finite interval $(0, 1)$ and thus create a new, transformed equation for $s \in (0, 1)$. Therefore our main interest in this section is whether and how eigenfunctions and eigenvalues of the original problem on $(0, \infty)$ are carried over to the transformed problem on $(0, 1)$.

In the paragraphs following the introduction we specify the transformations we consider in this thesis and give a brief overview on the topic of this section.

In Subsection 4.1 we describe the steps of transforming the equation and provide a Sturm Liouville expression of the transformed equation.

In Subsection 4.2 we will see that the two equations share the same set of eigenvalues and that the eigenfunctions of the individual equations correspond to each other in a one-to-one fashion.

In Subsections 4.4 and 4.3 we apply the results of the previous subsections on the radial Schrödinger equation with the two specific transformations TCII (*transformation compressing the infinite interval*) and ATCII (*alternative transformation compressing the infinite interval*).

The set of transformations t that we consider in this thesis can be specified as follows

$$t : \begin{cases} (0, \infty) & \rightarrow (0, 1), \\ r & \mapsto t(r) =: s, \end{cases} \quad t \in C^\infty((0, \infty)), \quad \text{bijective.} \quad (176)$$

We then apply the change of variable $r \mapsto s = t(r)$ in (175), so that (175) becomes

$$-a(s)z''(s) - b(s)z'(s) + c(s)z(s) = \lambda z(s), \quad s \in (0, 1), \quad (177)$$

where $a(s), b(s), c(s)$ are yet to be determined coefficient functions and $z(s)$ is defined by $u(r) = z(t(r))$. The relationship between u, z and t can also be seen in the following commutative diagram

$$\begin{array}{ccc} & u(r) & \\ & \curvearrowright & \\ r \in (0, \infty) & \xleftrightarrow[t^{-1}(s)]{t(r)} & s \in (0, 1) \xrightarrow{z(s)} z(s), u(r) \in \mathbb{R}. \end{array}$$

In Section 3.1 we have seen that the eigenfunctions of (175) are characterized by the boundary conditions

$$u(0) = u(\infty) = 0. \quad (178)$$

The equivalent set of boundary conditions for (177) is given by

$$z(0) = z(1) = 0. \quad (179)$$

These boundary conditions characterize the eigenfunctions of the transformed problem (177) in exactly the same way as the boundary conditions (178) characterize the eigenfunctions of the original problem. This will become apparent in Lemma 4.2 in Section 4.2, where we will see that the eigenfunctions of (177) are exactly the transformed eigenfunctions of the original problem (175). Additionally, we will see that the eigenfunctions of the transformed equation are again smooth functions on the entire interval.

The specific transformations of type (176) that we study in this section are the TCII transformations (*transformation compressing the infinite interval*)

$$t_\xi : \begin{cases} (0, \infty) & \rightarrow (0, 1), \\ r & \mapsto \frac{r}{r+\xi} = 1 - (1 + \frac{r}{\xi})^{-1}, \end{cases} \quad (180)$$

where $\xi > 0$ is a free parameter of the transformation, and the ATCII transformations (*alternative transformation compressing the infinite interval*)

$$t_\beta : \begin{cases} (0, \infty) & \rightarrow (0, 1), \\ r & \mapsto 1 - (1 + r)^{-\beta}, \end{cases} \quad (181)$$

with the free parameter $\beta > 0$.

4.1 Transformation by a change of the independent variable

The substitution $r \mapsto s = t(r)$ transforms the radial Schrödinger equation on $r \in (0, \infty)$ to a second-order, linear ODE with eigenvalue λ on $s \in (0, 1)$. Both eigenvalue problems can be represented by their SL expressions. In this section we carry out the steps of the transformation to connect them to each other.

Following the notation of the last paragraph in Subsection 3.3 we denote the coefficient of $u(r)$ as V_{eff} , so that (175) is of the form

$$-u''(r) + V_{\text{eff}}(r)u(r) = \lambda u(r), \quad r \in (0, \infty). \quad (182)$$

The left-hand side of this equation is equivalent to the SL expression

$$\tau_1 = \frac{1}{w_1(r)} \left(-\frac{d}{dr} p_1(r) \frac{d}{dr} + q_1(r) \right), \quad r \in (0, \infty), \quad (183)$$

where the coefficients are given by

$$p_1(r) = 1, \quad q_1(r) = V_{\text{eff}}(r), \quad w_1(r) = 1. \quad (184)$$

We replace $u(r)$ by $(z \circ t)(r) := z(t(r))$, where t is given by (176), and obtain

$$\begin{aligned} & - (z'' \circ t)(r) \cdot (t'(r))^2 - (z' \circ t)(r) \cdot (t''(r)) \\ & + V_{\text{eff}}(r) (z \circ t)(r) = \lambda (z \circ t)(r), \quad r \in (0, \infty), \end{aligned} \quad (185)$$

according to the conventional chain rule of calculus. The substitution $t(r) = s$, $r = t^{-1}(s)$ now yields

$$\begin{aligned} & - z''(s) \cdot ((t' \circ t^{-1})(s))^2 - z'(s) \cdot (t'' \circ t^{-1})(s) \\ & + (V_{\text{eff}} \circ t^{-1})(s) z(s) = \lambda z(s), \quad s \in (0, 1). \end{aligned} \quad (186)$$

Hence, we retrieved an eigenvalue problem given on the domain $(0, 1)$.

We can find the suitable SL expression τ_2 for the left hand side of (186), so that the whole equation becomes $\tau_2 z = \lambda z$, if we multiply the equation with an appropriate integrating factor. The integrating factor for a general, linear 2nd order ODE of the form

$$-a(s)z''(s) - b(s)z'(s) + c(s)z(s) = \lambda z(s) \quad (187)$$

is given by

$$m(s) := \frac{1}{a(s)} \exp \left(\int_{s_0}^s \frac{b(x)}{a(x)} dx \right). \quad (188)$$

Collecting terms then gives the following Sturm Liouville form

$$-(a(s)m(s) \cdot z'(s))' + c(s)m(s) \cdot z(s) = \lambda \cdot m(s) \cdot z(s). \quad (189)$$

(see also [12], p.36; [8], 2.1, p.24)

With the coefficients of Equation (186) we have

$$\begin{aligned} \int_{s_0}^s \frac{b(x)}{a(x)} dx &= \int_{s_0}^s \frac{t'' \circ t^{-1}(x)}{(t' \circ t^{-1}(x))^2} dx = \int_{s_0}^s \left(\frac{t''}{t'} \right) \circ t^{-1}(x) \cdot \frac{1}{t' \circ t^{-1}(x)} dx \\ &= \int_{t^{-1}(s_0)}^{t^{-1}(s)} \frac{t''(x)}{t'(x)} dx = \log((t' \circ t^{-1})(s)), \end{aligned} \quad (190)$$

which yields the integrating factor

$$m(s) = \frac{1}{a(s)} \exp \left(\int_{s_0}^s \frac{b(x)}{a(x)} dx \right) = \frac{t' \circ t^{-1}(s)}{(t' \circ t^{-1}(s))^2} = \frac{1}{t' \circ t^{-1}(s)}. \quad (191)$$

Thus, the eigenvalue problem given by (186) can be rewritten as

$$\begin{aligned} -\frac{d}{ds} \left((t' \circ t^{-1})(s) \cdot \frac{d}{ds} z(s) \right) + \frac{V_{\text{eff}} \circ t^{-1}(s)}{t' \circ t^{-1}(s)} \cdot z(s) \\ = \lambda \frac{1}{(t' \circ t^{-1})(s)} z(s), \quad s \in (0, 1) \end{aligned} \quad (192)$$

or $\tau_2 z = \lambda z$, where τ_2 is given by

$$\tau_2 = \frac{1}{w_2(s)} \left(-\frac{d}{ds} p_2(s) \frac{d}{ds} + q_2(s) \right), \quad s \in (0, 1) \quad (193)$$

and the SL coefficients are defined as

$$p_2(s) = t' \circ t^{-1}(s), \quad q_2(s) = \frac{V_{\text{eff}} \circ t^{-1}(s)}{t' \circ t^{-1}(s)}, \quad w_2(s) = \frac{1}{t' \circ t^{-1}(s)}. \quad (194)$$

4.2 Connecting the equations via a Liouville transformation L

More formally, we can describe the step from (186) to (192) by a special unitary mapping L , a generalization of *Liouville's* transformation [12]. This will enable us to connect the set of eigenvalues and the eigenfunctions of the radial Schrödinger equation to the set of eigenvalues and the eigenfunctions of the transformed equation. In fact, we will see that the two equations share the same set of eigenvalues and that the eigenfunctions of the two equations correspond to each other in a one-to-one fashion.

For transformations of type (176) we define the associated *Liouville transformation* as

$$L : \begin{cases} \mathcal{L}^2(I) & \rightarrow \mathcal{L}^2(J, w_2), \\ u & \mapsto z = u \circ t^{-1}, \end{cases} \quad (195)$$

where we have set $I = (0, \infty)$ and $J = (0, 1)$ (see also [12], 3.1).

First of all, L is well-defined and isometric. This can be seen from the following (where we apply the rule of integration by substitution)

$$\begin{aligned} \|z\|_{\mathcal{L}^2(J, w_2)}^2 &= \int_J u^2(t^{-1}(s)) \cdot \frac{1}{t'(t^{-1}(s))} ds \\ &= \int_{t^{-1}(J)} u^2(r) dr = \int_I u^2(r) dr = \|u\|_{\mathcal{L}^2(I)}^2. \end{aligned} \quad (196)$$

From the definition it can also be seen that L is linear and that its inverse is the Liouville transformation

$$L^{-1} : \begin{cases} \mathcal{L}^2(J, w_2) & \rightarrow \mathcal{L}^2(I), \\ z & \mapsto u = z \circ t. \end{cases} \quad (197)$$

Hence, L is bijective.

The definition of the Liouville transformation makes it easier to connect the radial Schrödinger equation to the transformed equation. In fact, we can reiterate the steps in Subsection 4.1 in terms of u , λ , τ_1 , τ_2 and L . Starting with

$$\tau_1 u = \lambda u \quad (198)$$

in (182), Equation (186) then becomes

$$L\tau_1 u = \lambda Lu, \quad (199)$$

which is finally transformed to

$$\tau_2 Lu = \lambda Lu \quad (200)$$

in (192). Thus, we can describe the relation between τ_1 , τ_2 and L as

$$L\tau_1 u = \tau_2 Lu \quad (201)$$

when $u \in \mathcal{D}_{max}(\tau_1)$, $Lu \in \mathcal{D}_{max}(\tau_2)$.

The mapping L also links the maximal domains of τ_1 and τ_2 . This is the content of the following lemma.

Lemma 4.1. *Let L, τ_1, τ_2 be given, so that (201) holds. Then L maps the maximal domain of τ_1 on the maximal domain of τ_2 ,*

$$L(\mathcal{D}_{max}(\tau_1)) = \mathcal{D}_{max}(\tau_2). \quad (202)$$

Proof. In Section 2.2, (91) we defined the maximal domain of a Sturm Liouville expression τ in the following way

$$\mathcal{D}_{max} = \{u : I \rightarrow \mathbb{C} \mid u, pu' \in AC_{loc}(I), u, \tau u \in \mathcal{L}^2(I)\}. \quad (203)$$

With this the desired statement follows from the equalities

$$\begin{aligned} L\mathcal{D}_{max}(\tau_1) &= L \{u : I \rightarrow \mathbb{C} \mid u, p_1u' \in AC_{loc}(I), u, \tau_1u \in \mathcal{L}^2(I)\} \\ &= \{Lu : J \rightarrow \mathbb{C} \mid Lu, L(p_1u') \in AC_{loc}(J), Lu, L\tau_1u \in \mathcal{L}^2(J, w_2)\} \\ &= \{Lu : J \rightarrow \mathbb{C} \mid Lu, p_2(Lu)' \in AC_{loc}(J), Lu, \tau_2Lu \in \mathcal{L}^2(J, w_2)\} \\ &= \{z : J \rightarrow \mathbb{C} \mid z, p_2z' \in AC_{loc}(J), z, \tau_2z \in \mathcal{L}^2(J, w_2)\} \\ &= \mathcal{D}_{max}(\tau_2). \end{aligned}$$

□

Finally, we formulate the main result, which links eigenfunctions and eigenvalues of τ_1 and τ_2 via the Liouville transformation L .

Lemma 4.2. *Let Sturm Liouville expressions τ_1, τ_2 and Liouville transformation L be given, so that (201) holds.*

Then L maps eigenfunctions of τ_1 for eigenvalue λ on the eigenfunctions of τ_2 for eigenvalue λ in a one-to-one correspondence.

In particular, we say that u is an eigenfunction of τ_1 with eigenvalue λ ,

$$\tau_1u = \lambda u, \quad (204)$$

if and only if $z = Lu$ is eigenfunction of τ_2 to the eigenvalue λ ,

$$\tau_2z = \lambda z. \quad (205)$$

Proof. This directly follows from (201). Suppose u is an eigenfunction of τ_1 with eigenvalue λ . Then

$$\tau_2z = \tau_2Lu = L\tau_1u = L\lambda u = \lambda Lu = \lambda z. \quad (206)$$

reveals that z as well is an eigenfunction of τ_2 with eigenvalue λ .

Conversely, if z is eigenfunction of τ_2 with eigenvalue λ , then

$$\tau_1u = L^{-1}L\tau_1u = L^{-1}\tau_2Lu = L^{-1}\tau_2z = L^{-1}\lambda z = L^{-1}\lambda Lu = \lambda u. \quad (207)$$

shows that u as well is an eigenfunction of τ_1 for the eigenvalue λ . □

As a consequence of Lemma 4.2, we can characterize the smoothness of the eigenfunctions z of τ_2 . In Section 3.1 we have seen that the eigenfunctions u of τ_1 are smooth functions on the entire interval $I = (0, \infty)$. Also, transformations $t : I \rightarrow J = (0, 1)$ of type (176) are bijective and smooth and therefore have an inverse $t^{-1} : J \rightarrow I$, which is bijective and smooth as well. With this it follows that the eigenfunctions z of τ_2 , which are exactly the images of u under L , are smooth as composition of smooth functions, $z = Lu = u \circ t^{-1}$.

In the last two subsections of this section, we discuss the transformed radial Schrödinger equation for two specific transformations of type (176).

4.3 A transformation compressing the infinite interval - TCII

The first transformation that we study here is

$$t_\xi : \begin{cases} (0, \infty) & \rightarrow (0, 1), \\ r & \mapsto \frac{r}{r+\xi}, \end{cases} \quad (208)$$

where $\xi > 0$ is a free parameter of the transformation.

At first we are going to calculate the coefficients of the transformed Equation (192) with transformation t_ξ . Here, the derivative is given by

$$t'_\xi(r) = \frac{(r+\xi) - r}{(r+\xi)^2} = \frac{\xi}{(r+\xi)^2} \quad (209)$$

Since the transformation t_ξ can be rewritten as

$$t_\xi(r) = \frac{1}{1 + (\xi/r)} = \left(1 + \frac{\xi}{r}\right)^{-1} \quad (210)$$

the inverse function is given by

$$t_\xi^{-1}(s) = \xi \cdot \left(\frac{1}{s} - 1\right)^{-1} = \xi \cdot \frac{s}{1-s}, \quad s \in (0, 1). \quad (211)$$

With this it also holds that

$$t_\xi^{-1}(s) + \xi = \xi \left(\frac{s}{1-s} + 1\right) = \xi \cdot \frac{1}{1-s}. \quad (212)$$

Thus, the computation of the coefficient $t'_\xi \circ t_\xi^{-1}(s)$ yields

$$t'_\xi \circ t_\xi^{-1}(s) = \frac{(1-s)^2}{\xi}. \quad (213)$$

Finally, the transformed Equation (192) with transformation t_ξ is given by

$$-\left(\frac{(1-s)^2}{\xi} z'\right)' + \frac{\xi V_{\text{eff}}\left(\frac{\xi s}{1-s}\right)}{(1-s)^2} z = \lambda \frac{\xi}{(1-s)^2} z, \quad s \in (0, 1). \quad (214)$$

However, the numerical calculations have been carried out via the equivalent equation

$$-\frac{(1-s)^4}{\xi^2} z'' + \frac{2(1-s)^3}{\xi^2} z' + V_{\text{eff}}\left(\frac{\xi s}{1-s}\right) z = \lambda z, \quad s \in (0, 1), \quad (215)$$

which we obtain from Equation (214) by multiplying with $(1-s)^2/\xi$, and the boundary conditions

$$z(0) = z(1) = 0. \quad (216)$$

For later use we denote the coefficients of Equation (215) in the following way:

$$a_2 = -\frac{(1-s)^4}{\xi^2}, \quad a_1 = \frac{2(1-s)^3}{\xi^2}, \quad a_0 = V_{\text{eff}}\left(\frac{\xi s}{1-s}\right). \quad (217)$$

4.4 An alternative transformation compressing the infinite interval - ATCII

The second transformation is given by

$$t_\beta : \begin{cases} (0, \infty) & \rightarrow & (0, 1), \\ r & \mapsto & 1 - (1+r)^{-\beta}, \end{cases} \quad (218)$$

where $\beta > 0$ is a free parameter of the transformation. For the numerical calculations we set $\beta = \frac{1}{2}$.

The coefficients of the transformed Equation (192) with transformation t_ξ are calculated as follows. Here we have

$$t'_\beta(r) = \beta(1+r)^{-(\beta+1)} \quad (219)$$

and

$$t_\beta^{-1} : \begin{cases} (0, 1) & \rightarrow & (0, \infty), \\ s & \mapsto & (1-s)^{-1/\beta} - 1, \end{cases} \quad (220)$$

which yields

$$t'_\beta \circ t_\beta^{-1}(s) = \beta(1-s)^{1+1/\beta} = \frac{(1-s)^{1+k}}{k}, \quad (221)$$

where we have set $1/\beta = k$ for convenience. Hence, the transformed Equation (192) with transformation t_β is given by

$$-\left(\frac{(1-s)^{1+k}}{k}z'\right)' + \frac{kV_{\text{eff}}((1-s)^{-k}-1)}{(1-s)^{1+k}}z = \lambda\frac{k}{(1-s)^{1+k}}z, \quad s \in (0, 1). \quad (222)$$

Here, again, we carried out the numerical calculations via the equivalent equation

$$-\frac{(1-s)^{2k+2}}{k^2}z'' + \frac{(1+k)(1-s)^{2k+1}}{k^2}z' + V_{\text{eff}}((1-s)^{-k}-1)z = \lambda z, \quad s \in (0, 1), \quad (223)$$

which we obtain from Equation (222) by multiplication with $(1-s)^{1+k}/k$, and the boundary conditions

$$z(0) = z(1) = 0. \quad (224)$$

For later use we denote the coefficients of Equation (223) as

$$\begin{aligned} a_2 &= -\frac{(1-s)^{2k+2}}{k^2}, & a_1 &= \frac{(1+k)(1-s)^{2k+1}}{k^2}, \\ a_0 &= V_{\text{eff}}((1-s)^{-k}-1). \end{aligned} \quad (225)$$

5 Numerical solution

In this section we present a way how to compute the eigenvalues and eigenfunctions of the radial Schrödinger equation numerically. We will use a finite difference scheme and apply it to the transformed equations (215) and (223) that we have derived in the last section. The continuous eigenvalue problem then becomes an algebraic eigenvalue problem, which we can solve by the Matlab function `eig` for instance.

5.1 The finite difference scheme

For the finite difference scheme we use the uniform mesh

$$t_i = ih, \quad i = 0, \dots, N, \quad h = \frac{1}{N}, \quad (226)$$

on the interval $[0, 1]$. For the value of z at the meshpoints we use the notation

$$z_i = z(t_i).$$

From the boundary conditions (224) and (216) we know that the eigenfunctions z vanish at the endpoints of the mesh

$$z_0 := z(t_0) = z(0) = 0, \quad z_N := z(t_N) = z(1) = 0. \quad (227)$$

The first and second derivative are approximated by special $2k$ -step central difference formulas, which are introduced in [2]. We consider only the derivatives of the inner meshpoints $i = 1, \dots, N - 1$. At the innermost meshpoints $i = k, \dots, N - k$ we approximate the derivatives by the arithmetic means

$$z'(t_i) \approx \frac{1}{h} \sum_{j=-k}^k \beta_{j+k} z_{i+j}, \quad z''(t_i) \approx \frac{1}{h^2} \sum_{j=-k}^k \alpha_{j+k} z_{i+j}, \quad (228)$$

with weights $\alpha_i, \beta_i \in \mathbb{R}$. However, when $k > 1$, we cannot use the above formulae for the first and last $(k - 1)$ meshpoints. In this case we then add the approximations ($\alpha_{ij}, \beta_{ij} \in \mathbb{R}$)

$$z'(t_i) \approx \frac{1}{h} \sum_{j=1}^{2k} \beta_{ij} z_j, \quad z''(t_i) \approx \frac{1}{h^2} \sum_{j=1}^{2k+1} \alpha_{ij} z_j, \quad (229)$$

for the meshpoints with indices $i = 1, \dots, k - 1$, and

$$z'(t_i) \approx \frac{1}{h} \sum_{j=N-2k}^{N-1} \beta_{ij} z_j, \quad z''(t_i) \approx \frac{1}{h^2} \sum_{j=N-(2k+1)}^{N-1} \alpha_{ij} z_j, \quad (230)$$

for the meshpoints with indices $i = N - (k - 1), \dots, N - 1$.

This finite difference scheme has consistency order $2k$, when the weights $\alpha_i, \alpha_{ij}, \beta_i, \beta_{ij}$ are chosen in a specific way [2]. In fact, the finite difference scheme then also becomes symmetric in the sense that

$$\alpha_j = \alpha_{2k-j}, \quad \beta_j = \beta_{2k-j}, \quad j = 0, \dots, k, \quad (231)$$

where $p = 2k$ denotes the order of the finite difference scheme, and set $\beta = 1/2$ in ATCII.

In Figures 2, 3 and 4 we plotted the relative error for several eigenvalues of Hydrogen Atom potential, Hulthén potential and Yukawa potential against the number of meshpoints N in the finite difference scheme. As the true value in

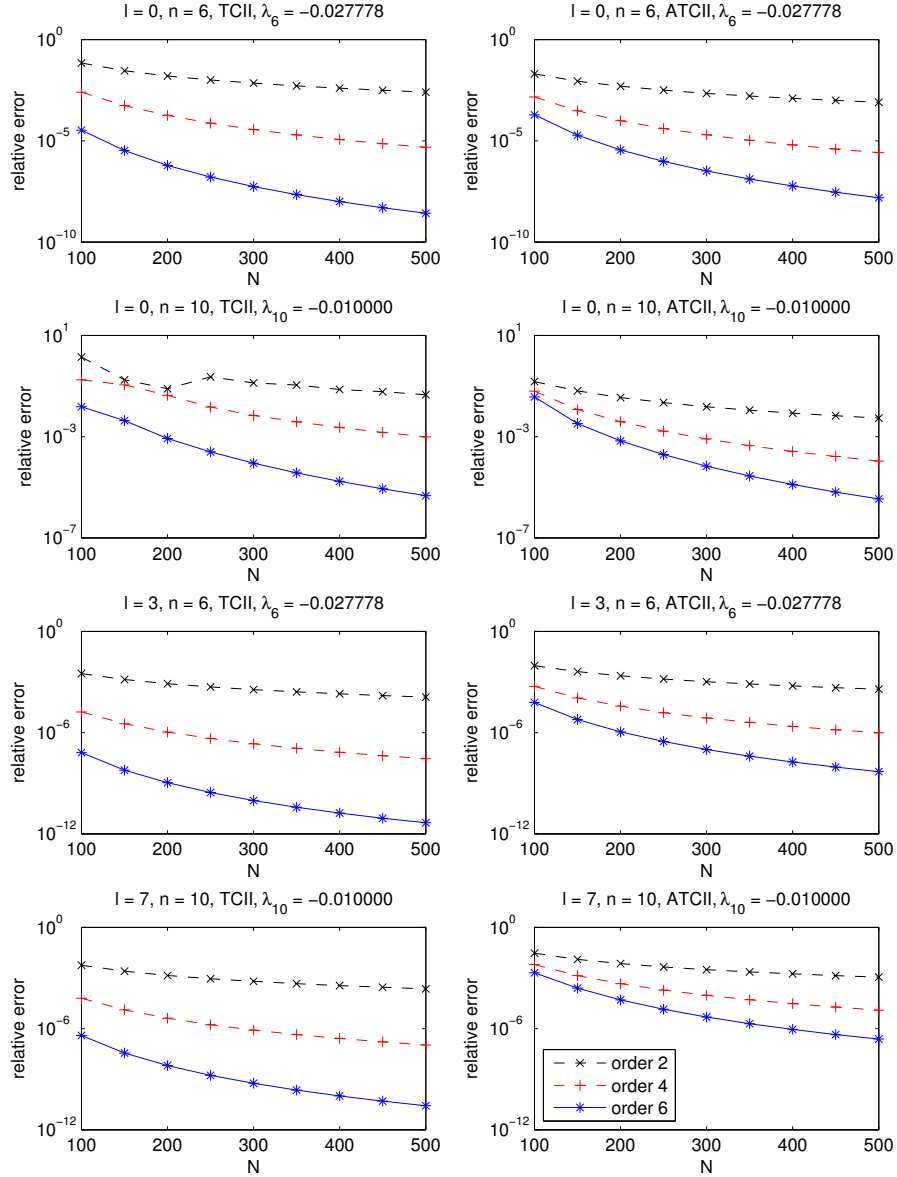


Figure 2: Relative errors for eigenvalues of the radial Schrödinger equation with **Hydrogen Atom** potential and transformation TCII (left) or ATCII (right). As can be seen in the plots the eigenvalues converge faster when using TCII, particularly for high values of ℓ .

the relative error we used the known exact eigenvalues of the Hydrogen Atom potential and the Hulthén potential with $\ell = 0$, or the reference eigenvalues that are calculated from the finite difference scheme with order $p = 8$ and $N = 1500$. The plots on the right hand side are related to TCII, while those on the left hand side to ATCII.

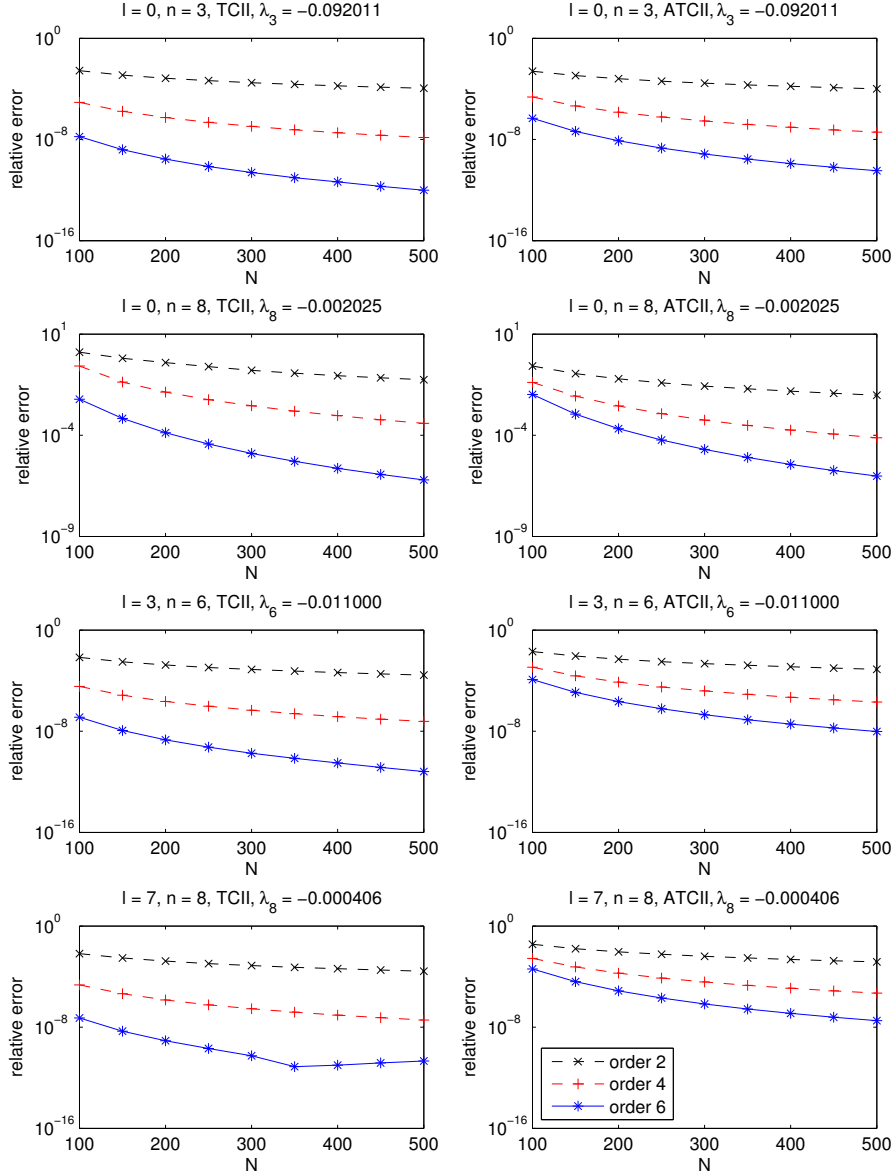


Figure 3: Relative errors for eigenvalues of the radial Schrödinger equation with **Hulthén** potential ($\alpha = 0.02$) and transformation TCII (left) or ATCII (right). As can be seen in the plots the transformation TCII proves to be advantageous over the alternative transformation ATCII.

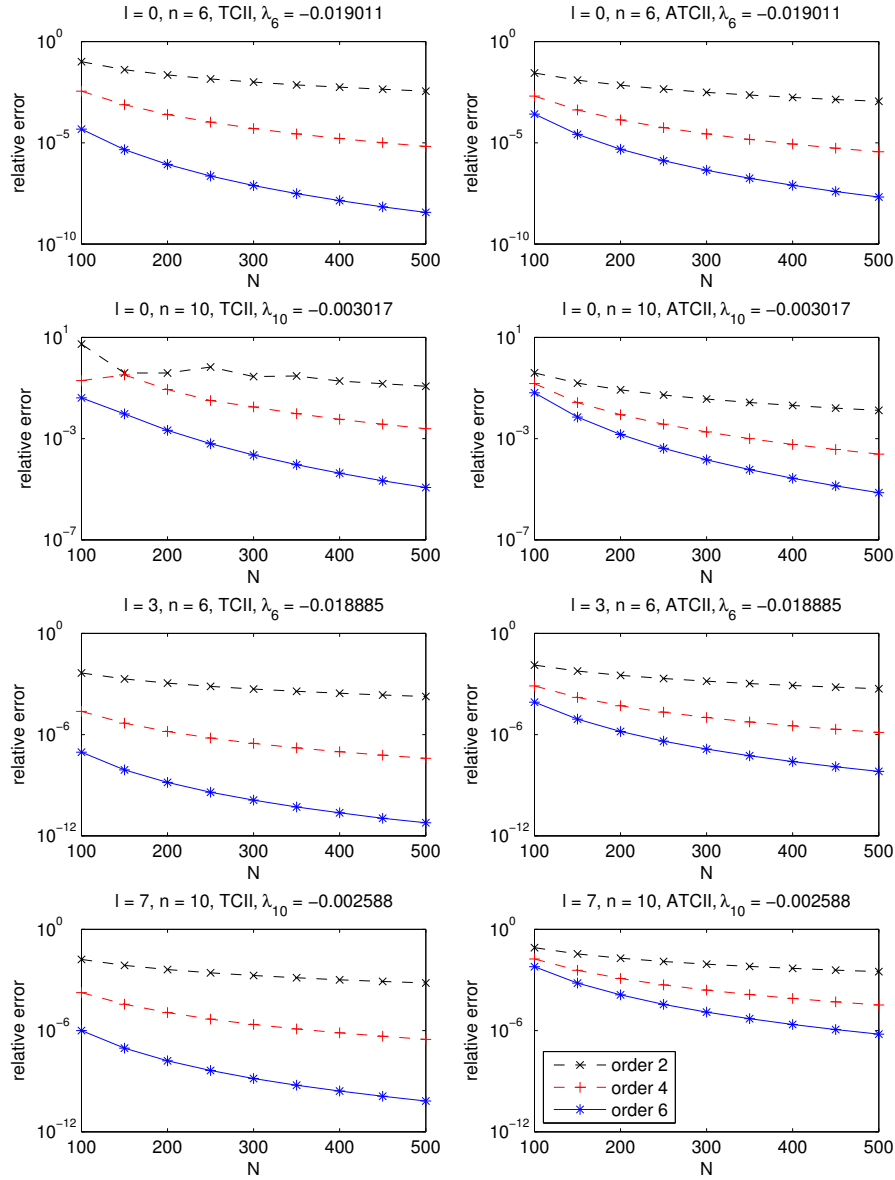


Figure 4: Relative errors for eigenvalues of the radial Schrödinger equation with **Yukawa** potential ($\alpha = 0.005$) and transformation TCII (left) or ATCII (right). Apart from the case with $\ell = 0$ and high values of n , the transformation TCII again appears to be advantageous over the alternative transformation ATCII.

5.3 Numerical Code

finiteDifferences.m

```
function [lambda,Y,t] = finiteDifferences(param,N,n)
% [lambda,Y,t] = finiteDifferences(param,N,n)
% This function returns eigenvalues of the transformed radial
% Schrödinger equation according to a finite difference scheme.
%
% Input:
% param ... Parameter object (see Parameter.m), which stores the
% values of l, alpha, xi and beta as well as the potential
% (Hydrogen Atom, Hulthén or Yukawa potential) and the used
% transformation (TCII or ATCII).
% N ... number of meshpoints
% n ... indices of desired eigenvalues
%
% Output:
% lambda ... desired eigenvalues
% Y ... matrix of columns of associated eigenfunctions
% t ... mesh

% After the application of the change of variable the EVP reads
%  $A_2(t)y''(t) + A_1(t)y'(t) + A_0(t)y(t) = \lambda y(t)$ 
[A2,A1,A0] = equationCoefficients(param);

% compute the uniform mesh over [0,1] and the stepsize
t = linspace(0,1,N+2);
t([1 end]) = [];
h = t(2)-t(1);

% evaluate the coefficient functions at the interior meshpoints
D2 = diag(feval(A2,t));
D1 = diag(feval(A1,t));
D0 = diag(feval(A0,t));

% compute the coefficients of the difference schemes which
% approximate the second and the first order derivative
[A,B] = coeffMatrices(param.order,N+1);
% these columns can be removed due to the condition  $y(0)=y(1)=0$ 
A(:, [1 end]) = [];
B(:, [1 end]) = [];

% assemble the matrix of the algebraic EVP
R = D2*A/h^2 + D1*B/h + D0;

% Compute the numerical eigenvalues
[Y,lambda] = eig(R);
lambda = diag(lambda);
```

```

% Remove any infinite eigenvalues
i = (abs(lambda)==inf);
lambda(i)=[]; Y(:,i)=[];
% Sort the numerical eigenvalues by increasing real part
[~,i]=sort(real(lambda)); lambda=lambda(i); Y=Y(:,i);

% compute the indices of the eigenvalues
n = n - param.l;
n = n(n>0);

% Extract the eigenvalues and the eigenfunctions with the
% desired indexes
lambda=lambda(n);
Y=Y(:,n);

end

```

Parameter.m

```

% This class stores the essential information about the
% particular radial Schroedinger equation and the transformation
% as well as the order of the finite difference scheme.

classdef Parameter
    properties
        l
        potentialName
        potential
        alpha
        order
        transformationName
        beta
        xi
    end

    methods
        function this = set.potentialName(this,in)
            if ismember(in,['Hydrogen Atom','Hulthen','Yukawa'])
                this.potentialName = in;
            else
                error('potential must be either Hydrogen Atom, ' ...
                    'Hulthen or Yukawa');
            end
        end

        function V = get.potential(this)
            switch this.potentialName
                case 'Hydrogen Atom', V = @(r) -2./r;
                case 'Hulthen', V = @(r) -2*this.alpha* ...
                    exp(-this.alpha*r)./(1-exp(-this.alpha*r));
            end
        end
    end
end

```

```

        case 'Yukawa', V = @(r) -2*exp(-this.alpha*r)./r;
    end
end

function out = get.xi(this)
    out = (1.35)^(this.order)*(this.l+1);
end

function this = set.transformationName(this,in)
    if ismember(in,['TCII','ATCII'])
        this.transformationName = in;
    else
        error('transformation must be either set to TCII ...
            or ATCII');
    end
end
end
end
end
end

```

equationCoefficients.m

```

function [A2,A1,A0] = equationCoefficients(param)
% [A2,A1,A0] = equationCoefficients(param)
% This functions returns the coefficient functions
% of a radial Schrödinger equation given by param.
%
% A2 ... coefficient of the second derivative
% A1 ... coefficient of the first derivative
% A0 ... coefficient of the linear term

switch param.transformationName

case 'TCII'
    rxi = 1/param.xi;

    A2=@(t) - rxi^2 * (1-t).^4;
    A1=@(t) 2*rxixi^2 * (1-t).^3;
    A0=@(t) rxi^2 * param.l*(param.l+1)*((1./t)-1).^2 ...
        + param.potential(param.xi*(t./(1-t)));

case 'ATCII'
    k = 1/param.beta;

    A2=@(t) - param.beta^2.*(1-t).^(2*k+2);
    A1=@(t) param.beta*(param.beta+1).*(1-t).^(2*k+1);
    A0=@(t) param.l*(param.l+1)*(1-t).^(2*k)./ ...
        (1-(1-t).^k).^2 + param.potential((1-t).^(-k)-1);

end
end

```

coeffMatrices.m

```
function [A,B]=coeffMatrices(p, N)
% [A,B]=coeffMatrices(p, N)
% This function computes the coefficients of the difference
% quotients which approximate the first and second derivative
% on a equidistant mesh with N meshpoints.
%
% Input:
% p ... order of the difference scheme
% N ... number of mehspoints.
%
% Output:
% A ... matrix of rows of coefficients for the second derivative
% B ... matrix of rows of coefficients for the first derivative

k=p/2;

load('coeff.mat');

C2L = secondDerivative{k,1};
C2 = secondDerivative{k,2};
C2R = reshape(C2L(end:-1:1),size(C2L));

C1L = firstDerivative{k,1};
C1 = firstDerivative{k,2};
C1R = -reshape(C1L(end:-1:1),size(C1L));

A = [C2L; repmat([C2 0], N-p, 1); [0 C2]; C2R];
B = [C1L; repmat(C1, N-p+1, 1); C1R];
[NA,MA] = size(A);
[NB,MB] = size(B);

I = repmat((1:NA)',1,MA);
J = repmat( 1:MA ,NA,1);
temp = min(N-k-1,I);
temp = max(0,temp-k);
J = J+temp;
A = sparse(I,J,A(:));

I = repmat((1:NB)',1,MB);
J = repmat( 1:MB ,NB,1);
temp = min(N-k,I);
temp = max(0,temp-k);
J = J+temp;
B = sparse(I,J,B(:));
end
```

exactEigenvalue.m

```
function lambda = exactEigenvalue(param,n)
% lambda = exactEigenvalue(param,n)
% This function returns sufficiently accurate eigenvalues to the
% indices n for a radial Schroedinger equation given by param.
% For the Hydrogen Atom potential and the Hulthen potential with
% l=0 this function relies on the exact formulas, in all other
% cases it computes the eigenvalues via 'finiteDifferences'
% with order p=8 and N=1500.

    if strcmp(param.potentialName,'Hydrogen Atom')
        lambda = -(n).^(-2);
    elseif strcmp(param.potentialName,'Hulthen') && param.l==0
        if param.alpha < 2
            lambda = -(n.^(-1) - n*(param.alpha/2)).^2;
        else
            lambda = [];
        end
    else
        param.order = 8;
        lambda = finiteDifferences(param,1500,n);
    end
end
```

Table 1: Cell entries of the variable `firstDerivative` in `coeff.mat`:

{1,2}	$\frac{1}{2}$	$[-1 \ 0 \ 1]$
{2,1}	$\frac{1}{12}$	$[-3 \ -10 \ 18 \ -6 \ 1]$
{2,2}	$\frac{1}{12}$	$[1 \ -8 \ 0 \ 8 \ -1]$
{3,1}	$\frac{1}{60}$	$\begin{bmatrix} -10 & -77 & 150 & -100 & 50 & -15 & 2 \\ 2 & -24 & -35 & 80 & -30 & 8 & -1 \end{bmatrix}$
{3,2}	$\frac{1}{60}$	$[-1 \ 9 \ -45 \ 0 \ 45 \ -9 \ 1]$
{4,1}	$\frac{1}{840}$	$\begin{bmatrix} -105 & -1338 & 2940 & -2940 & 2450 & -1470 & 588 & -140 & 15 \\ 15 & -240 & -798 & 1680 & -1050 & 560 & -210 & 48 & -5 \\ -5 & 60 & -420 & -378 & 1050 & -420 & 140 & -30 & 3 \end{bmatrix}$
{4,2}	$\frac{1}{840}$	$[3 \ -32 \ 168 \ -672 \ 0 \ 672 \ -168 \ 32 \ -3]$
{5,1}	$\frac{1}{2520}$	$\begin{bmatrix} -252 & -4609 & 11340 & -15120 & 17640 & -15876 & 10584 & -5040 & 1620 & -315 & 28 \\ 28 & -560 & -3069 & 6720 & -5880 & 4704 & -2940 & 1344 & -420 & 80 & -7 \\ -7 & 105 & -945 & -1914 & 4410 & -2646 & 1470 & -630 & 189 & -35 & 3 \\ 3 & -40 & 270 & -1440 & -924 & 3024 & -1260 & 480 & -135 & 24 & -2 \end{bmatrix}$
{5,2}	$\frac{1}{2520}$	$[-2 \ 25 \ -150 \ 600 \ -2100 \ 0 \ 2100 \ -600 \ 150 \ -25 \ 2]$
{6,1}	$\frac{1}{27720}$	$\begin{bmatrix} -2310 & -55991 & 152460 & -254100 & 381150 & -457380 & 426888 & -304920 & 163350 & -63525 & 16940 & -2772 & 210 \\ 210 & -5040 & -39611 & 92400 & -103950 & 110880 & -97020 & 66528 & -34650 & 13200 & -3465 & 560 & -42 \\ -42 & 756 & -8316 & -27599 & 62370 & -49896 & 38808 & -24948 & 12474 & -4620 & 1188 & -189 & 14 \\ 14 & -224 & 1848 & -12320 & -17589 & 44352 & -25872 & 14784 & -6930 & 2464 & -616 & 96 & -7 \\ -7 & 105 & -770 & 3850 & -17325 & -8580 & 32340 & -13860 & 5775 & -1925 & 462 & -70 & 5 \end{bmatrix}$
{6,2}	$\frac{1}{27720}$	$[5 \ -72 \ 495 \ -2200 \ 7425 \ -23760 \ 0 \ 23760 \ -7425 \ 2200 \ -495 \ 72 \ -5]$

Table 2: Cell entries of the variable `secondDerivative` in `coeff.mat`:

{1,2}		[1 -2 1]		
{2,1}	$\frac{1}{12}$	[10 -15 -4 14 -6 1]		
{2,2}	$\frac{1}{12}$	[-1 16 -30 16 -1]		
{3,1}	$\frac{1}{180}$	[126 -70 -486 855 -670 324 -90 11]		
{3,2}	$\frac{1}{180}$	[2 -27 270 -490 270 -27 2]		
{4,1}	$\frac{1}{5040}$	[3044 2135 -28944 57288 -65128 51786 -28560 10424 -2268 223]		
		[-223 5274 -7900 -2184 10458 -8932 4956 -1800 389 -38]		
		[38 -603 6984 -12460 5796 882 -952 396 -90 9]		
{4,2}	$\frac{1}{5040}$	[-9 128 -1008 8064 -14350 8064 -1008 128 -9]		
{5,1}	$\frac{1}{25200}$	[13420 29513 -234100 540150 -804200 888510 -731976 444100 -192900 56825 -10180 838]		
		[-838 23476 -25795 -49740 125340 -140504 114198 -68280 29290 -8540 1517 -124]		
		[124 -2326 31660 -53075 11640 27132 -25928 15990 -6900 2010 -356 29]		
		[-29 472 -4240 38040 -67430 34608 336 -2960 1635 -520 96 -8]		
{5,2}	$\frac{1}{25200}$	[8 -125 1000 -6000 42000 -73766 42000 -6000 1000 -125 8]		
{6,1}	$\frac{1}{831600}$	[397020 1545544 -11009160 29331060 -53967100 76285935 -83567088 70858920 -46112220 22619850 -8099080 $\frac{8585828603265023}{4294967296}$ -304260 21535]		
		[-21535 698510 -414141 -3170420 7774525 -10854030 11616330 -9658968 6189315 -2999150 1063315 $-\frac{8945214286725119}{34359738368}$ 39359 -2770]		
		[2770 -60315 950580 -1422421 -397650 2228985 -2535720 2109690 -1340658 643775 $-\frac{7778357571747839}{34359738368}$ 55035 -8270 579]		
		[-579 10876 -113004 1161336 -2002000 761508 $\frac{8422396507717633}{17179869184}$ -548592 370953 -181500 64196 -15624 2346 -164]		
		[164 -2875 25800 -172700 1325500 -2330328 1254000 -72600 -56100 42625 -17336 4500 -700 50]		
{6,2}	$\frac{1}{831600}$	[-50 864 -7425 44000 -222750 1425600 -2480478 1425600 -222750 44000 -7425 864 -50]		

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