Sinc Collocation Methods for Solving Quantum Mechanical Problems

by

Philippe Gaudreau

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Department of Mathematical and Statistical Sciences
University of Alberta

Abstract

In quantum mechanics, the Schrödinger equation is the staple for investigating and understanding quantum phenomena. Adjunct with the Schrödinger equation, the mathematical and physical laboratory that are anharmonic oscillator potentials provide a powerful tool for modelling complex quantum systems. In this work, we successfully apply the the double exponential Sinc-collocation method (DESCM) to the classical anharmonic potential for the numerical evaluation of energy eigenvalues. The DESCM was able to achieve unprecedented accuracy even in the case of multiple wells. This great success has lead us to our current research endeavours. In our current work, we wish to adapt the DESCM to the rational-anharmonic potential as well as the Coulombic-anharmonic potential. The rational-anharmonic potential has several complex singularities which impede the convergence of the DESCM. As a result, we investigate conformal mappings in order to relocate these complex singularities accelerating the convergence of the DESCM. The Coulombic-anharmonic potential has singularities at the end points of its domain which can affect the numerical stability of the DESCM. Subsequently, we investigate methods to remedy these numerical problems. Additionally, we wish to exploit the added symmetrical properties of the matrices generated by the DESCM in the presence of even potentials. We have been able to show that this added symmetry results in centrosymmetry. This added symmetry can be exploited to reduce the complexity of the DESCM by half.

This thesis is dedicated to my parents: Nicole Lepage and Michel Gaudreau.

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Introduction

1.1 The Schrödinger equation

In quantum physics, physicists describe the properties of a physical system by an abstract function known as the wave function. Axiomatically, the wave function of a particle denoted by Ψ should be a function of its space coordinate $\mathbf{r}$ as well as time t. With this formulation, there is a need to generate the wave function of more complicated particle systems. Analogous to Newton's laws in classical physics, the Schrödinger equation allows us to construct wave functions for particle systems in the quantum world. Otherwise stated, the Schrödinger equation is one of the fundamental equations of physics for describing quantum mechanical behaviour. The celebrated Schrödinger equation for a particle moving in a potential $V(\mathbf{r}, t)$ was proposed by Ernest Schrödinger in 1926. The Schrödinger equation is a linear complex valued partial differen-

tial equation given by the following equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = H\Psi(\mathbf{r},t) \doteq \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t), \tag{1.1}$$

where i is the imaginary unit, $\hbar \approx 1.0546 \times 10^{-34}\mathrm{m}^2\mathrm{kg/s}$ is h-bar, a famous physical constant, $V(\mathbf{r},t)$ is the potential, and H is the Hamiltonian operator.

Although there still exists some debate for the interpretation of the wave function still ongoing today, the most popular interpretation in the physics community was given by Max Born. Born won the 1954 Nobel Prize in physics for his "fundamental research in quantum mechanics, especially in the statistical interpretation of the wave function". Born postulated that, if a particle is described by a wave function $\Psi(\mathbf{r},t)$ normalized to unity over its domain of existence, the probability of finding the particle at time t within the volume element $d\mathbf{r} = dxdydz$ about the point $\mathbf{r} = (x,y,z)$ is given by:

$$P(\mathbf{r},t)d\mathbf{r} = |\Psi(\mathbf{r},t)|^2 d\mathbf{r} \tag{1.2}$$

1.1.1 The time-independent Schrödinger equation

In the case where the potential function V does not depend on time, the Hamiltonian operator H is time independent. As a result, equation (1.1) simplifies considerably:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r},t), \tag{1.3}$$

In particular, we can show that a solution decomposes as a product of two functions:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) f(t). \tag{1.4}$$

More generally, the full solution can be expressed as the sum of such a product. Inserting the decomposition (1.4) into equation (1.1) in the case where V does not depend on time, we obtain:

$$i\hbar\, \psi(\mathbf{r}) \frac{\partial f(t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) \right] f(t). \tag{1.5}$$

Separating the variables, we obtain:

$$i\hbar\, \frac{1}{f(t)} \frac{\partial f(t)}{\partial t} = \frac{1}{\psi(\mathbf{r})} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) \right]. \tag{1.6}$$

Since the left-hand side depends only on t and the right-hand side depends only on $\mathbf{r}$, both sides must be equal to a constant. This constant has units of energy and as such is denoted by E. Therefore, we obtain the following two equations:

$$i\hbar\, \frac{\partial f(t)}{\partial t} = E f(t), \tag{1.7}$$

and

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E \psi(\mathbf{r}). \tag{1.8}$$

Equation (1.7) can be solved directly since this equation is separable to obtain:

$$f(t) = Ce^{-iEt/\hbar}, \tag{1.9}$$

for some constant C which without loss of generality can be set to one. Equation (1.8) is known as the time-independent Schrödinger equation. The time-independent Schrödinger equation is a differential eigenvalue equation. If the potiential $V(\mathbf{r})$ is unbounded and diverge to infinity at the edges of its domain, solving equation (1.8) gives us the following solution to equation (1.3):

$$\Psi(\mathbf{r}, t) = \sum_n \psi_n(\mathbf{r}) e^{-iE_n t/\hbar}, \tag{1.10}$$

where $\{(\psi_n(\mathbf{r}), E_n)\}_{n=0}^{\infty}$ are the eigenpairs solutions associated with equation (1.8).

1.1.2 The time-independent Schrödinger equation in one dimension

The time-independent Schrödinger equation in one dimension can be written as follows:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z)\right]\psi(z) = E\psi(z). \tag{1.11}$$

To reduce the number of parameters of this equation the following change of variables is often used:

$$x = \sqrt{\frac{2m}{\hbar^2}}\, z. \tag{1.12}$$

Potential	Form of $V(x)$	Domain
Anharmonic Oscillator Potential	$V(x) = \sum_{i=1}^{m} c_i x^{2i}$	$x \in (-\infty, \infty)$
Rational Potential	$V(x) = \omega x^{2m} + \dfrac{\sum_{i=0}^{k} \lambda_i x^i}{1 + \sum_{i=1}^{2l} g_i x^i}$	$x \in (-\infty, \infty)$
Coulombic Potential	$V(x) = \sum_{i=-2}^{m} a_i x^i$	$x \in (0, \infty)$

Table 1.1: Table of important one-dimensional potentials.

Using this change of variable, we obtain the following equation:

$$\left[-\frac{d^2}{dx^2} + \tilde{V}(x)\right] \psi(x) = E\psi(x). \tag{1.13}$$

In this thesis, we will focus on solving (1.13) for different types of potentials. More specifically, the potentials we will tackle can be broken down into three categories displayed in Table 1.1:

All potentials presented in table 1.1 can be seen as a perturbation from the classical harmonic oscillator $V(x) = x^2$. Despite the name of the first potential in table 1.1, all three fall under the umbrella term of anharmonic potentials i.e. potentials that deviate from harmonicity. As early as the 1950's, one dimensional anharmonic oscillators have had multiple applications in modern physics. Over 60 years ago, the quartic anharmonic oscillator was of great interest to field theoreticians because it modeled complicated fields in one-dimensional spacetime [22]. Quantum field theory concerns with the mechanical models of subatomic particles in particle physics and quasiparticles

in condensed matter physics. This particular field theory model involved no space dimensions resulting in no asymptotic states and no particle scattering. As a result, this theory was an adequate model for a universe which sits at one point and oscillated. Despite its simplicity, this model predicted observed behaviours in more realistic field theory [93]. Hence, it was a great starting point for studying such complexity. Application of these theories can and are still found today [7, 93, 112, 137, 165]. With advances in mathematical techniques, computer architecture, numerical analysis and asymptotic theories, higher order anharmonic oscillators are being used to model higher dimensional fields. Hence, a more complete overview of quantum anharmonic oscillators would lead to a better understanding of the realistic analytic structure of field theory.

Secondly, outside the realm of field theory, double-well anharmonic potentials are among the most important potentials in quantum mechanics [85, 95]. The wave functions for such potentials are known to be the linear superposition of so called "classical states". This revelation is very important in the study of quantum information theory or quantum computing. Concisely, quantum information theory attempts to generalize the ideas of classical information theory to the quantum world. Recently, systems of two particles in double well potentials have been studied experimentally with ultracold atoms [11, 178]. In 2009, it was theoretically proposed that neutral atoms held in double well potentials could be used to create quantum logic gates to be used for quantum information processing [78]. Recently, Murmann et al. demonstrated that the quantum state of two ultracold fermionic atoms in an isolated double-well potential was completely controllable [122]. They were able to control the in-

teraction strength between these two particles, the tilt of the potential as well as their tunneling rates between the two wells. These experiments provide a starting point for quantum computation with neutral atoms. Hence, further investigations into quantum systems with multiple wells could be an asset in constructing an efficient and reliable quantum computer.

Thirdly, other problems in quantum physics that are modelled with the help of anharmonic potentials include the tunnelling of protons in hydrogen bonded systems, quantum phase transitions in ion traps, the spectra of molecules such as ammonia and hydrogen-bonded solids and quantum coherence in Josephson junction superconductors [103, 136, 138]. The Josephson effect occurs when a current flows without any voltage across two superconductors coupled by a weak link. The weak link can take various forms from a thin insulating barrier to a short section of non-superconducting metal or even a physical constriction that weakens the superconductivity at the point of contact. Its applications are very diverse and include superconducting quantum interference devices, precision metrology, superconducting single-electron transistors, rapid single flux quantum digital electronics and superconducting tunnel junction detectors. Moroever, Josephson junctions are crucial in superconducting quantum computing using qubits instead of classical bits.

Last but not least, one dimensional anharmonic oscillators also provides an excellent approximation to more complicated quantum potentials near a stable stationary point. Potential energy in quantum systems can be modelled mathematically by complicated functions adjunct with differential equations. In such models, particles prefer to settle themselves in stable stationary point. Mathematically, this corresponds to the local minimums of the potential energy

function. It is known that every local minimum of a function can be approximated by a much simpler quadratic function. In such case, we obtain the famous well-studied harmonic oscillator. For a better approximation around the stable stationary point, more polynomial terms or a rational function can be added to the quadratic function. This simple yet powerful approximation yields precisely the anharmonic oscillator potentials.

Chapter 2

The Anharmonic Oscillator

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Abstract.

In the present contribution, we derive an asymptotic expansion for the energy eigenvalues of anharmonic oscillators for potentials of the form $V(x) = \kappa x^{2q} + \omega x^2$, $q = 2, 3, \ldots$ as the energy level n approaches infinity. The asymptotic expansion is obtained using the WKB theory and series reversion. Furthermore, we construct an algorithm for computing the coefficients of the asymptotic expansion for quartic anharmonic oscillators, leading to an efficient and accurate computation of the energy values for $n \geq 6$.

2.1 Introduction

The quantum anharmonic oscillator energy eigenvalues have been studied extensively during the last three decades [21, 28, 33, 42, 70, 72, 100, 124, 150, 180, 183–186, 192]. For a quantum anharmonic oscillator, the Hamiltonian in the time-independent Schrödinger equation is $\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$, where the potential $V(x) = \omega\, x^2 + \kappa\, x^{2q}$ with $\omega \in \mathbb{R}$, $\kappa \in \mathbb{R}^+$ and $q \in \mathbb{N} \setminus \{1\}$. The quartic anharmonic oscillator corresponds to $q = 2$, the sextic anharmonic oscillator corresponds to $q = 3$, and the challenging octic anharmonic oscillator corresponds to $q = 4$.

In [22–24], a study of Rayleigh-Schrödinger perturbation series is presented using techniques from the Wentzel-Kramers-Brillouin (WKB) method as well as a difference equation method. The WKB method proved very useful in the calculation of higher-order energy states as the convergence is quite rapid. We refer the interested readers to [21] for an introduction of the WKB method as well as several examples for potentials of the form $V(x) = \lambda\, x^{2m}$ for $m = 2, 3, \ldots$ with $\lambda > 0$. In [2], an averaging method is proposed to calculate energy eigenvalues for potentials of the form $V(x) = \lambda\, x^{2m}$ for $m = 2, 3, \ldots$ with $\lambda > 0$, $V(x) = \mu\, x^2 + \lambda\, x^4 + \eta\, x^6$ with $\eta > 0$ and $V(x) = (a\, x^3 + b\, x)^2$ using a supersymmetric WKB approach.

In [124], an asymptotic energy expansion is presented for potentials $V(x) = \sum_{i=1}^{N} a_i\, x^i + \sum_{j=1}^{M} c_j\, x^{-j}$. This method allows for an easier way to obtain the symbolic coefficients for WKB expansions. As examples of application, in [124] Nanayakkara derived explicit analytic expressions for the first seven coefficients of the WKB expansion for the energy eigenvalues for the potentials

$V(x) = x^4 + \omega\, x^2$ and $V(x) = x^6$. Although this method is very efficient for obtaining symbolic coefficients for WKB expansions, it is cumbersome to obtain several terms in these expansions due to the complexity of the integrals involved in the calculation. A considerably large number of terms are in fact needed if one desires to obtain high accuracy particularly for low energy levels.

In the present work, we derive an asymptotic expansion for the energy eigenvalues of anharmonic oscillators for potentials of the form $V(x) = \kappa\, x^{2q} + \omega\, x^2$ for $q = 2, 3, \ldots$ using the WKB approach. This leads to an asymptotic series relating the energy levels to their corresponding energy values. This form is quite cumbersome from a numerical point of view as it would require the use of a root finding method to compute the energy values. Therefore, using series reversion theory, we revert this series to obtain an analytic expression for the energy values in terms of their corresponding energy levels. This is significantly more efficient as it requires only the summation of a series for different values of n eliminating the need for a root-finding method. The difficulty in evaluating the coefficients of the asymptotic expansion numerically increases significantly as q increases. Nevertheless, we construct an algorithm capable of obtaining a large number of the coefficients for quartic anharmonic oscillators (see Table 2.2). The numerical results obtained using the proposed method are in a complete agreement with those obtained using explicit analytic expressions obtained in [124] and leads to a highly accurate computation of the energy values for $n \geq 6$.

2.2 WKB for anharmonic oscillators

When a differential equation demonstrates dissipative or dispersive phenomena characterized by exponential behavior, one can seek an approximation of the solution of the form:

$$\psi(x) \sim A(x) \exp\left(\frac{S(x)}{\delta}\right) \qquad \text{as} \qquad \delta \to 0^+, \tag{2.1}$$

where the solution has a boundary layer of thickness δ.

For the approximation $\psi(x)$ in (2.1), which is known as the WKB approximation, to be valid we assume that the phase $S(x)$ is non constant and slowly varying in the breakdown region.

The form given by equation (2.1) is not ideal for deriving asymptotic approximations since both the amplitude and the phase functions $A(x)$ and $S(x)$ depend implicitly on δ. To simplify this matter, it is best to expand $A(x)$ and $S(x)$ as series in powers of δ and combine them into a single exponential power series of the form:

$$\psi(x) \sim \exp\left(\frac{1}{\delta}\sum_{n=0}^{\infty} \delta^n S_n(x)\right) \qquad \text{as} \qquad \delta \to 0^+. \tag{2.2}$$

WKB approximations for the solution of 2^{nd} order differential equations are derived from equation (2.2).

Now, let us consider the time-independent Schrödinger equation which is defined by the following equation:

$$\mathcal{H}\,\psi(x) \;=\; E\,\psi(x) \qquad \text{with} \qquad \mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \tag{2.3}$$

where the potential V is given by:

$$V(x) \;=\; \kappa\, x^{2q} + \omega\, x^2, \tag{2.4}$$

where $\kappa \in \mathbb{R}^+$, $\omega \in \mathbb{R}$ and $q \in \mathbb{N} \setminus \{1\}$.

Equation (2.3) can be re-written as follows:

$$\psi'' \;=\; Q(x)\,\psi \qquad \text{with} \qquad Q(x) = \kappa x^{2q} + \omega x^2 - E \neq 0. \tag{2.5}$$

By perturbing the second derivative ψ'' by a factor ϵ^2, we obtain:

$$\epsilon^2\,\psi'' \;=\; Q(x)\,\psi. \tag{2.6}$$

Inserting the expression of ψ given by (2.2) in the above equation and simplifying the exponential factors, one can obtain :

$$\epsilon^2 \left[\left(\frac{1}{\delta} \sum_{n=0}^{\infty} \delta^n S_n''(x) \right) + \frac{1}{\delta^2} \left(\sum_{n=0}^{\infty} \delta^n S_n'(x) \right)^2 \right] \;=\; Q(x). \tag{2.7}$$

Setting $\delta = \epsilon$, we obtain:

$$\epsilon \sum_{n=0}^{\infty} \epsilon^n S_n''(x) + \left(\sum_{n=0}^{\infty} \epsilon^n S_n'(x) \right)^2 = Q(x). \tag{2.8}$$

By equating both sides in powers of ϵ, we obtain the following recurrence

relations [21]:

$$\begin{cases} {S'_0}^2 & = & Q(x) & & \\ 2S'_0S'_1 + S''_0 & = & 0 & & \\ 2S'_0S'_n + S''_{n-1} + \displaystyle\sum_{j=1}^{n-1} S'_jS'_{n-j} & = & 0 & \text{for} \quad & n \geq 2. \end{cases} \tag{2.9}$$

The use of the above recurrence relations has been prevented due to the challenging calculations required to solve for the energy value E.

In 1932, Dunham found that the sum of the contour integrals of S'_n around the two turning points (real solutions of $Q(x) = 0$) was asymptotic to the energy levels [55]:

$$\frac{1}{2i}\oint_C \frac{1}{\epsilon}\sum_{k=0}^{\infty} \epsilon^k S'_k(z)\mathrm{d}z \sim n\pi \qquad \text{as} \qquad \epsilon \to 0^+. \tag{2.10}$$

Using the second relation $2S'_0S'_1 + S''_0 = 0$ in (2.9), Dunham was able to simplify further by noticing that:

$$S'_1(z) = -\frac{1}{4}\frac{\mathrm{d}}{\mathrm{d}z}\ln(Q(z)) \qquad \Rightarrow \qquad \frac{1}{2i}\oint_C S'_1(z)\mathrm{d}z = -\frac{1}{8i}(4\pi i) = -\frac{\pi}{2}. \tag{2.11}$$

Moreover, since all S'_i for $i = 3, 5, 7, \ldots$ are total derivatives by construction, they do not contribute to the calculation of the eigenvalues. The expression is therefore simplified to [55]:

$$\frac{1}{2i}\oint_C \frac{1}{\epsilon}\sum_{k=0}^{\infty} \epsilon^{2k} S'_{2k}(z)\mathrm{d}z \sim \left(n + \frac{1}{2}\right)\pi \qquad \text{as} \qquad \epsilon \to 0^+. \tag{2.12}$$

2.3 Properties of the functions $S'_k(z)$

The following Theorem establishes a form for all $S'_k(z)$ and simplifies their computation using a more efficient and simple recursive algorithm compared with the algorithm that can be obtained from equations (2.9).

Theorem 2.3.1. *If $Q(z) = V(z) - E$ where $V(z)$ is a polynomial of degree $l \geq 2$, then the functions $S'_k(z)$ have the following form:*

$$S'_k(z) = \frac{f_k(z)}{(Q(z))^{\frac{3k-1}{2}}} \qquad for \qquad k = 0, 1, 2, \ldots, \tag{2.13}$$

where $f_k(z)$ are polynomials in z and $\deg(f_k(z)) = k(l-1)$. Moreover, the polynomials $f_k(z)$ are given recursively by:

$$\begin{cases} f_0(z) & = & 1 \\ \displaystyle\sum_{j=0}^{k} f_j(z) f_{k-j}(z) & = & -Q(z)^{\frac{3k-2}{2}} \dfrac{d}{dz}\left(f_{k-1}(z) Q(z)^{\frac{4-3k}{2}}\right), \end{cases} \tag{2.14}$$

which can be rewritten as:

$$f_k(z) = -\frac{1}{2} Q(z)^{\frac{3k-2}{2}} \frac{d}{dz}\left(f_{k-1}(z) Q(z)^{\frac{4-3k}{2}}\right) - \frac{1}{2}\sum_{j=1}^{k-1} f_j(z) f_{k-j}(z). \tag{2.15}$$

Proof. We will proceed by induction.

The property is true for $k = 0$ since we have:

$$\begin{aligned} S'_0(z) &= \sqrt{Q(z)} \\ &= \frac{f_0(z)}{(Q(z))^{\frac{3(0)-1}{2}}}. \end{aligned} \tag{2.16}$$

We assume that the functions $S'_n(z)$ have the form given by (2.13) for $n = 1, 2, \ldots, k$. From this it follows that for $n = 1, 2, \ldots, k$, we have:

$$S'_n(z) = \frac{f_n(z)}{(Q(z))^{\frac{3n-1}{2}}}. \tag{2.17}$$

From the recurrence relations in (2.9), we have for $k \geq 1$:

$$2S'_0 S'_{k+1} + S''_k + \sum_{j=1}^{k} S'_j S'_{k+1-j} = 0. \tag{2.18}$$

Inserting equation (2.17) in equation (2.18) and isolating $S'_{k+1}(z)$, we obtain:

$$S'_{k+1}(z) = -\frac{\frac{f'_k(z)(Q(z)) - f_k(z)(\frac{3k-1}{2})Q'(z)}{(Q(z))^{\frac{3k+1}{2}}} + \sum_{j=1}^{k} \frac{f_j(z)}{(Q(z))^{\frac{3j-1}{2}}} \frac{f_{k+1-j}(z)}{(Q(z))^{\frac{3(k+1-j)-1}{2}}}}{2(Q(z))^{\frac{1}{2}}}. \tag{2.19}$$

Simplifying, we obtain:

$$S'_{k+1}(z) = \frac{f_{k+1}(z)}{(Q(z))^{\frac{3(k+1)-1}{2}}}, \tag{2.20}$$

where:

$$\begin{aligned} f_{k+1}(z) &= -\left(\frac{f'_k(z)}{2}\right) Q(z) + f_k(z) \left(\frac{3k-1}{4}\right) Q'(z) - \frac{1}{2} \sum_{j=1}^{k} f_j(z) f_{k+1-j}(z) \\ &= -\frac{1}{2} Q(z)^{\frac{3(k+1)-2}{2}} \frac{d}{dz} \left(f_k(z) Q(z)^{\frac{4-3(k+1)}{2}} \right) - \frac{1}{2} \sum_{j=1}^{k} f_j(z) f_{k+1-j}(z). \end{aligned} \tag{2.21}$$

Next, we will prove that $\deg(f_k(z)) = k(l-1)$ by induction.

It is obvious that the property is satisfied for $f_0(z) = 1$.

We assume that $\deg(f_n(z)) = n(l-1)$ for $n = 1, 2, \ldots, k-1$. From this it follows that:

$$\begin{cases} \deg(f'_{k-1}(z)) & = & k(l-1) - l \\ \deg(f_j(z)f_{k-j}(z))) & = & (j(l-1)) + ((k-j)(l-1)) = k(l-1). \end{cases} \tag{2.22}$$

Expanding expression (2.15), we obtain:

$$f_k(z) = -\left(\frac{f'_{k-1}(z)}{2}\right) Q(z) + f_{k-1}(z)\left(\frac{3k}{4} - 1\right) Q'(z) - \frac{1}{2}\sum_{j=1}^{k-1} f_j(z)f_{k-j}(z). \tag{2.23}$$

From the above equation, it follows that:

$$\begin{aligned} \deg(f_k(z)) &= \max\left\{ \begin{array}{c} \deg(f'_{k-1}(z)) + \deg(Q(z)) \\ \deg(f_{k-1}(z)) + \deg(Q'(z)) \\ \deg(f_j(z)f_{k-j}(z)))) \end{array} \right\} \\ &= k(l-1). \end{aligned} \tag{2.24}$$

□

Proposition 2.3.2. *If V(z) is an even function, then for $k \in \mathbb{N}_0$, $f_{2k}(z)$ are even functions and $f_{2k+1}(z)$ are odd functions.*

Proof. We will proceed by induction. Since $f_0(z)$ is constant, it is an even function.

First, we notice that if $V(z)$ is even then $Q(z)$ is even. From this, it follows

that:

$$f_1(-z) = -\frac{1}{4}V'(-z) = \frac{1}{4}V'(z) = -f_1(z) \qquad \Rightarrow \qquad f_1(z) \quad \text{is an odd function.} \tag{2.25}$$

Assume that $f_{2n}(z)$ are even functions and $f_{2n+1}(z)$ are odd functions for $n = 1, 2, \ldots, k-1$.

When $f_j(z)$ is an odd function, f_{2k-j} is also an odd function and f_{2k+1-j} is an even function. Similarly, when $f_j(z)$ is an even function, f_{2k-j} is also an even function and f_{2k+1-j} is an odd function. From this and (2.15), it follows that:

$$\begin{aligned} f_{2k}(-z) &= -\frac{1}{2}Q(-z)^{\frac{6k-2}{2}}\frac{d}{d(-z)}\left(f_{2k-1}(-z)Q(-z)^{\frac{4-6k}{2}}\right) - \frac{1}{2}\sum_{j=1}^{2k-1} f_j(-z)f_{2k-j}(-z) \\ &= -\frac{1}{2}Q(z)^{\frac{6k-2}{2}}\frac{d}{dz}\left(f_{2k-1}(z)Q(z)^{\frac{4-6k}{2}}\right) - \frac{1}{2}\sum_{j=1}^{2k-1} f_j(z)f_{2k-j}(z) \\ &= f_{2k}(z), \end{aligned} \tag{2.26}$$

$$\begin{aligned} f_{2k+1}(-z) &= -\frac{1}{2}Q(-z)^{\frac{6k+1}{2}}\frac{d}{d(-z)}\left(f_{2k}(-z)Q(-z)^{\frac{1-6k}{2}}\right) - \frac{1}{2}\sum_{j=1}^{2k} f_j(-z)f_{2k+1-j}(-z) \\ &= \frac{1}{2}Q(z)^{\frac{6k+1}{2}}\frac{d}{dz}\left(f_{2k}(z)Q(z)^{\frac{1-6k}{2}}\right) - \frac{(-1)}{2}\sum_{j=1}^{2k} f_j(z)f_{2k+1-j}(z) \\ &= -f_{2k+1}(z). \end{aligned} \tag{2.27}$$

□

The following Theorem establishes the asymptotic behavior of the integrals in (2.12) as E tends to infinity. It also demonstrates that we do not need to know explicitly the solutions to $Q(z) = 0$ to evaluate the contour integrals

involved in (2.12). As we shall see, all the zeros of $Q(z)$ follow the same pattern as E tends to infinity. Prior to this development, it would have been impossible to deal with anharmonic oscillators where $q \geq 4$ as it would have been impossible to find explicit analytic expressions for the zeros.

Theorem 2.3.3. *If $V(z)$ is an even function as described in theorem 2.3.1 and $V(\pm\infty) = \infty$, then:*

$$\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z = O\left(E^{-\frac{(l+2)(2k-1)}{2l}}\right) \quad \text{as} \quad E \to \infty. \tag{2.28}$$

Proof. Using equation (2.13), we obtain:

$$\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z = \frac{1}{2i}\oint_C f_{2k}(z)Q(z)^{\frac{1}{2}-3k}\mathrm{d}z. \tag{2.29}$$

We need to parametrize $S'_{2k}(z)$ around the two real zeros of $Q(z)$. We can do this by setting $z = R(E)e^{it}$ for $\alpha < t \leq \alpha+2\pi, \alpha \in \mathbb{R}$. α is chosen according to the branch cut of $Q(z)^{\frac{1}{2}-3k}$. $R(E)$ is the radius of the circle as a function of E. Thus, we have:

$$\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z = \frac{1}{2i}\int_\alpha^{\alpha+2\pi} R(E)\, i\, e^{it}\, f_{2k}(R(E)\, e^{it})\, (Q(R(E)e^{it}))^{\frac{1}{2}-3k}\, \mathrm{d}t. \tag{2.30}$$

The optimal choice for $R(E)$ is $(\frac{E}{a_l})^{\frac{1}{l}}$ where a_l is the non-zero coefficient of the leading order term z^l in $V(z)$. This is due to the fact that all the solutions of $Q(z) = 0$ (*i.e.* $V(z) = E$) tend to $(\frac{E}{a_l})^{\frac{1}{l}}$ in modulus as $E \to \infty$. This can be demonstrated by a regular perturbation analysis.

Making the substitution $R(E) = (\frac{E}{a_l})^{\frac{1}{l}}$ in (2.30), we obtain:

$$\frac{1}{2i}\oint_C S'_{2k}(z)\,\mathrm{d}z = \quad E^{\frac{1}{l}}\int_\alpha^{\alpha+2\pi}\frac{1}{2}a_l^{-\frac{1}{l}}e^{it}f_{2k}\left((a_l^{-1}E)^{\frac{1}{l}}e^{it}\right)Q\left((a_l^{-1}E)^{\frac{1}{l}}e^{it}\right)^{\frac{1}{2}-3k}\mathrm{d}t. \tag{2.31}$$

Since $\deg(Q(z)) = l$, we can extract E from $Q\left((a_l^{-1}E)^{\frac{1}{l}}e^{it}\right)$. Moreover, we can extract $E^{\frac{2k(l-1)}{l}}$ from $f_{2k}\left((a_l^{-1}E)^{\frac{1}{l}}\,e^{it}\right)$ since $\deg(f_{2k}(z)) = 2k(l-1)$. From this, it follows that as $E\to\infty$:

$$E^{\frac{1}{l}}\int_\alpha^{\alpha+2\pi}\frac{1}{2}a_l^{-\frac{1}{l}}e^{it}f_{2k}\left((a_l^{-1}E)^{\frac{1}{l}}e^{it}\right)Q\left((a_l^{-1}E)^{\frac{1}{l}}e^{it}\right)^{\frac{1}{2}-3k}\mathrm{d}t = O\left(E^{-\frac{(l+2)(2k-1)}{2l}}\right) \tag{2.32}$$

□

Theorem 2.3.4. *For an anharmonic oscillator potential $V(z) = \kappa z^{2q} + \omega z^2$ of order $q = 2, 3, \ldots$, we have:*

$$\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z \sim E^{-\frac{(q+1)(2k-1)}{2q}}\sum_{j=0}^{\infty}d_j(k,q,\kappa,\omega)E^{-\frac{j}{q}} \quad \text{as} \quad E\to\infty. \tag{2.33}$$

Proof. Using equation (2.31) with $l = 2q$, we obtain:

$$\begin{aligned}\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z &= E^{\frac{1}{2q}}\int_\alpha^{\alpha+2\pi}\frac{e^{it}}{2\kappa^{\frac{1}{2q}}}f_{2k}(\kappa^{-\frac{1}{2q}}E^{\frac{1}{2q}}e^{it})(\kappa(\kappa^{-\frac{1}{2q}}E^{\frac{1}{2q}}e^{it})^{2q}+\omega(\kappa^{-\frac{1}{2q}}E^{\frac{1}{2q}}e^{it})^2-E)^{\frac{1}{2}-3k}\mathrm{d}t\\ &= E^{\frac{1}{2q}+\frac{1}{2}-3k}\int_\alpha^{\alpha+2\pi}\frac{e^{it}}{2\kappa^{\frac{1}{2q}}}f_{2k}(\kappa^{-\frac{1}{2q}}E^{\frac{1}{2q}}e^{it})\left((e^{2qit}-1)+\frac{\omega E^{\frac{1}{q}-1}}{\kappa^{\frac{1}{q}}}e^{2it}\right)^{\frac{1}{2}-3k}\mathrm{d}t.\end{aligned} \tag{2.34}$$

Taking into consideration that $f_{2k}(z)$ is even for such a potential and expand-

ing $f_{2k}\left(\kappa^{-\frac{1}{2q}}E^{\frac{1}{2q}}e^{it}\right)$ into an asymptotic series in E, we obtain:

$$f_{2k}(\kappa^{-\frac{1}{2q}}E^{\frac{1}{2q}}e^{it}) = E^{\frac{k(2q-1)}{q}}\sum_{j=0}^{2k(2q-1)} p_j(k,q,\kappa,\omega,e^{it})E^{-\frac{j}{q}} \quad \text{as} \quad E\to\infty, \tag{2.35}$$

where $p_j(k,q,\kappa,\omega,e^{it})$ are polynomials in e^{it} that depend on k,q,ω and κ.

Expanding $\left((e^{2qit}-1)+\frac{\omega E^{\frac{1}{q}-1}}{\kappa^{\frac{1}{q}}}e^{2it}\right)^{1/2-3k}$ into a binomial series, we obtain:

$$\begin{aligned}\left((e^{2qit}-1)+\frac{\omega E^{\frac{1}{q}-1}}{\kappa^{\frac{1}{q}}}e^{2it}\right)^{\frac{1}{2}-3k} &= \sum_{m=0}^{\infty}\binom{\frac{1}{2}-3k}{m}\frac{(e^{2qit}-1)^{\frac{1}{2}-3k-m}\omega^m e^{2imt}}{\kappa^{\frac{m}{q}}E^{(1-\frac{1}{q})m}}\\ &= \sum_{m=0}^{\infty} h_m\, E^{-(1-\frac{1}{q})m},\end{aligned} \tag{2.36}$$

where:

$$\begin{aligned}h_m &= h_m(k,q,\kappa,\omega,e^{it})\\ &= \binom{\frac{1}{2}-3k}{m}\frac{(e^{2qit}-1)^{\frac{1}{2}-3k-m}\omega^m e^{2imt}}{\kappa^{\frac{m}{q}}}.\end{aligned} \tag{2.37}$$

Using equations (2.35) and (2.36) along with (2.34) and letting $E\to\infty$, we obtain:

$$\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z \sim E^{-\frac{(q+1)(2k-1)}{2q}}\sum_{m=0}^{\infty}\sum_{j=0}^{2k(2q-1)}\left[\int_{\alpha}^{\alpha+2\pi} h_m\, p_j(k,q,\kappa,\omega,e^{it})\,\frac{e^{it}}{2\kappa^{\frac{1}{2q}}}\mathrm{d}t\right]E^{-\frac{(q-1)m+j}{q}} \tag{2.38}$$

$$= E^{-\frac{(q+1)(2k-1)}{2q}}\sum_{m=0}^{\infty}\sum_{\eta=0}^{2k(2q-1)}\tau_{\eta,m}(k,q,\kappa,\omega)\,E^{-\frac{(q-1)m+\eta}{q}}, \tag{2.39}$$

and by combining the two summation in the RHS of the above equation, we

obtain:

$$\frac{1}{2i}\oint_C S'_{2k}(z)\mathrm{d}z \sim E^{-\frac{(q+1)(2k-1)}{2q}} \sum_{\lambda=0}^{\infty} d_\lambda(k,q,\kappa,\omega)\, E^{-\frac{\lambda}{q}}. \tag{2.40}$$

□

Using (2.40), we obtain:

$$\begin{aligned}\frac{1}{2i}\oint_C \sum_{k=0}^{\infty} S'_{2k}(z)\mathrm{d}z &\sim \sum_{k=0}^{\infty}\left(E^{-\frac{(q+1)(2k-1)}{2q}} \sum_{\lambda=0}^{\infty} d_\lambda(k,q,\kappa,\omega)\, E^{-\frac{\lambda}{q}}\right)\\ &= E^{\frac{q+1}{2q}} \sum_{k=0}^{\infty}\sum_{\lambda=0}^{\infty} d_\lambda(k,q,\kappa,\omega)\, E^{-\frac{\lambda+(q+1)k}{q}},\end{aligned}$$

and here again, we combine the two summation in the RHS of the above equation and we obtain:

$$\frac{1}{2i}\oint_C \sum_{k=0}^{\infty} S'_{2k}(z)\mathrm{d}z \sim E^{\frac{q+1}{2q}} \sum_{j=0}^{\infty} \beta_j(q,\kappa,\omega) E^{-\frac{j}{q}}. \tag{2.41}$$

By setting $\epsilon = 1$ in (2.12) and using the above equation, we obtain:

$$E^{\frac{q+1}{2q}} \sum_{j=0}^{\infty} \beta_j(q,\kappa,\omega)\, E^{-\frac{j}{q}} \sim \left(n+\frac{1}{2}\right)\pi \quad \text{as} \quad n\to\infty. \tag{2.42}$$

The difficulty in evaluating the integrals in (2.33) numerically stems from the coefficients $h_m(k,q,\kappa,\omega,e^{it})$ in equation (2.36). As q increases the number of branch cuts in the term $(e^{2qit}-1)^{\frac{1}{2}-3k-m}$ also increases. For $q=2$, we derived an algorithm capable of computing the coefficients $\beta_j(q,\kappa,\omega)$.

Equation (2.42) gives a direct correlation between the energy values E and the energy levels n for all $q \geq 2$. However, this expression is not practical from

a computational point of view. In order to obtain the energy value E, one would have to truncate the sum and use a root-finding method for each value of n. It would be much more efficient if we could derive an analytic expression for E in terms of n. This is the focus of the next section where we make use of the theory of series reversion.

2.4 Asymptotic Series Reversion

The reversion of series is not a new topic in mathematical analysis. One of the most famous Theorems published by Lagrange on the reversion of power series dates back to 1770 [98]. Since then, several new discoveries have been made in this field. In [61], Fabijonas and Olver used an asymptotic series reversion to calculate the zeros of the Airy functions to high accuracy.

In the following section, we will be extending the Fabijonas and Olver formula for the reversion of an asymptotic expansion [61] for a different type of asymptotic series.

Now, we shall state two Theorems presented in [61, Theorem 2.1].

Theorem 2.4.1. *[61, Theorem 2.1] Let $f(z)$ be analytic at $z = z_0$, $f(z_0) = \omega_0$ and $f'(z_0) \neq 0$. The equation $\omega = f(z)$ has a unique solution $z = F(\omega)$ such that $F(\omega_0) = z_0$ and $F(\omega)$ is analytic at $\omega = \omega_0$.* □

Theorem 2.4.1 is a standard theorem of complex analysis and its proof can be found in [45, Chapter 6] or [189, Chapter 7].

Theorem 2.4.2. *[61, Theorem 2.3] Let $f(z)$ be analytic in a domain that includes a closed annular sector* **S** *with vertex at the origin and angle less than*

2π, *and satisfy an asymptotic expansion of the form:*

$$f(z) \sim z + \sum_{k=0}^{\infty} \frac{a_k}{z^k} \quad \text{as} \quad z \to \infty, \tag{2.43}$$

in $\mathbf{S}$ *uniformly with respect to* ph z. *Also, let* $\mathbf{S_1}$ *and* $\mathbf{S_2}$ *be closed annular sectors with vertices at the origin,* $\mathbf{S_1}$ *being properly interior to* $\mathbf{S}$ *and* $\mathbf{S_2}$ *being properly interior to* $\mathbf{S_1}$.

(i) If the boundary arcs of $\mathbf{S_1}$ *and* $\mathbf{S_2}$ *are of sufficiently large radius, the equation* $\omega = f(z)$ *has exactly one root* $z = F(\omega)$ *say in* $\mathbf{S_1}$ *for each* $\omega \in \mathbf{S_2}$.

(ii) $F(\omega)$ *is analytic within* $\mathbf{S_2}$.

(iii) As $\omega \to \infty$ *in* $\mathbf{S_2}$, *we have:*

$$z \sim \omega - \sum_{j=0}^{\infty} \frac{F_j}{\omega^j}. \tag{2.44}$$

□

The proof for (i) can be found in section 6 of chapter 1 in [131]. The proof for (ii) comes from Theorem 2.4.1. Part (iii) is proved in section 8.4 of chapter 1 in [131].

Theorem 2.4.3. *Let* $f(z)$ *satisfy the same conditions as in Theorem 2.4.2 with an asymptotic expansion of the form:*

$$f(z) \sim z^{\alpha} \sum_{k=0}^{\infty} \frac{a_k}{z^{\delta k}} \quad \text{as} \quad z \to \infty, \tag{2.45}$$

then as $\omega \to \infty$ *in* $\mathbf{S_2}$*, we have:*

$$z \sim \left(\left(\frac{\omega}{a_0} \right)^{\frac{\delta}{\alpha}} - \sum_{j=0}^{\infty} \frac{F_j}{\omega^{\frac{\delta j}{\alpha}}} \right)^{\frac{1}{\delta}}. \tag{2.46}$$

Proof. We start by making the following substitutions in (2.45):

$$z^{\delta} = \frac{1}{x} \qquad \text{and} \qquad f(z) = \omega = \frac{1}{y^{\frac{\alpha}{\delta}}}. \tag{2.47}$$

Equation (2.45) then becomes:

$$\begin{aligned} \frac{1}{y^{\frac{\alpha}{\delta}}} \sim \frac{\sum_{k=0}^{\infty} a_k x^k}{x^{\frac{\alpha}{\delta}}} \quad \text{as} \quad x \to 0^+ \qquad &\Rightarrow \qquad y^{\frac{\alpha}{\delta}} \sim \frac{x^{\frac{\alpha}{\delta}}}{\sum_{k=0}^{\infty} a_k x^k} \quad \text{as} \quad x \to 0^+ \\ &\Rightarrow \qquad y \sim \frac{x}{\left(\sum_{k=0}^{\infty} a_k x^k \right)^{\frac{\delta}{\alpha}}} = \phi(x) \quad \text{as} \quad x \to 0^+. \end{aligned} \tag{2.48}$$

It can be shown that for all sufficiently small values of $|x|, \phi(x)$ is analytic at $x = 0$. In addition:

$$\phi(0) = 0 \qquad \text{and} \qquad \phi'(0) = a_0^{-\frac{\delta}{\alpha}}. \tag{2.49}$$

By Theorem 2.1, when y lies in the neighbourhood Υ of the origin, the equation $\phi(t) = y$ has a single root $t = x$ such that:

(a) $x = 0$ when $y = 0$;

(b) x is an analytic function of y.

Let C be a circle centred at the origin and within Υ. If $|y|$ is sufficiently small, then both x and y lie within C. Hence, by the residue Theorem, we have:

$$\begin{aligned}\frac{1}{2\pi i}\oint_C \frac{\phi'(t)}{t(\phi(t)-y)}\,\mathrm{d}t &= \frac{1}{x}+\frac{\phi'(0)}{\phi(0)-y}\\ &= \frac{1}{x}-\frac{a_0^{-\frac{\delta}{\alpha}}}{y}.\end{aligned} \tag{2.50}$$

The last quantity has a removable singularity at $y=0$ and can therefore be expanded in a series of the form:

$$\begin{aligned}&\frac{1}{x}-\frac{a_0^{-\frac{\delta}{\alpha}}}{y} = -\sum_{j=0}^{\infty} F_j y^j \quad \text{as} \quad y\to 0^+\\ \Rightarrow \qquad & z\sim\left(\left(\frac{\omega}{a_0}\right)^{\frac{\delta}{\alpha}}-\sum_{j=0}^{\infty}\frac{F_j}{\omega^{\frac{\delta j}{\alpha}}}\right)^{\frac{1}{\delta}} \quad \text{as} \quad \omega\to\infty.\end{aligned} \tag{2.51}$$

□

Now, we shall state a Theorem that will establish a relationship between the coefficients of the initial series and those of the reversed series.

Theorem 2.4.4. *For $j=0,1,2,3,\ldots$, F_j are given by:*

$$\begin{cases} F_0 &= \dfrac{\delta}{\alpha}\dfrac{a_1}{a_0}\\ F_j &= \dfrac{1}{j(j+1)!}\dfrac{\mathrm{d}^{\mathrm{j}+1}}{\mathrm{d}t^{j+1}}\left(\displaystyle\sum_{k=0}^{\infty}a_k t^k\right)^{\frac{\delta j}{\alpha}}\Bigg|_{t=0} \quad \text{for} \quad j\geq 1.\end{cases} \tag{2.52}$$

Proof. We will start by proving the equation for F_j for $j=1,2,\ldots$ in (2.52).

Differentiating (2.50) and (2.51) and integrating by parts, we find that:

$$\begin{aligned}\sum_{j=1}^{\infty} jF_j y^{j-1} &= -\frac{1}{2\pi i}\oint_C \frac{\phi'(t)}{t(\phi(t)-y)^2}\,\mathrm{d}t \\ &= \frac{1}{2\pi i}\oint_C \frac{1}{t^2(\phi(t)-y)}\mathrm{d}t. \end{aligned} \tag{2.53}$$

We can expand the last integrand in ascending powers of y:

$$\sum_{j=1}^{\infty} jF_j y^{j-1} = \frac{1}{2\pi i}\sum_{k=0}^{\infty} y^k \oint_C \frac{1}{t^2(\phi(t))^{k+1}}\mathrm{d}t. \tag{2.54}$$

Equating powers of y, we obtain:

$$\begin{aligned} jF_j &= \frac{1}{2\pi i}\oint_C \frac{1}{t^2(\phi(t))^j}\mathrm{d}t \\ &= \frac{1}{2\pi i}\oint_C \frac{(\frac{t}{\phi(t)})^j}{t^{j+2}}\,\mathrm{d}t. \end{aligned} \tag{2.55}$$

By the Cauchy integral formula, we obtain for $j \geq 1$:

$$jF_j = \frac{1}{(j+1)!}\frac{\mathrm{d}^{\mathrm{j}+1}}{\mathrm{d}t^{j+1}}\left(\frac{t}{\phi(t)}\right)^j\Bigg|_{t=0} \quad \Rightarrow \quad F_j = \frac{1}{j(j+1)!}\frac{\mathrm{d}^{\mathrm{j}+1}}{\mathrm{d}t^{j+1}}\left(\sum_{k=0}^{\infty} a_k t^k\right)^{\frac{\delta j}{\alpha}}\Bigg|_{t=0}. \tag{2.56}$$

We shall now prove the equation for F_0 in (2.52). In fact, F_0 is simply a

limiting case of (2.52) as $j \to 0$:

$$\begin{aligned} F_j(t) &= \frac{1}{j(j+1)!}\frac{\mathrm{d}^{\mathrm{j}+1}}{\mathrm{d}t^{j+1}}\left(\sum_{k=0}^{\infty} a_k t^k\right)^{\frac{\delta j}{\alpha}} \\ &= \frac{1}{j(j+1)!}\frac{\mathrm{d}^{\mathrm{j}}}{\mathrm{d}t^{j}}\left[j\frac{\delta}{\alpha}\left(\sum_{k=0}^{\infty} a_k t^k\right)^{\frac{\delta j}{\alpha}-1}\sum_{k=1}^{\infty} k a_k t^{k-1}\right] \\ &= \frac{\delta}{\alpha}\frac{1}{(j+1)!}\frac{\mathrm{d}^{\mathrm{j}}}{\mathrm{d}t^{j}}\left[\left(\sum_{k=0}^{\infty} a_k t^k\right)^{\frac{\delta j}{\alpha}-1}\sum_{k=1}^{\infty} k a_k t^{k-1}\right]. \end{aligned} \tag{2.57}$$

Taking the limit as $j \to 0$, we obtain:

$$F_0(t) = \frac{\delta}{\alpha}\left[\left(\sum_{k=0}^{\infty} a_k t^k\right)^{-1}\sum_{k=1}^{\infty} k a_k t^{k-1}\right] \qquad \Rightarrow \qquad F_0 = \frac{\delta}{\alpha}\frac{a_1}{a_0}. \tag{2.58}$$

□

Corollary 2.4.5. *The analytic expression for the coefficients F_j given by* (2.52) *can be simplified to:*

$$F_j = \frac{1}{j(j+1)!}\frac{\mathrm{d}^{\mathrm{j}+1}}{\mathrm{d}t^{j+1}}\left(\sum_{k=0}^{j+1} a_k t^k\right)^{\frac{\delta j}{\alpha}}\Bigg|_{t=0} \qquad \text{for} \quad j \geq 1. \tag{2.59}$$

Proof. We make use of the Faà di Bruno formula generalizing the chain rule to higher order derivatives to prove the validity of the equation given in the Corollary.

The Faà di Bruno formula is given by [52, 53]:

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n} f(g(t)) = \sum_{i=0}^{n} f^{(i)}(g(t)) B_{n,i}(g'(t), g''(t), \ldots, g^{(n-i+1)}(t)), \tag{2.60}$$

where $B_{n,i}$ are the Bell polynomials [18].

Applying the formula to $F_j(t)$, we obtain:

$$F_j(t) = \frac{1}{j(j+1)!}\sum_{i=0}^{j+1}\prod_{m=1}^{i}\left(\frac{\delta j}{\alpha}-m+1\right)\left(\sum_{k=0}^{\infty}a_k t^k\right)^{\frac{\delta j}{\alpha}-i} \times B_{j+1,i}\left[\sum_{k=1}^{\infty}a_k k t^{k-1}, \sum_{k=2}^{\infty}a_k k(k-1)t^{k-2}, \ldots, \sum_{k=j+2-i}^{\infty}a_k \prod_{n=1}^{j+2-i}(k-n+1)t^{k-j-2+i}\right]. \tag{2.61}$$

By setting $t = 0$, we obtain:

$$F_j = \frac{1}{j(j+1)!}\sum_{i=0}^{j+1}\prod_{m=1}^{i}\left(\frac{\delta j}{\alpha}-m+1\right)(a_0)^{\frac{\delta j}{\alpha}-i}\, B_{j+1,i}\left(a_1, 2a_2, \ldots, (j+2-i)!\; a_{j+2-i}\right). \tag{2.62}$$

As we can see, the F_j's depend only on the coefficients $a_0, a_1, \ldots, a_{j+1}$. □

We now have all the tools required to revert the series (2.42) obtained in the previous section. By using Corollary 2.4.3 with $z = E$, $\omega = \left(n+\frac{1}{2}\right)\pi$, $\alpha = \frac{q+1}{2q}$ and $\delta = \frac{1}{q}$, we arrive at the following equation:

$$E = E_n \sim \left[\left(\frac{(n+\frac{1}{2})\pi}{\beta_0(q,\kappa,\omega)}\right)^{\frac{2}{q+1}} - \sum_{j=0}^{\infty}\frac{F_j(q,\kappa,\omega)}{\left((n+\frac{1}{2})\pi\right)^{\frac{2j}{q+1}}}\right]^q \quad \text{as} \quad n\to\infty. \tag{2.63}$$

2.5 Numerical Discussion

In this section, we will discuss the numerical procedure used to calculate the energy values for a quartic anharmonic oscillator $V(z) = \kappa z^4 + \omega z^2$. All the numerical procedures were done using Maple with 20 decimal precision. The

form of the $S_k'(z)$ proved in Theorem 2.3.1 greatly improves the efficiency and simplifies considerably the calculations required by WKB. One will quickly notice that the form of the $S_k'(z)$ in 2.3.1 and the recurrence relations (2.14) can be generalized for any well defined potential $V(z)$. Previously, the recurrence relation (2.9) involved differentiating rational functions whereas the recurrence relation for the numerator (2.14) involves only differentiation of polynomials. Lastly, the general form found in Theorem 2.3.4 for any anharmonic oscillator of order q and its reverted series found through Theorem 2.4.3, offer an efficient method for computing the energy values without having to resort to root finding methods.

Theorems presented in this work are useful in determining the general form of the asymptotic expansions for potentials of the form $V(z) = \kappa x^4 + \omega x^2$. However, the approach we used to compute the coefficients $\beta_j(2, \kappa, \omega)$ differs slightly from our theoretical development presented in the Theorems.

First, we use the symbolic programming language Maple to compute the polynomials $f_{2k}(z)$ using the expression (2.15). Second, from the form of the integrand $S_k'(z)$ in Theorem 2.3.1, it is very easy to create a list of integrands $S_{2k}'(z)$ that are needed since we can simply divide the polynomials $f_{2k}(z)$ by $Q(z)^{\frac{6k-1}{2}}$ which will be required in the asymptotic expansions presented in equation (2.12). Next, we make a slightly different change of variable than the one presented in the proof of Theorem 2.3.3. Instead of substituting $z = \left(\frac{E}{\kappa}\right)^{\frac{1}{2q}} e^{it}$ into our integrands $S_{2k}'(z)$, we enlarge our radius by a constant $C > \kappa$, say $\left(\frac{E}{\kappa}\right)^{\frac{1}{2q}} \to \left(C\frac{E}{\kappa}\right)^{\frac{1}{2q}}$ and take the real part after integrating $S_{2k}'(z)$ over $(-\pi, \pi]$. This leads to a less cumbersome numerical integration for Maple.

The expansion of $Q\left(\left(C\frac{E}{\kappa}\right)^{\frac{1}{2q}} e^{it}\right)^{\frac{6k-1}{2}}$ using the binomial formula can be

done in a similar fashion than the one presented in Theorem 2.3.4. Once, this integration is done, we can simply collect the coefficients in front of the powers of E presented in equation (2.42). These coefficients correspond to the coefficients $\beta_j(2,\kappa,\omega)$. If we uses $2n$ functions $S'_{2k}(z)$ in their expansion, we would obtain $3(n+1)$ coefficients $\beta_j(2,\kappa,\omega)$. This relation was obtained empirically.

Since only finitely many coefficients $\beta_j(2,\kappa,\omega)$ can be calculated, we use (2.63) and truncate the sum. To calculate the $F_j(2,\kappa,\omega)$ coefficients, we simply use (2.63).

In [124], Nanayakkara presented explicitly the analytical expressions of the first seven coefficients $\beta(2,1,\omega)$ for the potential $V(z) = z^4 + \omega z^2$. These analytic expressions are given by:

$$\begin{aligned}
\beta_0 &= \frac{\sqrt{\pi}\,\Gamma(1/4)}{3\,\Gamma(3/4)} \\
\beta_1 &= -\frac{\omega\sqrt{\pi}\,\Gamma(3/4)}{\Gamma(1/4)} \\
\beta_2 &= \frac{\omega^2\sqrt{\pi}\,\Gamma(1/4)}{32\,\Gamma(3/4)} \\
\beta_3 &= -\left(\frac{\omega^3}{32}+\frac{1}{4}\right)\frac{\sqrt{\pi}\,\Gamma(3/4)}{\Gamma(1/4)} \\
\beta_4 &= -\left(\frac{5\omega^4}{6144}+\frac{\omega}{192}\right)\frac{\sqrt{\pi}\,\Gamma(1/4)}{\Gamma(3/4)} \\
\beta_5 &= \left(\frac{21\omega^5}{10240}+\frac{5\omega^2}{128}\right)\frac{\sqrt{\pi}\,\Gamma(3/4)}{\Gamma(1/4)} \\
\beta_6 &= \left(\frac{5\omega^6}{65536}+\frac{5\omega^3}{2048}+\frac{11}{1536}\right)\frac{\sqrt{\pi}\,\Gamma(1/4)}{\Gamma(3/4)}.
\end{aligned} \tag{2.64}$$

We used equation (2.63) to reverse the series and we obtain:

$$E_n(1,\omega) \approx \left[\left(\frac{(n+\frac{1}{2})\pi}{\beta_0(2,1,\omega)} \right)^{\frac{2}{3}} - \sum_{j=0}^{5} \frac{F_j(2,1,\omega)}{\left((n+\frac{1}{2})\pi\right)^{\frac{2j}{3}}} \right]^2, \tag{2.65}$$

where:

$$\begin{aligned}
F_0 &= -\frac{\omega\,\Gamma\left(3/4\right)^4}{\pi^2} \\
F_1 &= \frac{\sqrt[3]{6}\,\omega^2\left(\pi^4 - 4\,\Gamma\left(3/4\right)^8\right)}{48\pi^3\Gamma\left(3/4\right)^{4/3}} \\
F_2 &= -\frac{\sqrt[3]{36}\;\Gamma\left(3/4\right)^{4/3}\;\left(3\,\pi^4\omega^3 + 12\,\pi^4 - 4\,\Gamma\left(3/4\right)^8\omega^3\right)}{216\pi^4} \\
F_3 &= \frac{\omega\;\left(36\,\Gamma\left(3/4\right)^8\omega^3 + 288\,\Gamma\left(3/4\right)^8 + \pi^4\omega^3 - 8\,\pi^4\right)}{576\pi\,\Gamma\left(3/4\right)^4} \\
F_4 &= -\frac{\sqrt[3]{6}\,\omega^2\left(40\,\Gamma\left(3/4\right)^{16}\;\omega^3 + 50\,\Gamma\left(3/4\right)^8\;\pi^4\omega^3 + 600\,\Gamma\left(3/4\right)^8\pi^4 + 7\,\pi^8\omega^3 - 50\,\pi^8\right)}{1080\Gamma\left(3/4\right)^{4/3}\pi^6} \\
F_5 &= \left(\frac{\sqrt[3]{36}\left(1680\,\Gamma\left(3/4\right)^{16}\pi^4 + 15\,\pi^{12} + 1092\,\pi^8\Gamma\left(3/4\right)^8 + 2240\,\Gamma\left(3/4\right)^{24}\right)}{62208\Gamma\left(3/4\right)^{\frac{20}{3}}\;\pi^7} \right)\omega^6 \\
&\quad + \left(\frac{5\sqrt[3]{36}\left(56\,\Gamma\left(3/4\right)^{16} + \pi^8 - 14\,\Gamma\left(3/4\right)^8\pi^4\right)}{648\pi^3\Gamma\left(3/4\right)^{\frac{20}{3}}} \right)\omega^3 + \frac{5\sqrt[3]{36}\pi\;\left(11\,\pi^4 + 84\,\Gamma\left(3/4\right)^8\right)}{1296\Gamma\left(3/4\right)^{\frac{20}{3}}}.
\end{aligned} \tag{2.66}$$

We used the analytic expressions (2.64) and (2.66) to compute the coefficients $\beta_j(2,1,2)$ and $F_j(2,1,2)$ and we examined the relative error between these exact values with those obtained using our algorithm. These values are listed in Table 2.1. In this Table, the relative errors are defined respectively

by:

$$\rho(j) = \left| \frac{\beta_j(2,1,2)^\sharp - \beta_j(2,1,2)^\dagger}{\beta_j(2,1,2)^\sharp} \right| \qquad \text{for} \qquad j = 0, 1, \ldots, 6 \tag{2.67}$$

$$\varepsilon(j) = \left| \frac{F_j(2,1,2)^\sharp - F_j(2,1,2)^\dagger}{F_j(2,1,2)^\sharp} \right| \qquad \text{for} \qquad j = 0, 1, \ldots, 5, \tag{2.68}$$

where $\beta_j(2,1,2)^\sharp$ and $F_j(2,1,2)^\sharp$ are obtained using (2.64) and (2.66) and $\beta_j(2,1,2)^\dagger$ and $F_j(2,1,2)^\dagger$ are the values obtained using our algorithm.

From Table 2.1, it is clear that our numerical results are in complete agreement with the values obtained using the analytic expressions (2.64) and (2.66). Moreover, our algorithm is able to compute a large number of the coefficients $\beta_j(q,\kappa,w)$ and $F_j(q,\kappa,w)$. In Table 2.2, we list the first 32 coefficients $\beta(2,1,2)$ and the first 31 coefficients $F(2,1,2)$ obtained using our algorithm.

Since only finitely many coefficients $\beta_j(2,\kappa,\omega)$ can be calculated, we use (2.63) and truncate the sum. To calculate the $F_j(2,\kappa,\omega)$ coefficients, we simply use the corollary 2.4.5:

$$E_n(\kappa,\omega,m) = \left[\left(\frac{(n+\frac{1}{2})\pi}{\beta_0(2,\kappa,\omega)} \right)^{\frac{2}{3}} - \sum_{j=0}^{m-1} \frac{F_j(2,\kappa,\omega)}{\left((n+\frac{1}{2})\pi\right)^{\frac{2j}{3}}} \right]^2 . \tag{2.69}$$

To approximate the error of our energy values for each additional term added to the series, we used the absolute error defined as:

$$\epsilon_n(\kappa,\omega,m) = |E_n(\kappa,\omega,m) - E_n(\kappa,\omega,m-1)| \qquad \text{for} \qquad m \geq 1. \tag{2.70}$$

Figure 2.2 shows the absolute error of the energy values for $n = 6, 9, 12, 15, 18, 21$

with $\kappa = 1$ and $\omega = 2$. As one would suspect when dealing with an asymptotic formula, the amount of accuracy increases significantly as $n \to \infty$. In addition, it is clear from this figure that using only the first 6 explicit $F_j(2,1,2)$ coefficients would only yield to 6 significant digits for $n = 6$.

The authors struggled to derive any analytical and asymptotic properties associated with either of the sequences $\{\beta_j\}_{j\geq 0}$ or $\{F_j\}_{j\geq 1}$. Herein, we will try to explain the difficulties that arise. The asymptotics of the sequence $\{\beta_j\}_{j\geq 0}$ are firmly rooted in the asymptotics of the $\{S_n'(x)\}_{n\geq 0}$, as their dominant term will be related to the dominant contribution of the contour integrals, and will therefore contribute to the sequence $\{\beta_j\}_{j\geq 0}$. One of the most powerful techniques used in ascertaining the asymptotics of a sequence is to examine the sequence's generating function. It should come as no surprise that the generating function for the sequence $\{S_n'(x)\}_{n\geq 0}$ indeed satisfies:

$$G(z,x) = \sum_{n=0}^{\infty} S_n'(x) z^n \qquad \Longrightarrow \qquad z\frac{\partial G(z,x)}{\partial x} = G^2(z,x) - Q(x). \tag{2.71}$$

With $z = 1$, we quickly recover the Riccati equation for the logarithmic derivative of the solution to the Schrödinger equation. Therefore, the generating function implies that ascertaining the asymptotics of the sequence $\{S_n'(x)\}_{n\geq 0}$ is as complicated of a problem as the problem for which the sequence $\{S_n'(x)\}_{n\geq 0}$ is used to solve. This suggests that any analytical study of the asymptotics found in this manuscript is probably hopeless.

Nevertheless, we are able to observe some heuristics on the growth of the sequence $\{\beta_j\}_{j\geq 0}$. From Table 2, an alternating sign pattern of period two, i.e. $++--++--\ldots$ appears to emerge. This suggests a governing oscillatory

behaviour. In a numerical analysis of the ratios of successive coefficients, the following leading-order approximation is obtained:

$$\beta_j(2,1,2) \approx c_0\,\Gamma(j+c_1)\,c_2^j\,\sin\left(\frac{\pi}{2}j-\frac{\pi}{4}\right) \qquad \text{as} \qquad j\to\infty, \tag{2.72}$$

where:

$$c_0 = 4.75\times 10^{-7}, \qquad c_1 = 9.68 \qquad \text{and} \qquad c_2 = 9.88\times 10^{-2}. \tag{2.73}$$

This approximation is shown in Figure 2.1. While heuristic, this result suggests that the series (41) may not converge for any value of E as the factors of $E^{-\frac{1}{q}}$ are but geometric and are dwarfed by the factorial growth. We also note that the highly nonlinear process of reverting the series is somewhat damaging to the alternations in sign and would provide yet another difficulty in an analytical treatment of the sequence $\{F_j\}_{j\geq 1}$.

2.6 Conclusion

The form of the $S_k'(z)$ proved in Theorem 2.3.1 greatly improves the efficiency as well as reduces the amount of calculations required by WKB. By comparing the exact values obtained using (2.64) and (2.66) and the numerical values obtained using our algorithm, we showed that they agree completely. The asymptotic behavior of the non-linear recurrence relations in (2.14) would allow one to know the asymptotic behavior of the integrands $S_k'(z)$ which in turn would lead to the asymptotic behavior of the coefficients $\beta_j(q,\kappa,\omega)$. Only then, could we find the form of the error of the non-inverted sum in equation (2.42).

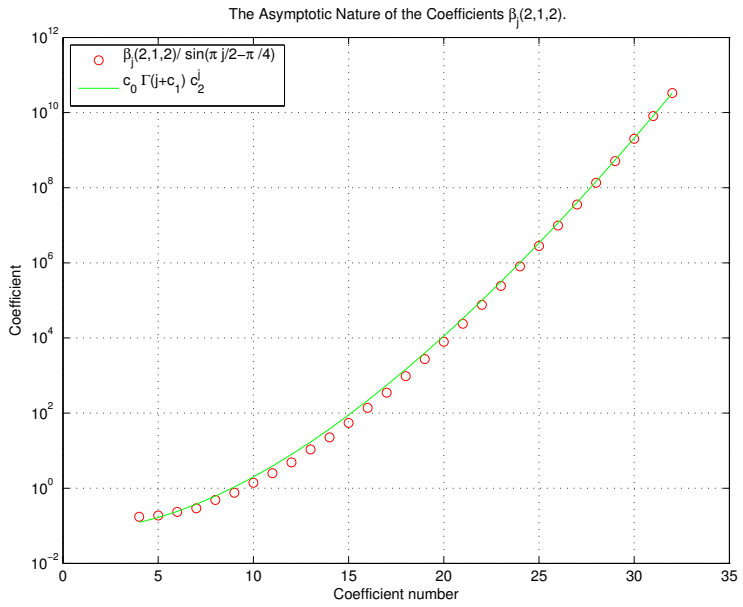

Figure 2.1: Heuristic asymptotics of the sequence $\{\beta_j(2,1,2)\}_{j\geq 0}$.

Furthermore, through the use of Corollary 2.4.5, it would be interesting to be able to find how the form of the error changes once the series is reversed. This would allow for a better understanding of the convergence of this algorithm. Additionally, further knowledge of numerical complex integration would allow for the computation of the coefficients $\beta_j(q,\kappa,\omega)$ for $q > 2$. With numerical estimates of these coefficients, one would simply have to use (2.63) to revert the series and obtain an expression for any desired energy value.

A Graph and numerical tables

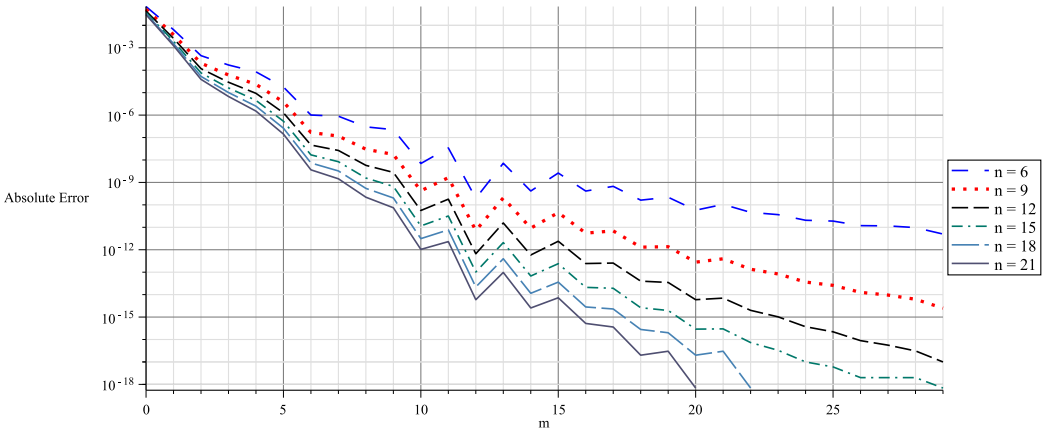

Figure 2.2: The values on the abscissa represent the number of terms in the series. The values on the ordinate represent the absolute error. This is the numerical calculation of the absolute error for energy level $n = 6, 9, 12, 15, 18, 21$ for the potential $V(z) = x^4 + 2x^2$.

Table 2.1: Relative error between the coefficients found using the exact formula and numerical estimates.

j	$\beta_j(2,1,2)^\natural$	$\beta_j(2,1,2)^\dagger$	$\rho(j)$ (2.67)
0	1.7480383695280798736	1.7480383695280798735	8.1(-20)
1	-1.1981402347355922074	-1.1981402347355922074	3.3(-20)
2	0.6555143885730299526	0.6555143885730299525	5.5(-20)
3	-0.2995350586838980518	-0.2995350586838980518	6.7(-20)
4	-0.1229089478574431161	-0.1229089478574431161	4.5(-20)
5	0.1329186822909797605	0.1329186822909797605	9.7(-20)
6	0.1655856658634997536	0.1655856658634997536	9.5(-20)
j	$F_j(2,1,2)^\sharp$	$F_j(2,1,2)^\dagger$	$\varepsilon(j)$ (2.68)
0	-0.45694658104446362537	-0.45694658104446362540	1.1(-20)
1	0.28702969557805425191	0.28702969557805425191	3.5(-20)
2	-0.34408378420502949543	-0.34408378420502949539	1.4(-19)
3	0.23925667034870999927	0.23925667034870999925	5.6(-20)
4	-0.12467471923834294258	-0.12467471923834294260	8.2(-19)
5	0.35723759046141083291	0.35723759046141083283	2.4(-19)

$^\natural$ Coefficients computed using equations (2.64). $^\sharp$ Coefficients computed using equations (2.66).
† Coefficients computed using the numerical algorithm presented in this work.
Numbers in parentheses represent powers of 10.

Table 2.2: Computation of $\beta_j(2,1,2)$ and $F_j(2,1,2)$ using the algorithm presented in this work.

j	$\beta_j(2,1,2)$	$F_j(2,1,2)$
0	1.7480383695280798736(00)	-4.5694658104446362537(-01)
1	-1.1981402347355922074(00)	2.8702969557805425191(-01)
2	6.5551438857302995258(-01)	-3.4408378420502949538(-01)
3	-2.9953505868389805184(-01)	2.3925667034870999925(-01)
4	-1.2290894785744311611(-01)	-1.2467471923834294257(-01)
5	1.3291868229097976050(-01)	3.5723759046141083284(-01)
6	1.6558566586349975365(-01)	-1.3214849643052383146(00)
7	-2.0639837637437350134(-01)	2.0742620237808097990(00)
8	-3.4369237595627648147(-01)	8.7661786242052607910(-01)
9	5.3512396506917389018(-01)	-5.8027220848957686410(00)
10	9.8826990293494178549(-01)	-1.4527363727230401800(01)
11	-1.7727104172802503849(00)	8.1645013033374835214(01)
12	-3.4603320054219551427(00)	1.8888577144524697440(01)
13	7.6250489841030361588(00)	-6.9761752532798225917(02)
14	1.5996737098879811614(01)	-2.9730788039683265380(01)
15	-3.8746606752926469393(01)	8.0967218371063755555(03)
16	-9.7718718838695330848(01)	3.5047762978500328260(03)
17	2.4658544977041937142(02)	-1.6557706930368463153(05)
18	6.8127124140934458226(02)	1.9451891117092241490(05)
19	-1.9347776095320305941(03)	2.3576379474121149423(06)
20	-5.5917614279028342511(03)	-4.2674693742846836160(06)
21	1.6946577183838210440(04)	-4.3029864503539416628(07)
22	5.3740662904165215028(04)	8.4840418648295838800(07)
23	-1.7196455150728807293(05)	1.1513747610584117254(09)
24	-5.7154842554279465430(05)	-3.7947723566734150700(09)
25	1.9947297545959578757(06)	-2.2471348739202700242(10)
26	6.9774955493224775978(06)	9.4247294262547014757(10)
27	-2.5295885095113634269(07)	6.4705017160340005390(11)
28	-9.5582266340499649945(07)	-3.0328400791282728668(12)
29	3.6243387414615841710(08)	-2.2096776597420553290(13)
30	1.4161712974011493534(09)	1.3816693658929721364(14)
31	-5.7365962696111560159(09)	5.3295402762012514065(14)
32	-2.3384167179932367473(10)	———

Numbers in parentheses represent powers of 10.

Chapter 3

Sturm-Liouville Eigenvalue Problems

This chapter has been published as:

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Abstract.

The double exponential transformation coupled with Sinc methods has sparked a lot of interest in numerical analysis over the last two decades. In the following paper, we introduce a method based on the double exponential transformation combined with the Sinc collocation method for computing eigenvalues of singular Sturm-Liouville problems. This method produces a symmetric positive-definite generalized eigenvalue system. The theoretical convergence rate of our algorithm is established and numerical examples are presented comparing our method with the single exponential Sinc collocation

method.

3.1 Introduction

The following chapter follows from our published work in [84]. Sturm-Liouville equations are abundant in the numerical treatment of scientific and engineering problems. For example, Sturm-Liouville equations describe the vibrational modes of various systems, such as the energy eigenfunctions of a quantum mechanical oscillator, in which case the eigenvalues correspond to the energy levels. Sturm-Liouville problems arise directly as eigenvalue problems in one space dimension. They also commonly arise from linear PDEs in several space dimensions when the equations are separable in some coordinate system, such as cylindrical or spherical coordinates. Classical methods for computing the eigenvalues of singular Sturm-Liouville problems often rely on approximations of the differential equations using finite-difference techniques or Prüfer transformations in order to obtain a matrix eigenvalue system [126]. Other alternatives where coefficient functions of the given problem are approximated by piecewise polynomial functions were also introduced [134]. Asymptotic methods also surfaced as an efficient tool to evaluate higher order eigenvalues [135].

Recently, new algorithms based on collocation and spectral methods have become increasingly popular and have shown great promise [16]. More specifically, Sinc collocation methods (SCM) [8, 94] have been shown to yield exponential convergence. The SCM have been used extensively during the last

30 years to solve many problems in numerical analysis. Their applications include numerical integration, linear and non-linear ordinary differential equations, partial differential equations, interpolation, and approximations to functions [155, 158]. The SCM consists of expanding the solution of a Sturm-Liouville problem using a basis of Sinc functions. By evaluating the resulting approximation at the Sinc collocation points, one arrives at a matrix eigenvalue problem or generalized matrix eigenvalue problem for which the resulting eigenvalues are approximations to the eigenvalues of the Sturm-Liouville operator.

In [56, 94], a method combining the SCM and the single exponential (SE) transformation is introduced. This method, which will be referred to as SESCM leads to an efficient and accurate algorithm for computing the eigenvalues for singular Sturm-Liouville problems. The SE transformation is a conformal mapping which allows for the function being approximated by a Sinc expansion to decay single exponentially at both infinities. In [56], Eggert et al. introduced such a transformation where the resulting matrices in the generalized eigenvalue problem are symmetric and positive definite. Moreover, they were able to show that their method converges at the rate $\mathcal{O}(N^{3/2}e^{-c\sqrt{N}})$ where N refers to the index of the $2N+1$ collocation points.

Recently, combination of the SCM with the double exponential (DE) transformation has sparked a great interest. The DE transformation is a conformal mapping which allows for the function being approximated by a Sinc basis to decay double exponentially at both infinities. Since its introduction by Takahasi and Mori [166], many have studied its effectiveness in numerically evaluating integrals [121, 163, 164]. As is stated in [164], the DE Sinc col-

location method (DESCM) method yields the best available convergence for problems with end point singularities or infinite sized domains.

It is well known that the DE enables the Sinc expansion to achieve a much higher rate of convergence than the SE. However, it should be noted that the assumption for DE convergence is more severe than the one for SE. A key feature in Sinc numerical methods is the distance from the real axis for which the function of interest is analytic. This strip is traditionally denoted by $\mathscr{D}_d = \{z \in \mathbb{C} : |\Im(z)| < d\}$ for some $d > 0$. For simplicity, the larger the value of d, the better Sinc numerical methods typically performs. As in [129, 167], we denote the class of functions for which SE is suitable by $\mathcal{F}_{SE}$ and the class of functions for which DE is suitable by $\mathcal{F}_{DE}$. Given the fact that $\mathcal{F}_{DE} \subsetneq \mathcal{F}_{SE}$, there exist examples such that Sinc expansion with SE achieves its usual rate, whereas it does not with DE [129, 167] and consequently the DESCM is not better than the SESCM for functions in $\mathcal{F}_{SE} \backslash \mathcal{F}_{DE}$. However, in [129, 167], the authors present a theoretical convergence analysis for Sinc methods with DE for functions in $\mathcal{F}_{SE} \backslash \mathcal{F}_{DE}$ for which DE does not achieve its usual rate of $\mathcal{O}\left(e^{-\kappa_1 N/\log(\kappa_2 N)}\right)$, and they were able to prove that DE still works for these functions with errors bounded by $\mathcal{O}\left(e^{-\kappa_3\sqrt{N}/\log(\kappa_4 N)}\right)$ which is slightly lower than the rate of SE; however, as stated in [129, 167] one can consider that there is almost no difference between the two transformations. This result also illustrates the great advantage of using DE over SE. Concrete examples of functions belonging to $\mathcal{F}_{SE} \backslash \mathcal{F}_{DE}$ are presented in [129, 167]. Such examples present somewhat complicated functions which depend on several factors involved in Sinc numerical analysis. For example, one function presented in [129]

concerning numerical integration which belongs to $\mathcal{F}_{SE}\backslash\mathcal{F}_{DE}$ is given by:

$$f(t) = \frac{2(1-t^2)}{\cos(4\text{arctanh}\, t) + \cosh(2)}, \qquad \text{with} \qquad \int_{-1}^{1} f(t)dt = 0.7119438.... \tag{3.1}$$

Applying the single-exponential variable transformation $t = \psi_{SE}(x) = \tanh\left(\frac{x}{2}\right)$, results in the new integrand $f(\psi_{SE}(x))$ to have an infinite number of complex poles at the points:

$$\zeta = \left(\frac{\pi}{2} + m\pi\right) \pm i, \quad \text{with} \quad m \in \mathbb{Z} \tag{3.2}$$

As we can see, this new function is analytic in the strip $\{z \in \mathbb{C} : |\Im(z)| < 1\}$. However, applying the double-exponential variable transformation $t = \psi_{DE}(x) = \tanh\left(\frac{\pi}{2}\sinh(x)\right)$, results in the new integrand $f(\psi_{DE}(x))$ to have an infinite number of complex poles at the points:

$$\zeta = \text{arcsinh}\left[\frac{1}{\pi}\left\{\left(\frac{\pi}{2} + m\pi\right) \pm i\right\}\right], \quad \text{with} \quad m \in \mathbb{Z} \tag{3.3}$$

As we can see, the complex poles go to zero as $|m| \to \infty$. Hence, there exist no strip in the complex plane around the real axis for which the function $f(\psi_{DE}(x))$ is analytic. This lack of an analytic strip about the real axis is the reason for $f(t) \in \mathcal{F}_{SE}\backslash\mathcal{F}_{DE}$.

In the present work, we demonstrate that the DESCM leads to an extremely efficient computation of eigenvalues of singular Sturm-Liouville problems. Implementing the DESCM leads to a generalized eigenvalue problem where the matrices are symmetric and positive definite. We also show that the conver-

gence of the DESCM algorithm is of the rate $\mathcal{O}\left(\frac{N^{5/2}}{\log(N)^2}\, e^{-\kappa N/\log(N)}\right)$ where N refers to the index of the $2N+1$ collocation points. Our convergence result helps to explain the performance enhancement that Sinc collocation methods receive when using variable transformations with DE decay instead of SE decay. Three singular Sturm-Liouville problems are treated and comparisons with the SE transformation are presented for each example clearly illustrating the superiority of the DESCM. Lastly, we demonstrate through an example how the conformal mapping presented in the Eggert et al.'s transformation [56] can be used to improve convergence of the DESCM when the coefficients functions of the Sturm-Liouville problem are not analytic.

3.2 Definitions and basic properties

The sinc function is defined by the following expression:

$$\operatorname{sinc}(z) = \frac{\sin(\pi z)}{\pi z}, \tag{3.4}$$

where $z \in \mathbb{C}$ and the value at $z = 0$ is taken to be the limiting value $\operatorname{sinc}(0) = 1$. In figure 3.1, we display the sinc function over the interval $(-10, 10)$.

For $j \in \mathbb{Z}$ and h a positive number, The Sinc function $S(j,h)(x)$ by:

$$S(j,h)(x) = \operatorname{sinc}\left(\frac{x}{h} - j\right). \tag{3.5}$$

It is possible to expand well-defined functions as series of Sinc functions. Such expansions are known as Sinc expansions or Whittaker Cardinal expansions.

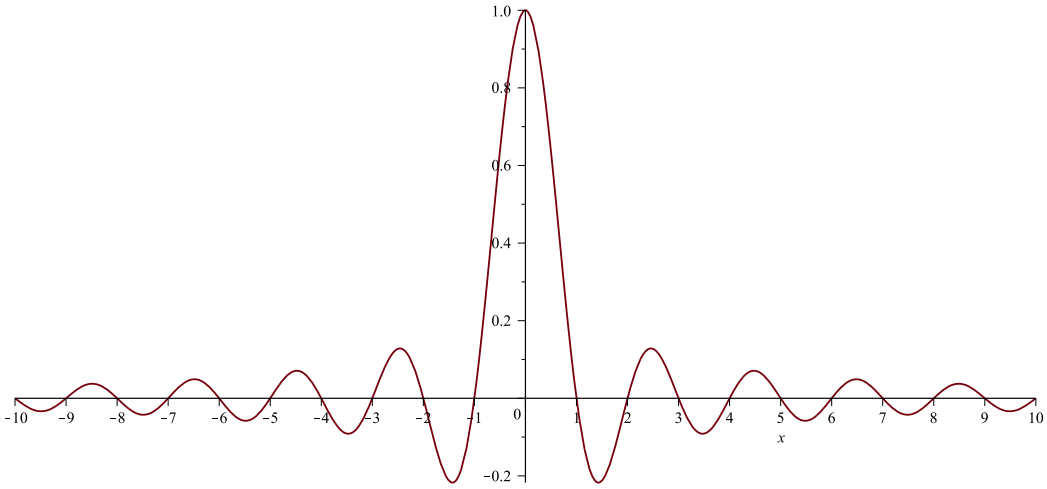

Figure 3.1: The following figure displays the sinc function over the interval $(-10, 10)$.

Definition 3.2.1. *[155] Given any function $v(x)$ defined everywhere on the real line and any $h > 0$, the Sinc expansion of $v(x)$ is defined by*

$$C(v,h)(x) = \sum_{j=-\infty}^{\infty} v(jh)S(j,h)(x). \tag{3.6}$$

Whenever, the above series converges, it is called the cardinal function of v. The truncated Sinc expansion of $v(x)$ is defined by

$$C_{M,N}(v,h)(x) = \sum_{j=-M}^{N} v(jh)\, S(j,h)(x) \quad for \quad M, N \in \mathbb{N}. \tag{3.7}$$

The symmetric truncated Sinc expansion is obtained by taking $M = N$ in the above equation.

The Sinc functions form an interpolatory set of functions with the discrete

orthogonality property:

$$S(j,h)(kh) = \begin{cases} 1 & \text{for} \quad j = k \\ 0 & \text{for} \quad j \neq k \end{cases} \qquad \text{with} \qquad j,k \in \mathbb{Z}. \tag{3.8}$$

In other words, $C(v,h)(x) = v(x)$ at all the Sinc grid points $x_k = kh$.

A class of functions for which the cardinal function of v, $C(v,h)(x)$ converges to $v(x)$ is characterized in the following definition:

Definition 3.2.2. *[108] Let h be a positive constant. The Paley-Wiener class of functions $W(\pi/h)$ is the family of entire functions v such that on the real line, $v \in L^2(\mathbb{R})$ and in the complex plane, v is of exponential type π/h, that is $|v(z)| \leq K \exp\left(\frac{\pi|z|}{h}\right)$ for some $K > 0$.*

Functions in the family $W(\pi/h)$ share many important properties for which we will state a few bellow. This first theorem characterizes the convergence of the cardinal function for function belonging to $W(\pi/h)$.

Theorem 3.2.3. *[108] If $v \in W(\pi/h)$, then for all $z \in \mathbb{C}$, we have $v(z) = C(v,h)(z)$.*

The following corollary establishes a connection between cardinal expansions and the trapezoidal rule.

Corollary 3.2.4. *[108] If $v \in W(\pi/h)$, and $v \in L^1(\mathbb{R})$, then $\int_{-\infty}^{\infty} v(t)\mathrm{d}t = h \sum_{k=-\infty}^{\infty} v(kh)$.*

If a function $v \in W(\pi/h)$, then the generalized Fourier series of v relative

to the complete orthogonal set $\left\{\frac{S(k,h)(t)}{\sqrt{h}}\right\}_{k=-\infty}^{\infty}$ is given by $\sum_{k=-\infty}^{\infty} \frac{c_k}{\sqrt{h}}\, S(k,h)(t)$ where $c_k = \sqrt{h}v(kh)$, by Theorem 3.2.3.

In [155], a class of functions which are successfully approximated by Sinc expansions is introduced. Now, we shall present the definition for this class of functions.

Definition 3.2.5. *[155] Let $d > 0$ and let $\mathscr{D}_d$ denote the strip of width $2d$ about the real axis:*

$$\mathscr{D}_d = \{z \in \mathbb{C} : |\,\Im(z)| < d\}. \tag{3.9}$$

In addition, for $\epsilon \in (0,1)$, let $\mathscr{D}_d(\epsilon)$ denote the rectangle in the complex plane:

$$\mathscr{D}_d(\epsilon) = \{z \in \mathbb{C} : |\,\Re(z)| < 1/\epsilon,\ |\,\Im(z)| < d(1-\epsilon)\}. \tag{3.10}$$

Let $\mathbf{B}_2(\mathscr{D}_d)$ denote the family of all functions g that are analytic in $\mathscr{D}_d$, such that:

$$\int_{-d}^{d} |\,g(x+iy)|\,dy \to 0 \qquad as \qquad x \to \pm\infty, \tag{3.11}$$

and such that:

$$\mathcal{N}_2(g,\mathscr{D}_d) = \lim_{\epsilon\to 0}\left(\int_{\partial\mathscr{D}_d(\epsilon)} |\,g(z)|^2\,|dz|\right)^{1/2} < \infty. \tag{3.12}$$

A figure of the strip $\mathscr{D}_d$ and the rectangle $\mathscr{D}_d(\epsilon)$ is provided in figure 3.2.

The Sturm-Liouville (SL) equation in Liouville form is defined as follows:

$$\begin{aligned} Lu(x) = -u''(x) + q(x)u(x) \;&=\; \lambda\rho(x)u(x) \\ a < x < b \qquad\qquad & u(a) = u(b) = 0, \end{aligned} \tag{3.13}$$

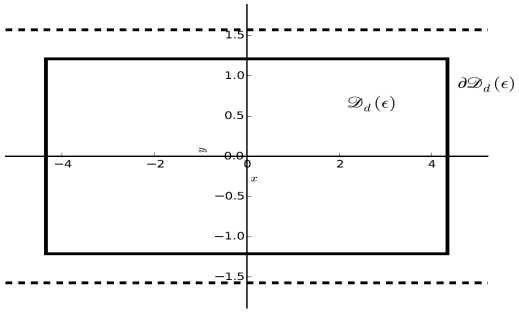

Figure 3.2: Representive plot of the strip $\mathscr{D}_d$ and the rectangle in the complex plane $\mathscr{D}_d(\epsilon)$.

where $-\infty \leq a < b \leq \infty$. Additionally, the function $q(x)$ is assumed non-negative and the weight function $\rho(x)$ is assumed positive. The values λ are known as the eigenvalues of the SL equation. The SL equation (3.13) is classified as either regular or singular depending on the behaviour of $q(x)$ and $\rho(x)$ at the endpoints a and b [193].

In [56], Eggert et al. demonstrate that when using Sinc expansion approximations for solving the SL boundary value problem (3.13), an appropriate change of variables results in a symmetric discretized system. The change of variable they propose is of the form [56]:

$$v(x) = \left(\sqrt{(\phi^{-1})'}\, u\right) \circ \phi(x) \qquad \Longrightarrow \qquad u(x) = \frac{v \circ \phi^{-1}(x)}{\sqrt{(\phi^{-1}(x))'}}, \tag{3.14}$$

where $\phi^{-1}(x)$ a conformal map of a simply connected domain in the complex plane with boundary points $a \neq b$ such as $\phi^{-1}(a) = -\infty$ and $\phi^{-1}(b) = \infty$. Examples of such conformal maps are given in Table 3.1, where conformal maps inducing SE decay are given as ϕ_{SE} and DE decay as ϕ_{DE}.

Table 3.1: Table of exponential variable transformations.

Interval	ϕ_{SE}	ϕ_{DE}
$(0,1)$	$\frac{1}{2}\tanh(t)+\frac{1}{2}$	$\frac{1}{2}\tanh(\sinh(t))+\frac{1}{2}$
$(0,\infty)$	$\operatorname{arcsinh}(e^t)$	$\operatorname{arcsinh}(e^{\sinh(t)})$
$(-\infty,\infty)$	t	$\sinh(t)$

Applying the change of variable (3.14) to (3.13), one obtains [56]:

$$\mathcal{L}\,v(x) = -v''(x) + \tilde{q}(x)v(x) = \lambda\rho(\phi(x))(\phi'(x))^2 v(x), \tag{3.15}$$

where:

$$\tilde{q}(x) = -\sqrt{\phi'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\phi'(x)}\frac{\mathrm{d}}{\mathrm{d}x}(\sqrt{\phi'(x)})\right) + (\phi'(x))^2 q(\phi(x)). \tag{3.16}$$

To apply the SCM method, one begins by approximating the solution of (3.15) by the truncated Sinc expansion (3.7) where the terms $v(jh)$ are unknown scalar weights and h is a mesh size.

Inserting (3.7) into (3.15) and collocating at the Sinc points, we obtain the following system:

$$\begin{aligned}\mathcal{L}\,C_{M,N}(v,h)(x_k) &= \sum_{j=-M}^{N}\left[-\frac{\mathrm{d}^2}{\mathrm{d}x_k^2}S(j,h)(x_k) + \tilde{q}(x_k)S(j,h)(x_k)\right]v(jh)\\ &= \mu\sum_{j=-M}^{N} S(j,h)(x_k)(\phi'(x_k))^2\rho(\phi(x_k))v(jh),\end{aligned} \tag{3.17}$$

where $x_k = kh$ for $k = -M,\ldots,N$ and μ is the approximation of the eigenvalue λ in (3.15).

If we let $\delta_{j,k}^{(l)}$ be the l^{th} Sinc differentiation matrix with unit mesh size [157]:

$$\delta_{j,k}^{(l)} = h^l \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l S(j,h)(x)\bigg|_{x=kh}, \tag{3.18}$$

then we obtain equivalently:

$$\sum_{j=-M}^{N} \left[-\frac{1}{h^2}\,\delta_{j,k}^{(2)} + \tilde{q}(kh)\,\delta_{j,k}^{(0)}\right] v(jh) = \mu \sum_{j=-M}^{N} \delta_{j,k}^{(0)} (\phi'(kh))^2 \rho(\phi(kh)) v(jh). \tag{3.19}$$

Equation (3.19) can be rewritten in a matrix form as follows:

$$\mathcal{L}\,\mathbf{C}_{M,N}(v,h) = \mathbf{A}\mathbf{v} \;=\; \mu \mathbf{D}^2\mathbf{v} \quad \Longrightarrow \quad (\mathbf{A} - \mu\mathbf{D}^2)\mathbf{v} \;=\; 0, \tag{3.20}$$

where the vectors $\mathbf{v}$ and $\mathbf{C}_{M,N}(v,h)$ are given by:

$$\begin{aligned} \mathbf{v} &= (v(-Nh), \ldots, v(Nh))^T \\ \mathbf{C}_{M,N}(v,h) &= (C_{M,N}(v,h)(-Mh), \ldots, C_{M,N}(v,h)(Nh))^T. \end{aligned} \tag{3.21}$$

The entries $A_{j,k}$ of the $(N+M+1)\times(N+M+1)$ matrix $\mathbf{A}$ are given by:

$$A_{j,k} = -\frac{1}{h^2}\,\delta_{j,k}^{(2)} + \tilde{q}(kh)\,\delta_{j,k}^{(0)} \qquad \text{with} \qquad -M \le j,k \le N, \tag{3.22}$$

and the entries $D_{j,k}^2$ of the $(N+M+1)\times(N+M+1)$ diagonal matrix $\mathbf{D}^2$ are given by:

$$D_{j,k}^2 = (\phi'(kh))^2 \rho(\phi(kh))\,\delta_{j,k}^{(0)} \qquad \text{with} \qquad -M \le j,k \le N. \tag{3.23}$$

To obtain nontrivial solutions for $\mathbf{v}$, we set:

$$\det(\mathbf{A} - \mathbf{D}^2\mu) = 0. \tag{3.24}$$

To find an approximation of the eigenvalues of (3.15), one simply has to solve this generalized eigenvalue problem. From this it follows that there is no need to find the solution $v(x)$ of (3.15) in order to find its eigenvalues. However, most modern eigensolvers can give eigenvalues and eigenvectors at the same time.

To implement SESCM, one needs to find a function ϕ for the substitution (3.14) that would result in the solution of (3.15) to decay single exponentially. In [56], an upper bound for the error between the eigenvalues λ in (3.15) and their approximations μ in (3.20) is obtained when $|v(t)| \leq C\exp(-\alpha|t|))$ for some $\alpha > 0$ on the real line. The upper bound is given by [56]:

$$|\mu - \lambda| \leq K_{v,d}\sqrt{\delta\lambda}N^{3/2}\exp(-\sqrt{\pi d\alpha N}), \tag{3.25}$$

where $K_{v,d}$ is a constant that depends on v and d. The optimal step size h is given by:

$$h = \left(\frac{\pi d}{\alpha N}\right)^{1/2}. \tag{3.26}$$

In [56], Eggert et al. consider the case where $|v(t)| \leq C\exp(-\alpha|t|)$. For the more general case where $|v(t)| \leq C\exp(-\alpha|t|^\rho)$ for some $\rho > 0$, the optimal step size is given by [163]:

$$h = \left(\frac{\pi d}{(\alpha N)^\rho}\right)^{\frac{1}{\rho+1}}, \tag{3.27}$$

and in this case equation (3.25) becomes [163]:

$$|\mu - \lambda| = \mathcal{O}\left(\exp(-(\pi d\alpha N)^{\frac{\rho}{\rho+1}})\right) \qquad \text{as} \qquad N \to \infty. \tag{3.28}$$

3.3 The double exponential Sinc collocation method (DESCM)

In the DE transformation, the function $v(x)$ decays double exponentially at the endpoints of its domain.

Similarly to the SESCM, we approximate the solution $v(x)$ of (3.15) by the truncated Sinc expansion (3.7).

To analyse the convergence of the DESCM method, we need to consider the error of the second derivative of the truncated Sinc expansion of the solution $v(x)$:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}(C_{M,N}(v,h)(x)) = \sum_{k=-M}^{N}\left(v(jh)\frac{\mathrm{d}^2}{\mathrm{d}x^2}(S(k,h)(x))\right). \tag{3.29}$$

A bound for this error is established in the following lemma. First, let us denote by $W(x)$ the Lambert W function which is defined as follows:

Definition 3.3.1. *[46, Equation (1.5)] The Lambert W function denoted by $W(x)$ is defined implicitly by the solution of the following equation:*

$$z = W(x)e^{W(x)}. \tag{3.30}$$

In our case, we restrict the Lambert W function to be real valued with the additional constraint $W(x) \geq -1$. This additional constraint forces the Lambert

W function to be single-valued. This branch is commonly denoted by $W_0(x)$. For the numerical evaluation of the Lambert W function, we refer the readers to [46].

Let us also denote by $\lfloor x \rfloor$ the floor function, $\lceil x \rceil$ the ceiling function, and $x^+ = \max\{x, 0\}$. Let also $||\cdot||_2$ denote the L^2 norm for Lebesgue integrable functions:

$$||f(x)||_2 = \left(\int_{\mathbb{R}} |f(x)|^2 \, \mathrm{d}x \right)^{1/2}. \tag{3.31}$$

Lemma 3.3.2. *Let $E^{(2)}_{M,N}(g,h)(x)$ denote the error of approximating the second derivative of a function g by the second derivative of its truncated Sinc expansion:*

$$E^{(2)}_{M,N}(g,h)(x) = \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[g(x)\right] - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[C_{M,N}(g,h)(x)\right]. \tag{3.32}$$

Let:

$$|g(x)| \leq A \begin{cases} \exp(-\beta_L \exp(\gamma_L |x|)) & \text{for} \quad x \in (-\infty, 0] \\ \exp(-\beta_R \exp(\gamma_R |x|)) & \text{for} \quad x \in [0, \infty), \end{cases} \tag{3.33}$$

where $A, \beta_L, \beta_R, \gamma_L, \gamma_R > 0$.

Moreover, assume that $g \in \mathbf{B}_2(\mathscr{D}_d)$ with $d \leq \dfrac{\pi}{2\gamma}$, where $\gamma = \max\{\gamma_L, \gamma_R\}$. If the mesh size h is given by:

$$h = \frac{\log(\pi d \gamma n / \beta)}{\gamma n}, \tag{3.34}$$

where:

$$\begin{cases} n = M,\ N = \left\lceil \dfrac{\gamma_L}{\gamma_R} M \left(1 + \dfrac{\log\left(\beta_L/\beta_R\right)}{W(\pi d \gamma_L M/\beta_L)}\right)\right\rceil^+, \beta = \beta_L \ \ \textit{if}\ \ \gamma_L > \gamma_R \\ n = N,\ M = \left\lfloor \dfrac{\gamma_R}{\gamma_L} N \left(1 + \dfrac{\log\left(\beta_R/\beta_L\right)}{W(\pi d \gamma_R N/\beta_R)}\right)\right\rfloor^+, \beta = \beta_R \ \ \textit{if}\ \ \gamma_R > \gamma_L \\ n = M,\ N = \left\lceil M \left(1 + \dfrac{\log\left(\beta_L/\beta_R\right)}{W(\pi d \gamma_L M/\beta_L)}\right)\right\rceil, \beta = \beta_L \ \ \textit{if}\ \ \gamma_L = \gamma_R \ \ \textit{and}\ \ \beta_L \geq \beta_R \\ n = N,\ M = \left\lfloor N \left(1 + \dfrac{\log\left(\beta_R/\beta_L\right)}{W(\pi d \gamma_R N/\beta_R)}\right)\right\rfloor, \beta = \beta_R \ \ \textit{if}\ \ \gamma_L = \gamma_R \ \ \textit{and}\ \ \beta_R \geq \beta_L, \end{cases} \tag{3.35}$$

then:

$$||E^{(2)}_{M,N}(g,h)(x)||_2 \leq K_{g,d} \left(\frac{n}{\log(n)}\right)^{5/2} \exp\left(-\frac{\pi d \gamma n}{\log(\pi d \gamma n/\beta)}\right), \tag{3.36}$$

where $K_{g,d}$ is a positive constant that depends on the function g and d.

Proof. To begin, we re-write the Sinc expansion of g as follows:

$$\begin{aligned} E^{(2)}_{M,N}(g,h)(x) = &\left(g''(x) - \sum_{k=-\infty}^{\infty} g(kh) S(k,h)''(x)\right) \\ &+ \sum_{k=N+1}^{\infty} g(kh) S(k,h)''(x) + \sum_{k=-\infty}^{-M-1} g(kh) S(k,h)''(x). \end{aligned} \tag{3.37}$$

The difference of the first two terms in (3.37) is known as the sampling or discretization error while the sum of the last two terms corresponds to the truncation error.

Using the triangle inequality, we obtain:

$$\begin{aligned}||E^{(2)}_{M,N}(g,h)(x)||_2 \leq & \left|\left|g''(x) - \sum_{k=-\infty}^{\infty} g(kh)S(k,h)''(x)\right|\right|_2 \\ & + \left|\left|\sum_{k=N+1}^{\infty} g(kh)S(k,h)''(x)\right|\right|_2 \\ & + \left|\left|\sum_{k=-\infty}^{-M-1} g(kh)S(k,h)''(x)\right|\right|_2 . \end{aligned} \tag{3.38}$$

From [156], we have:

$$\left|\left|g''(x) - \sum_{k=-\infty}^{\infty} g(kh)S(k,h)''(x)\right|\right|_2 \leq B_{g,d}\frac{\exp(-\pi d/h)}{h^2}, \tag{3.39}$$

where $B_{g,d}$ is a constant that depends on g and d.

In the proof of [110], Lundin et al. derive the following result:

$$\left|\left|\sum_{k=N+1}^{\infty} g(kh)S(k,h)''(x)\right|\right|_2 \leq \frac{C_{g,d}}{h^{3/2}}\sum_{k=N+1}^{\infty}|g(kh)|. \tag{3.40}$$

for some constant $C_{g,d}$ that depends on the function g and d.

Utilizing this result with the bound in (3.33), we show that:

$$\begin{aligned}\left|\left|\sum_{k=N+1}^{\infty} g(kh)S(k,h)''(x)\right|\right|_2 &\leq D_{g,d}\,h^{-3/2}\left(\sum_{k=N+1}^{\infty} A\exp(-\beta_R\exp(\gamma_R kh))\right) \\ &\leq AD_{g,d}\,h^{-3/2}\left(\int_N^{\infty}\exp(-\beta_R\exp(\gamma_R kh))\mathrm{d}k\right) \\ &\leq AD_{g,d}\,h^{-5/2}\left(\frac{\exp(-\beta_R\exp(\gamma_R Nh))}{\gamma_R\beta_R\exp(\gamma_R Nh)}\right) \\ &\leq F_{g,d}\frac{\exp(-\beta_R\exp(\gamma_R Nh))}{h^{5/2}}, \end{aligned} \tag{3.41}$$

where $F_{g,d}$ is a constant that depends on g and d and similarly, we obtain the following upper bound:

$$\left|\left|\sum_{k=-\infty}^{-M-1} g(kh)S(k,h)''(x)\right|\right|_2 \leq G_{g,d}\frac{\exp(-\beta_L \exp(\gamma_L Mh))}{h^{5/2}}, \tag{3.42}$$

where $G_{g,d}$ is a constant that depends on g and d.

Equating the exponential terms in (3.41) and (3.42) and solving for N or M in $\mathbb{N}_0$, we obtain:

$$\begin{cases} N = \left\lceil \frac{\gamma_L}{\gamma_R} M + \frac{\log(\beta_L/\beta_R)}{\gamma_R h} \right\rceil^+ & \text{if} \quad \gamma_L > \gamma_R \\ M = \left\lfloor \frac{\gamma_R}{\gamma_L} N + \frac{\log(\beta_R/\beta_L)}{\gamma_L h} \right\rfloor^+ & \text{if} \quad \gamma_R > \gamma_L \\ N = \left\lceil M + \frac{\log(\beta_L/\beta_R)}{\gamma_R h} \right\rceil & \text{if} \quad \gamma_L = \gamma_R \quad \text{and} \quad \beta_L \geq \beta_R \\ M = \left\lfloor N + \frac{\log(\beta_R/\beta_L)}{\gamma_L h} \right\rfloor & \text{if} \quad \gamma_L = \gamma_R \quad \text{and} \quad \beta_R \geq \beta_L. \end{cases} \tag{3.43}$$

As can be seen from (3.43), M and N depend upon the step size h.

Combining (3.39), (3.41) and (3.42), we obtain:

$$||E^{(2)}_{M,N}(g,h)(x)||_2 \leq B_{g,d}\frac{\exp(-\pi d/h)}{h^2} + (F_{g,d} + G_{g,d})\frac{\exp(-\beta \exp(\gamma nh))}{h^{5/2}}, \tag{3.44}$$

where:

$$\begin{cases} n = M, \quad \beta = \beta_L \quad \text{if} \quad \gamma_L > \gamma_R \\ n = N, \quad \beta = \beta_R \quad \text{if} \quad \gamma_R > \gamma_L \\ n = M, \quad \beta = \beta_L \quad \text{if} \quad \gamma_L = \gamma_R \quad \text{and} \quad \beta_L \geq \beta_R \\ n = N, \quad \beta = \beta_R \quad \text{if} \quad \gamma_L = \gamma_R \quad \text{and} \quad \beta_R \geq \beta_L. \end{cases} \tag{3.45}$$

Equating the exponential terms in the RHS of (3.44) and solving for h, we obtain:

$$h = \frac{W(\pi d\gamma n/\beta)}{\gamma n}. \tag{3.46}$$

Substituting this result in (3.43), we obtain equation (3.35).

The first term in the asymptotic expansion of the Lambert W function as $x \to \infty$ is given by [46]:

$$W(x) \sim \log(x) \qquad \text{as} \qquad x \to \infty. \tag{3.47}$$

Consequently the asymptotic value for the mesh size h as $n \to \infty$ is given by:

$$h \sim \frac{\log(\pi d\gamma n/\beta)}{\gamma n} \qquad \text{as} \quad n \to \infty. \tag{3.48}$$

Substituting (3.48) into (3.44) and simplifying, we obtain equation (3.36).

□

We shall now state a theorem establishing the convergence of the eigenvalues of a discretized SL problem when the solution decays double exponentially.

Theorem 3.3.3. *Let λ and $v(x)$ be an eigenpair of the transformed differential equation* (3.15). *Assume there exist positive constants $A, \beta_L, \beta_R, \gamma_L, \gamma_R$ such*

that:

$$|\,v(x)| \leq A \begin{cases} \exp(-\beta_L \exp(\gamma_L|x|) & \text{for} \quad x \in (-\infty, 0] \\ \exp(-\beta_R \exp(\gamma_R|x|)) & \text{for} \quad x \in [0, \infty). \end{cases} \tag{3.49}$$

If $v \in \mathbf{B}_2(\mathscr{D}_d)$ *with* $d \leq \dfrac{\pi}{2\gamma}$, *where* $\gamma = \max\{\gamma_L, \gamma_R\}$.

If there is a constant $\delta > 0$ *such that* $\tilde{q}(x) \geq \delta^{-1}$ *and if the optimal mesh size* h *is given by:*

$$h = \frac{\log(\pi d\gamma n/\beta)}{\gamma n}, \tag{3.50}$$

where n *and* β *are given by* (3.35).

Then, there is an eigenvalue μ *of the generalized eigenvalue problem satisfying:*

$$|\mu - \lambda| \leq K_{v,d}\sqrt{\delta\lambda}\left(\frac{n^{5/2}}{\log(n)^2}\right)\exp\left(-\frac{\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right) \quad \text{as} \quad n \to \infty, \tag{3.51}$$

where $K_{v,d}$ *is a constant that depends on* v *and* d.

Proof. In general, SL differential equations and their transformed counterpart (3.15) have an infinite number of eigenpairs $\{(\lambda_i, v_i(x))\}_{i\in\mathbb{N}_0}$. Since the choice of the eigenpair is arbitrary for the procedure of this proof, we will abstain from using indices on the eigenvalues λ as well as on the eigenfunctions $v(x)$.

First, we assume that the arbitrary eigenpair λ and $v(x)$ of the transformed differential equation (3.15) can be normalized as follows:

$$\int_{-\infty}^{\infty} v(x)^2 \rho(\phi(x))(\phi'(x))^2 \mathrm{d}x = 1. \tag{3.52}$$

This is equivalent to normalization condition for the original system:

$$\int_a^b u(x)^2 \rho(x) \mathrm{d}x = 1. \tag{3.53}$$

Applying (3.15) to the collocation points $x = jh$ for $-M \leq j \leq N$ leads to:

$$\mathcal{L}\,\mathbf{v} \;=\; \lambda\, \mathrm{diag}(\rho\,(\phi')^2)\mathbf{v} \;=\; \lambda \mathbf{D}^2 \mathbf{v}, \tag{3.54}$$

where $\mathbf{v}$ is defined in (3.21), λ is the eigenvalue corresponding to the eigenfunction $v(x)$ and the matrix $\mathbf{D}$ is given by:

$$\mathbf{D} = \mathrm{diag}(\sqrt{\rho}\,(\phi')). \tag{3.55}$$

Taking the difference between (3.54) and (3.20), we obtain:

$$\Delta\mathbf{v} \;=\; \mathcal{L}\,\mathbf{C}_{M,N}(v,h) - \mathcal{L}\,\mathbf{v} \;=\; (\mathbf{A} - \lambda \mathbf{D}^2)\mathbf{v}, \tag{3.56}$$

where the vector $\mathbf{C}_{M,N}(v,h)$ is defined in (3.21).

Since $\mathbf{A}$ and $\mathbf{D}^2$ are symmetric positive definite matrices, there exist generalized orthogonal eigenvectors $\mathbf{z}_i$ and generalized positive real eigenvalues $\mu_{-M} \leq \mu_{-M+1} \leq \ldots \leq \mu_N$ such that:

$$\mathbf{Z}^T \mathbf{A} \mathbf{Z} = \mathrm{diag}((\mu_{-M}, \ldots, \mu_N)) \tag{3.57}$$

$$\mathbf{Z}^T \mathbf{D}^2 \mathbf{Z} = \mathbf{I} \tag{3.58}$$

$$\mathbf{A}\mathbf{z}_i = \mu_i \mathbf{D}^2 \mathbf{z}_i. \tag{3.59}$$

The matrix $\mathbf{Z}$ is simply a matrix with the generalized eigenvectors $\mathbf{z}_i$ as its columns. Equations (3.57), (3.58) and (3.59) are analogous to the spectral decomposition of one symmetric positive definite matrix, i.e. when $\mathbf{D}^2 = \mathbf{I}$. However, in this case $\mathbf{D}^2 \neq \mathbf{I}$ and we are dealing with a generalized eigenvalue problem with two symmetric positive definite matrices. It is important to note that the matrices $\mathbf{A}$ and $\mathbf{D}^2$ generate $N+M+1$ generalized eigenvalues. Since we are only interested in the generalized eigenvalue that approximates λ, $N+M$ of these generalized eigenvalues are not useful in this proof. The following demonstration will determine a systematic way to discard these remaining $N+M$ eigenvalues. In other words, we will demonstrate that there exists a sequence of generalized eigenvalues $\{\mu_n\}_{n\in\mathbb{N}}$ such that this sequence converges to the eigenvalue λ.

Since all the eigenvectors $\{\mathbf{z}_i\}_{i=-M}^{N}$ are linearly independent, there exists constants b_i such that:

$$\mathbf{v} = \sum_{i=-M}^{N} b_i \, \mathbf{z}_i. \tag{3.60}$$

Note that the values b_i depend on the vector $\mathbf{v}$ and consequently on the eigenfunction $v(x)$.

Substituting (3.60) in the RHS of (3.56) and using (3.59), we obtain:

$$\Delta\mathbf{v} = \sum_{i=-M}^{N} b_i(\mu_i - \lambda)\mathbf{D}^2\mathbf{z}_i. \tag{3.61}$$

Multiplying both sides of (3.61) by $\mathbf{z}_j^T$ and utilizing (3.58), we obtain:

$$\mathbf{z}_j^T \Delta\mathbf{v} = b_j(\mu_j - \lambda) \quad \text{for} \quad j = -M, \ldots, N. \tag{3.62}$$

Moreover, by multiplying both sides of (3.60) by the matrix $\mathbf{D}^2$, and taking the inner product of the resulting vector with $\mathbf{v}$ and using (3.59), we obtain:

$$||\mathbf{Dv}||_2^2 = \sum_{i=-M}^{N} b_i^2 \leq (N + M + 1)\, b_p^2, \tag{3.63}$$

where:

$$b_p = \max_{-M \leq i \leq N} \{|b_i|\}. \tag{3.64}$$

Note that the value of b_p depends on the vector $\mathbf{v}$ and consequently on the eigenfunction $v(x)$ as can be seen from (3.60). Moreover, the index p depends on the range $(-M, \ldots, N)$. Since $v \in \mathbf{B}^2(\mathscr{D}_d)$ and it satisfies the decay condition (3.49), we have the following relation when applying the trapezoidal quadrature rule to (3.52):

$$\begin{aligned} 1 &= h \sum_{k=-M}^{N} v(jh)^2 \rho(\phi(jh))(\phi'(jh))^2 + \epsilon(v, M, N) \\ &= h||\mathbf{Dv}||_2^2 + \epsilon(v, M, N). \end{aligned} \tag{3.65}$$

The assumptions on $v(x)$ guarantee that $|\epsilon(v, M, N)/h| \to 0$ as $M, N \to \infty$. From this it follows that there exist $N > 0$ and $M > 0$ such that $|\epsilon(v, M, N)/h| \leq 1/(2h)$, and this leads to $||\mathbf{Dv}||_2^2 \geq 1/(2h)$. Combining this with (3.63), we obtain a lower bound for b_p:

$$(2(N + M + 1)h)^{-1/2} \leq b_p. \tag{3.66}$$

Using the Rayleigh principle [12] and the assumption that there exists a

constant $\delta > 0$ such that $\tilde{q}(x) \geq \delta^{-1}$ implies that:

$$\begin{aligned} \delta^{-1} &\leq \min_{\alpha_j \in \sigma(\mathbf{A})} \{\alpha_j\} \\ &= \min_{\mathbf{x} \neq 0} \left\{ \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \right\} \\ &\leq \frac{\mathbf{z}_j^T \mathbf{A} \mathbf{z}_j}{||\mathbf{z}_j||_2^2}, \end{aligned} \tag{3.67}$$

where $\sigma(\mathbf{A})$ is the eigenspectrum of the matrix $\mathbf{A}$ and $\{\alpha_j\}_{j=-M}^{N}$ are its eigenvalues.

The equality in (3.57) indicates that $\mathbf{z}_i^T \mathbf{A} \mathbf{z}_i = \mu_i$ and when combined with (3.67) leads to the following upper bound for $||\mathbf{z}_j||_2^2$:

$$||\mathbf{z}_j||_2^2 \leq \delta \mu_j. \tag{3.68}$$

Let θ_j be the angle between $\mathbf{z}_j$ and $\Delta\mathbf{v}$ in (3.62). Taking the absolute value of (3.62) and expanding the inner product, we obtain:

$$|\mu_j - \lambda| = \frac{||\mathbf{z}_j||_2 ||\Delta\mathbf{v}||_2 |\cos(\theta_j)|}{|b_j|}. \tag{3.69}$$

Since we are looking to minimize the left hand side of (3.69), we have to select the index j such that we maximize the denominator of the right hand side of (3.69). Choosing the same index $l = p$ in (3.64) will certainly achieve this goal given fixed N and M. Hence, replacing $||\mathbf{z}_p||_2$ by its bound in (3.68), $|b_p|$ by its bound in (3.66) and taking into consideration that $|\cos(\theta_p)| \leq 1$, we obtain:

$$|\mu_p - \lambda| \leq \sqrt{\delta \mu_p}\, (2(N + M + 1)h)^{1/2}\, ||\Delta\mathbf{v}||_2. \tag{3.70}$$

In the following, we write μ instead of μ_p for simplicity.

We now have to consider two cases. For fixed N and M, we have:

$$\begin{aligned} |\mu-\lambda| \leq \lambda \quad &\Rightarrow \quad \mu = \mu - \lambda + \lambda \leq |\mu-\lambda| + \lambda \leq 2\lambda \\ |\mu-\lambda| > \lambda \quad &\Rightarrow \quad \mu = \mu - \lambda + \lambda \leq |\mu-\lambda| + \lambda \leq 2|\mu-\lambda|. \end{aligned} \tag{3.71}$$

Combining these inequalities with (3.70) leads to the following results:

$$\begin{aligned} |\mu-\lambda| &\leq 2\sqrt{\delta|\mu-\lambda|}\left((N+M+1)h\right)^{1/2}||\Delta\mathbf{v}||_2 \quad \text{when} \quad |\mu-\lambda| > \lambda \\ |\mu-\lambda| &\leq 2\sqrt{\delta\lambda}\left((N+M+1)h\right)^{1/2}||\Delta\mathbf{v}||_2 \qquad\quad \text{when} \quad |\mu-\lambda| \leq \lambda. \end{aligned} \tag{3.72}$$

Next, we will consider the quantity $||\Delta\mathbf{v}||_2$. It is easy to show that:

$$\begin{aligned} |\Delta v(jh)| &= |\mathcal{L}\, C_{M,N}(v,h)(x) - \mathcal{L}\, v(x)||_{x=jh} \\ &= \left|\frac{\mathrm{d}^2}{\mathrm{d}x^2} C_{M,N}(v,h)(x) - \frac{\mathrm{d}^2}{\mathrm{d}x^2} v(x)\right|\Bigg|_{x=jh} \\ &= |E^{(2)}_{M,N}(g,h)(jh)|. \end{aligned} \tag{3.73}$$

Hence, using lemma 3.3.2 with:

$$h = \frac{\log(\pi d\gamma n/B)}{\gamma n}, \tag{3.74}$$

we can derive the following result:

$$||\Delta\mathbf{v}||_2 \;\leq\; F_{v,d}\left(\frac{n}{\log(n)}\right)^{5/2} \exp\left(-\frac{\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right), \tag{3.75}$$

where $F_{v,d}$ is a constant that depends on v and d.

Combining (3.75) with (3.72), we obtain:

$$\begin{aligned}
|\mu-\lambda| &\leq K_{v,d}\sqrt{\delta|\mu-\lambda|}\frac{n^{5/2}}{\log(n)^2}\exp\left(-\frac{\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right) \quad \text{when} \quad |\mu-\lambda|>\lambda \\
|\mu-\lambda| &\leq K_{v,d}\sqrt{\delta\lambda}\frac{n^{5/2}}{\log(n)^2}\exp\left(-\frac{\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right) \quad \text{when} \quad |\mu-\lambda|\leq\lambda,
\end{aligned} \tag{3.76}$$

where $K_{v,d}$ is a constant that depends on v and d.

Simplifying, we obtain:

$$\begin{aligned}
|\mu-\lambda| &\leq K_{v,d}^2\,\delta\,\frac{n^5}{\log(n)^4}\exp\left(-\frac{2\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right) \quad \text{when} \quad |\mu-\lambda|>\lambda \\
|\mu-\lambda| &\leq K_{v,d}\sqrt{\delta\lambda}\frac{n^{5/2}}{\log(n)^2}\exp\left(-\frac{\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right) \quad \text{when} \quad |\mu-\lambda|\leq\lambda.
\end{aligned} \tag{3.77}$$

The bounds in (3.77) demonstrate that for fixed n, one of the generalized eigenvalues of the matrices $\mathbf{A}$ and $\mathbf{D^2}$ of size $(N+M+1)\times(N+M+1)$ will approximate the eigenvalues λ. As n increases, we will create a sequence of generalized eigenvalues that converge to the eigenvalue λ. Equation (3.77) also indicates that $|\mu-\lambda|\to 0$ as $n\to\infty$ for all eigenvalues λ. Moreover, as n increases, the second case in (3.77) will take precedence since $|\mu-\lambda|\leq\lambda$. Hence we obtain the following asymptotic error estimate:

$$|\mu-\lambda| \leq K_{v,d}\sqrt{\delta\lambda}\left(\frac{n^{5/2}}{\log(n)^2}\right)\exp\left(-\frac{\pi d\gamma n}{\log(\pi d\gamma n/\beta)}\right) \qquad \text{as} \qquad n\to\infty. \tag{3.78}$$

Since this process can be done for any arbitrary eigenpair $\{(\lambda_i, v_i(x))\}_{i\in\mathbb{N}_0}$,

it is clear from (3.78) that every eigenvalue λ will satisfy the error bound for the appropriate sequence of generalized eigenvalues μ. $\square$

The dependence on the value of λ in the right-hand side of (3.78) demonstrates that convergence for eigenvalues on the lower end of the eigenvalue spectrum will be slightly faster. Nevertheless, the exponential term decreases very rapidly to 0 as $n \to \infty$ regardless the value of λ.

3.4 Numerical Discussion

In the following section, we will investigate the convergence of the DESCM compared with the SESCM for various equations. Before we proceed with the examples, we would like to address the choice of the optimal mesh for the DESCM. As shown in [175], the use of the mesh size in (3.46) instead of (3.34) often leads to markedly superior results for intermediate values of N. Moreover, both these formulas for the mesh size h will lead to the same asymptotic error estimate in Theorem 3.3.3.

All calculations are performed using the programming language Julia [30] in double precision. The eigenvalue solvers in Julia utilize the famous linear algebra package *LAPACK* [13]. To produce our figures, we use the Julia package *Winston* [128]. The matrices $\mathbf{A}$ and $\mathbf{D}^2$ are constructed using (3.22) and (3.23) respectively.

To measure the performance of the DESINC method when the generalized eigenvalues of interest are known analytically, we use the absolute error as

follows:

$$\text{Absolute error} = |\mu_i(n) - \lambda_i| \qquad \text{for} \qquad n, i = 1, 2, \ldots, \tag{3.79}$$

where $\mu_i(n)$ is the n^{th} approximation to the i^{th} eigenvalue λ_i.

For the example 4.3, since the exact generalized eigenvalues are not known analytically, we computed approximations to absolute errors as follows:

$$\text{Absolute error approximation} = |\mu_i(n) - \mu_i(n-1)| \qquad \text{for} \qquad n, i = 1, 2, \ldots, \tag{3.80}$$

where $\mu_i(n)$ and $\mu_i(n-1)$ are the n^{th} and $(n-1)^{\text{th}}$ approximations to the i^{th} eigenvalue λ_i respectively.

3.4.1 Bessel Equation

An important eigenvalue problem related to the Bessel equation in Liouville form for $n \geq 1$ is defined by: [193]

$$\begin{aligned} -u''(x) + \frac{4n^2 - 1}{x^2}\, u(x) &= \lambda u(x), \qquad 0 < x < 1, \\ u(0) &= u(1) = 0. \end{aligned} \tag{3.81}$$

The solutions of (3.81) are given by:

$$u_m(x) = x^{1/2} J_n(x\sqrt{\lambda_m}) \quad \text{and} \quad \lambda_m = j_{m,n}^2 \quad \text{for} \quad m = 0, 1, \ldots, \tag{3.82}$$

where $j_{m,n}$ are the positive zeros of the Bessel function $J_n(x)$. In this case, the

point $x = 0$ is a regular singular point. The solution $u(x)$ has the following asymptotic behavior near the endpoints:

$$u(x) \sim \begin{cases} a_1 x^{n+1/2} & \text{as} \quad x \to 0 \\ a_2 (x-1) & \text{as} \quad x \to 1, \end{cases} \tag{3.83}$$

for some constants a_1 and a_2.

To implement the DE transformation, we use the first mapping in Table 3.1:

$$x = \phi_{DE}(t) \;=\; \frac{1}{2}\tanh(\sinh(t)) + \frac{1}{2} \;\sim\; \begin{cases} \dfrac{1}{2}\exp(-\exp(-t)) & \text{as} \quad t \to -\infty \\ 1 - \dfrac{1}{2}\exp(-\exp(t)) & \text{as} \quad t \to \infty. \end{cases} \tag{3.84}$$

Hence, the transformed equation (3.15) is given by:

$$\begin{aligned} -v''(t) + \left(\cosh^2(t) + \frac{1}{4} - \frac{3}{4}\mathrm{sech}^2(t) + \frac{(4n^2-1)\cosh^2(t)}{(e^{2\sinh(t)}+1)^2} \right) v(t) \\ = \lambda \left(\frac{\cosh(t)}{2\cosh^2(\sinh(t))} \right)^2 v(t). \end{aligned} \tag{3.85}$$

The solution of (3.85) has the following asymptotic behavior near infinities:

$$v(t) \sim \begin{cases} \alpha_1 \exp\left(\dfrac{t}{2} - n\exp(-t) \right) & \text{as} \quad t \to -\infty \\ \alpha_2 \exp\left(-\dfrac{t}{2} - \dfrac{1}{2}\exp(t) \right) & \text{as} \quad t \to \infty, \end{cases} \tag{3.86}$$

for some constants α_1 and α_2. Consequently, we can establish the following

bound for $v(t)$:

$$|v(t)| \leq A \exp(-n \exp(|\, t|)) \qquad \text{for} \qquad t \in \mathbb{R}, \tag{3.87}$$

for some constant A.

Using (3.46) with $\gamma = 1$, $\beta = n$ and $d = \dfrac{\pi}{2}$, we obtain:

$$h = \frac{W(\pi^2 N/2n)}{N}. \tag{3.88}$$

Before we conclude this numerical example, we mention that nonsymmetric Sinc expansions ($M \neq N$ in the Sinc expansion) can provide numerical efficiency in problems where the solutions to the transformed SL equation (3.15) have different asymptotic behaviour at both infinities. To illustrate this claim, we will compare the symmetric ($M = N$ in the Sinc expansion) and nonsymmetric Sinc expansions for this example.

For the transformed Bessel equation (3.85), using (3.35) with $B_L = n$, $B_R = 1/2$, $\gamma_L = 1$ and $\gamma_R = 1$, we obtain the following equation for the number of right collocation points:

$$N = \left\lceil M \left(1 + \frac{\log(2n)}{W(\pi^2 M/2n)} \right) \right\rceil. \tag{3.89}$$

Using (3.46), we obtain:

$$h = \frac{W(\pi^2 M/2n)}{M}. \tag{3.90}$$

Figure 3.3 displays the absolute error for the symmetric and nonsymmetric

DESCM and SESCM for the first eigenvalue of (3.81) with $n = 7$ and $\lambda_1 \approx 122.9076002036162$.

It is clear from Figure 3.3 that the symmetric DESCM outperforms the SESCM and more importantly the nonsymmetric DESCM proves to be far superior compared to both methods.

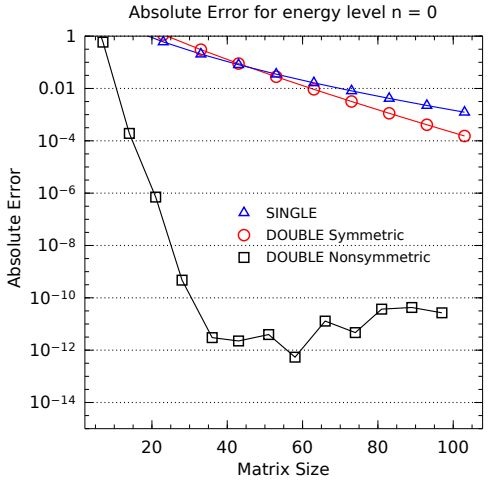

Figure 3.3: Plot of the absolute convergence of the SESCM as well as the symmetric and nonsymmetric DESCMs for the first eigenvalue $\lambda \approx 122.9076002036162$ of (3.81) with $n = 7$.

3.4.2 Laguerre Equation

The Laguerre equation in Liouville form [193] for $\alpha \in (-\infty, \infty)$ is defined by:

$$-u''(x) + \left(\frac{\alpha^2 - 1/4}{x^2} - \frac{\alpha + 1}{2} + \frac{x^2}{16}\right) u(x) = \lambda u(x), \qquad 0 < x < \infty$$
$$u(0) = u(\infty) = 0. \tag{3.91}$$

Equation (3.91) has the following analytic eigenvalues independent of α:

$$\lambda_n = n - 1, \qquad n = 1, 2, \ldots. \tag{3.92}$$

We will consider the case $\alpha > \dfrac{1}{2}$ where the point $x = 0$ is a regular singular point. The solution $u(x)$ has the following behavior near the endpoints:

$$u(x) \sim \begin{cases} Ax^{\alpha+1/2} & \text{as} \quad x \to 0 \\ Bx^{2\lambda+\alpha+1/2} \exp\left(-\dfrac{x^2}{8}\right) & \text{as} \quad x \to \infty, \end{cases} \tag{3.93}$$

for some constants A and B.

To implement the DE transformation, we use the second mapping in Table 3.1:

$$x = \phi_{DE}(t) \;=\; \operatorname{arcsinh}(e^{\sinh(t)}) \;\sim\; \begin{cases} \exp\left[-\dfrac{\exp(-t)}{2}\right] & \text{as} \quad t \to -\infty \\ \dfrac{\exp(t)}{2} & \text{as} \quad t \to \infty. \end{cases} \tag{3.94}$$

Hence, the transformed equation (3.15) is given by:

$$\begin{aligned} -v''(t) + \Bigg[& -\frac{3\cosh^2(x)}{16}\left(\tanh(\sinh(x)) + \frac{1}{3}\right)^2 + \frac{\cosh^2(x)}{3} + \frac{1}{4} - \frac{3}{4}\operatorname{sech}^2(x) \\ & + \left(\frac{\alpha^2 - 1/4}{\operatorname{arcsinh}^2(e^{\sinh(t)})} - \frac{\alpha+1}{2} + \frac{\operatorname{arcsinh}^2(e^{\sinh(t)})}{16}\right)\left(\frac{\cosh^2(t)}{1 + e^{-2\sinh(t)}}\right)\Bigg] v(t) \\ & = \left(\frac{\lambda \cosh^2(t)}{1 + e^{-2\sinh(t)}}\right) v(t). \end{aligned} \tag{3.95}$$

The solution of (3.95) has the following asymptotic behaviour near infini-

ties:

$$v(t) \sim \begin{cases} A' \exp(\frac{t}{2} - \frac{\alpha}{2}\exp(-t)) & \text{as} \quad t \to -\infty \\ B' \exp(t(\alpha + 2\lambda) - \frac{1}{32}\exp(2t)) & \text{as} \quad t \to \infty, \end{cases} \tag{3.96}$$

for some constants A' and B'. Consequently, we can establish the following bound for $v(t)$:

$$|v(t)| \leq \tilde{A} \exp\left(-\frac{1}{32}\exp(2|\,t|)\right) \qquad \text{for} \qquad t \in \mathbb{R}, \tag{3.97}$$

for some constant $\tilde{A}$.

Using (3.46) with $\gamma = 2$, $\beta = \dfrac{1}{32}$ and $d = \dfrac{\pi}{4}$, we obtain:

$$h = \frac{W(16\pi^2 N)}{2N}. \tag{3.98}$$

Since the solution to the transformed Laguerre equation (3.95) has different asymptotic behaviour at both infinities, we can use a nonsymmetric Sinc expansion. Using (3.46) with $B_L = \alpha/2$, $B_R = 1/32$, $\gamma_L = 1$ and $\gamma_R = 2$, we obtain the following equation for the number of left collocation points:

$$M = \max\left\{\left\lfloor 2N\left(1 - \frac{\log(16\alpha)}{W(16\pi^2 N)}\right)\right\rfloor, 0\right\}. \tag{3.99}$$

The step size in this case is given by (3.46) as:

$$h = \frac{W(16\pi^2 N)}{2N}. \tag{3.100}$$

Figure 3.4 displays the absolute error for the DESCM and SESCM for the first eigenvalue of (3.91) with $\alpha = 3$ and $\lambda_1 = 0$. Here again, the nonsymmetric case performs better than the symmetric case.

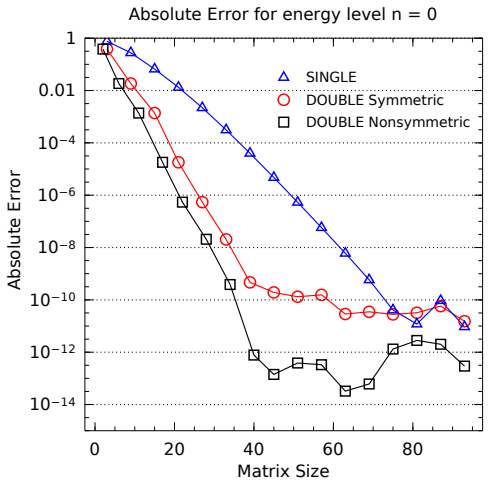

Figure 3.4: Plot of the absolute convergence of the SESCM as well as the symmetric and nonsymmetric DESCMs for the first eigenvalue of (3.91) with $\alpha = 3$ and $\lambda_1 = 0$.

3.4.3 Complex Singular equation

The following example illustrates the case where the coefficients $q(x)$ and $\rho(x)$ might have complex singularities close to the real line. In such instances the DESCM still outperforms the SESCM.

The singular equation that we consider is defined by the following:

$$-u''(x) + \left(x^2 + \frac{\tanh(x)}{\log(x^2+1.1)}\right) u(x) = \frac{\lambda}{x^2+\cos(x)} u(x), \qquad -\infty < x < \infty$$
$$u(-\infty) = u(\infty) = 0. \tag{3.101}$$

Equation (3.101) has several points where the coefficient functions are not analytic. Firstly, the coefficient function:

$$q(z) = z^2 + \frac{\tanh(z)}{\log(z^2 + 1.1)}, \tag{3.102}$$

has complex singularities at the points:

$$z = \pm i\sqrt{0.1} \qquad \text{and} \qquad z = i\pi\left(n + \frac{1}{2}\right) \quad \text{for} \quad n \in \mathbb{Z}. \tag{3.103}$$

Secondly, the weight function:

$$\rho(z) = \frac{1}{z^2 + \cos(z)}, \tag{3.104}$$

has complex singularities at the points:

$$z \approx \pm 1.621347946\, i \qquad \text{and} \qquad z \approx \pm 2.593916090\, i. \tag{3.105}$$

The solution $u(x)$ has the following behavior near the boundary points:

$$u(x) \sim A|x|^{-1/2} \exp\left(-\frac{1}{2}x^2\right) \qquad \text{as} \qquad |x| \to \infty, \tag{3.106}$$

for some constant A.

Since this example is not treated in literature, we will present the implementation of the SE transformation. Since the solution already exhibits SE decay, we use the third mapping in Table 3.1 $x = \phi_{SE}(t) = t$ to implement the SE transformation. Consequently, the transformed equation (3.15) is ex-

actly the same as (3.101). Moreover, we can obtain a bound for the solution of (3.15), which is given by:

$$|v(t)| \leq \tilde{A} \exp\left(-\frac{1}{2}t^2\right) \quad \text{for} \quad t \in \mathbb{R}. \tag{3.107}$$

Due to the complex singularities in (3.103) and (3.105), the optimal value for the strip width is $d = \sqrt{0.1}$. Hence using (3.27) with $\rho = 2$ and $\beta = \frac{1}{2}$, we obtain:

$$h = \left(\frac{4\pi\sqrt{0.1}}{N^2}\right)^{1/3}. \tag{3.108}$$

To implement the DE transformation, we use the third mapping in Table 3.1:

$$x = \phi_{DE}(t) \;=\; \sinh(t) \;\sim\; \begin{cases} -\dfrac{\exp(-t)}{2} & \text{as} \quad t \to -\infty \\ \dfrac{\exp(t)}{2} & \text{as} \quad t \to \infty. \end{cases} \tag{3.109}$$

Hence, the transformed equation (3.15) is given by:

$$\begin{aligned} -v''(t) + \left[\frac{1}{4} - \frac{3}{4}\operatorname{sech}^2(t) + \sinh(t)^2 + \frac{\tanh(\sinh(t))\cosh^2(t)}{\ln(\sinh^2(t) + 1.1)}\right] v(t) \\ = \left[\frac{\lambda \cosh^2(t)}{\sinh^2(t) + \cos(\sinh(t))}\right] v(t). \end{aligned} \tag{3.110}$$

The solution of (3.110) has the following asymptotic behavior near infinities:

$$v(t) \sim A' \exp\left(-|t| - \frac{1}{8}\exp(2|t|)\right) \qquad \text{as} \qquad |t| \to \infty, \tag{3.111}$$

for some constants A'. Consequently, $v(t)$ can be bounded as follows:

$$|\, v(t)| \leq \tilde{A} \exp\left(-\frac{1}{8}\exp(2|t|)\right) \qquad \text{for} \qquad t \in \mathbb{R}. \tag{3.112}$$

The conformal map $\phi(t) = \sinh(t)$ moves the singularities in (3.103) and (3.105) as follows. First, the coefficient function:

$$\tilde{q}(z) = \frac{1}{4} - \frac{3}{4}\text{sech}^2(z) + \sinh(z)^2 + \frac{\tanh(\sinh(z))\cosh^2(z)}{\ln(\sinh^2(z) + 1.1)}, \tag{3.113}$$

has complex singularities at the points:

$$\pm\, i \arcsin\left(\sqrt{0.1}\right),\, i\left(\frac{\pi}{2} + n\pi\right) \quad \text{and} \quad \pm\left(\text{arccosh}\left(\frac{\pi}{2} + \pi n\right) + \frac{\pi}{2}i\right), \quad n \in \mathbb{Z}. \tag{3.114}$$

Second, the weight function:

$$\rho(\sinh(z))\cosh^2(z) = \frac{\cosh^2(z)}{\sinh(z)^2 + \cos(\sinh(z))}, \tag{3.115}$$

has complex singularities at the points:

$$z \approx \pm\left[1.063876028 + \frac{\pi}{2}i\right] \quad \text{and} \quad z \approx \pm\left[1.606899463 + \frac{\pi}{2}i\right]. \tag{3.116}$$

Due to the complex singularities in (3.114) and (3.116), the optimal value for the strip width d is $d = \arcsin\left(\sqrt{0.1}\right)$.

Using (3.46) with $\gamma = 2$, $\beta = \dfrac{1}{8}$ and $d = \arcsin(\sqrt{0.1})$, we obtain:

$$h = \frac{W(16\pi \arcsin(\sqrt{0.1})N)}{2N}. \tag{3.117}$$

As can be seen from the above analysis, the conformal map $\phi(t) = \sinh(t)$ requires the solution of (3.110) to belong to $\mathbf{B}_2(\mathscr{D}_{\arcsin(\sqrt{0.1})})$. However, we will demonstrate that by choosing a conformal map of the form $\phi(t) = \kappa \sinh(t)$ for some parameter $0 < \kappa < 1$, we ware able to create a solution to (3.110) that belongs to the function space $\mathbf{B}_2(\mathscr{D}_{\frac{\pi}{4}})$. Since $\arcsin(\sqrt{0.1}) < \frac{\pi}{4}$, by Theorem 3.3.3 we expect eigenvalues of functions belonging to $\mathbf{B}_2(\mathscr{D}_{\frac{\pi}{4}})$ to converge faster. For more information on the use of conformal maps to accelerate convergence of Sinc numerical methods, we refer the interested reader to [152].

To implement the double exponential transformation for (3.110), we use the mapping:

$$x = \phi_{DE}(t) = \kappa \sinh(t) \sim \begin{cases} -\dfrac{\kappa \exp(-t)}{2} & \text{as} \quad t \to -\infty \\ \dfrac{\kappa \exp(t)}{2} & \text{as} \quad t \to \infty \end{cases} \quad \text{with} \;\; 0 < \kappa < 1. \tag{3.118}$$

Hence, the transformed equation (3.15) is given by:

$$\begin{aligned} -v''(t) + \left(\frac{1}{4} - \frac{3}{4}\operatorname{sech}^2(t) + \kappa^2 \sinh(t)^2 + \frac{\tanh(\kappa \sinh(t))\kappa^2 \cosh^2(t)}{\ln(\kappa^2 \sinh^2(t) + 1.1)} \right) v(t) \\ = \left(\frac{\lambda \kappa^2 \cosh^2(t)}{\kappa^2 \sinh^2(t) + \cos(\kappa \sinh(t))} \right) v(t). \end{aligned} \tag{3.119}$$

The solution of (3.110) has the following asymptotic behavior near infinities:

$$v(t) \sim A' \exp\left(-|t| - \frac{\kappa^2}{8} \exp(2|t|) \right) \qquad \text{as} \qquad |t| \to \infty, \tag{3.120}$$

for some constants A'. Consequently, $v(t)$ can be bounded as follows:

$$|\, v(t)| \leq \tilde{A} \exp\left(-\frac{\kappa^2}{8}\exp(2|t|)\right) \qquad \text{for} \qquad t \in \mathbb{R}. \tag{3.121}$$

The conformal map $\phi(t) = \kappa \sinh(t)$ moves the singularities in (3.103) and (3.105) as follows. Firstly, the coefficient function:

$$\tilde{q}(z) = \frac{1}{4} - \frac{3}{4}\text{sech}^2(t) + \kappa^2 \sinh(t)^2 + \frac{\tanh(\kappa \sinh(t))\kappa^2 \cosh^2(t)}{\ln(\kappa^2 \sinh^2(t) + 1.1)}, \tag{3.122}$$

has complex singularities at the points:

$$\pm i \arcsin\left(\frac{\sqrt{0.1}}{\kappa}\right),\ i\left(\frac{\pi}{2} + n\pi\right) \ \text{ and } \ \pm\left(\text{arccosh}\left(\frac{\pi}{2\kappa} + \frac{\pi n}{\kappa}\right) + \frac{\pi}{2}i\right),\ \ n \in \mathbb{Z}. \tag{3.123}$$

Secondly, the weight function:

$$\rho(\kappa \sinh(z))\kappa^2 \cosh^2(z) = \frac{\kappa^2 \cosh^2(z)}{\kappa^2 \sinh(z)^2 + \cos(\kappa \sinh(z))}, \tag{3.124}$$

has complex singularities at the points:

$$z \approx \pm\left[\text{arccosh}\left(\frac{1.621347946}{\kappa}\right) + \frac{\pi}{2}i\right] \ \text{ and } \ z \approx \pm\left[\text{arccosh}\left(\frac{2.593916090}{\kappa}\right) + \frac{\pi}{2}i\right]. \tag{3.125}$$

By Theorem 3.3.3, the optimal value for the strip width d can be at most $\frac{\pi}{4}$. Hence, by choosing $\kappa = \sqrt{0.2}$, the closest singularities of (3.119) lie on the lines $y = \pm i\frac{\pi}{4}$. Consequently, using (3.46) with $\gamma = 2$, $\beta = \frac{0.2}{8}$ and $d = \frac{\pi}{4}$, we obtain:

$$h = \frac{W(20\pi^2 N)}{2N}. \tag{3.126}$$

Figure 3.5 displays the convergence rate of the DESCM and SESCM in computing approximations of the the first eigenvalue $\lambda \approx 0.690894228848$ of the singular equation (3.101). It is clear that the convergence is further improved by using the adapted transformation $\phi(t) = \sqrt{0.2}\sinh(t)$.

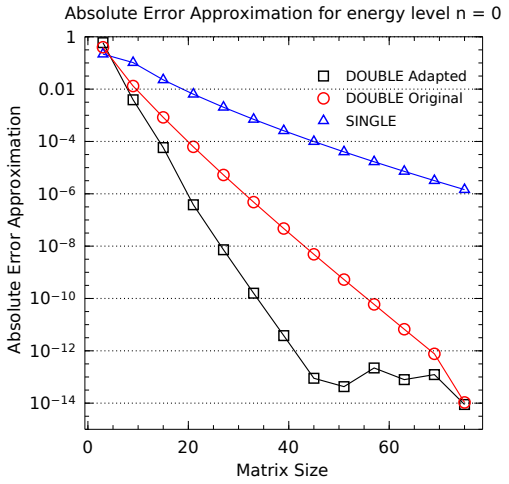

Figure 3.5: Plot of the absolute convergence of the SESCM as well as the symmetric and adapted DESCMs for the first eigenvalue $\lambda \approx 0.690894228848$ of (3.101).

3.5 Conclusion

Computing the eigenvalues of singular Sturm-Liouville equations can be numerically challenging. In this work, we compute the eigenvalues of such equations using the Sinc-collocation method coupled with double exponential variable transformation. The implementation of the DESCM leads to a generalized eigenvalue problem with symmetric and positive definite matrices. In addition, we also show that the convergence of the DESCM is of the rate $\mathcal{O}\left(\frac{N^{5/2}}{\log(N)^2}e^{-\kappa N/\log(N)}\right)$ for some $\kappa > 0$, as $N \to \infty$ where $2N+1$ is the dimen-

sion of the resulting generalized eigenvalue system. Consequently, DESCM outperforms SESCM proposed in [56]. We follow up this claim by conducting numerical studies of several Sturm-Liouville eigenvalue problems using both the SESCM and the DESCM. Finally, we also use adapted conformal mappings to accelerate the convergence of the DESCM to ensure the analyticity of the transformed coefficient functions in a strip of maximal width. In all our numerical examples, we were able to reach an unprecedented degree of accuracy.

Chapter 4

The Anharmonic Oscillator Revisited

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Abstract.

A quantum anharmonic oscillator is defined by the Hamiltonian $\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$, where the potential is given by $V(x) = \sum_{i=1}^{m} c_i x^{2i}$ with $c_m > 0$. Using the Sinc collocation method combined with the double exponential transformation, we develop a method to efficiently compute highly accurate approximations of energy eigenvalues for anharmonic oscillators. Convergence properties of the proposed method are presented. Using the principle of minimal sensitivity, we introduce an alternate expression for the mesh size for the Sinc collocation method which improves considerably the accuracy in comput-

ing eigenvalues for potentials with multiple wells.

We apply our method to a number of potentials including potentials with multiple wells. The numerical results section clearly illustrates the high efficiency and accuracy of the proposed method. All our codes are written in Julia and are available upon request.

4.1 Introduction

The following chapter follows from our published work in [83]. The one dimensional anharmonic oscillator is of great interest to field theoreticians because it models complicated fields in one-dimensional space-time [22]. A complete overview of quantum anharmonic oscillators would lead to a better understanding of the realistic analytic structure of field theory. Moreover, outside the realm of field theory, the one dimensional anharmonic oscillator also provides an approximation to more complicated quantum potentials near a stable stationary point. The study of quantum anharmonic oscillators as potentials in the Schrödinger equation has been on the edge of thrilling and exciting research during the past three decades [2, 4, 10, 20, 21, 24, 28, 33, 35, 39, 43, 50, 51, 54, 71, 72, 75, 97, 111, 124, 130, 133, 148–150, 170, 171, 184, 186, 192, 197]. With advances in asymptotic analysis and symbolic computing algebra, the interest in developing more efficient methods was renewed recently [17, 19, 82, 179, 180]. The Hamiltonian in the time-independent Schrödinger equation is given by $\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ for some potential function $V(x)$. In the case of quantum anharmonic oscillators, the potential $V(x)$ is an even function of the form $V(x) = \sum_{i=1}^{m} c_i x^{2i}$ with $c_m > 0$. Several approaches have been used for the nu-

merical evaluation of the differential eigenvalue problem $\mathcal{H}\psi = E\psi$. However, the existing numerical methods are mostly case specific and lack uniformity when faced with a general problem.

In [21,184,186], Rayleigh-Schrödinger perturbation series are used to evaluate the ground state energy for potentials of the form $V(x) = x^2 + \beta x^{2m}$ for $\beta \in [0, \infty)$ and $m = 2, 3, 4$. These summations are strongly divergent for $\beta \neq 0$. To sum them efficiently, Padé approximants combined with nonlinear sequence transformations are used. In [192], Rayleigh-Schrödinger perturbation series are also used to evaluate energies of the ground state and the first excited state for potentials of the form $V(x) = x^2 + \beta x^4$. In [133], Rayleigh-Schrödinger perturbation series are used to evaluate energies of the ground state and the first four excited states for the Hamiltonian of the form $\mathcal{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2 + \lambda x^4$ in the limits $\lambda \to 0^+$ and $\lambda \to \infty$. In [35], exact soluble models are used to construct Rayleigh-Schrödinger perturbation series for the eigenvalues of the anharmonic potentials of the form $V(A, E) = \frac{1}{2}Ax^2 + Ex^4$. In [10,20,24], a study of Rayleigh-Schrödinger perturbation series is presented using the Wentzel-Kramers-Brillouin (WKB) method and a difference equation method. In [2], an averaging method is proposed to calculate energy eigenvalues for potentials of the form $V(x) = \lambda x^{2m}$ for $m = 2, 3, \ldots$ with $\lambda > 0$, $V(x) = \mu x^2 + \lambda x^4 + \eta x^6$ with $\eta > 0$ and $V(x) = (ax^3 + bx)^2$ using a supersymmetric WKB approach. Their method yields appreciable accuracy for a variety of potentials and the accuracy increases as the energy level increases. In [50], the first four terms of the asymptotic expansion for the energy eigenvalues of the potential $V(x) = ax^2 + bx^4 + cx^6$ as $n \to \infty$ and in the large coupling limit $c \to \infty$ are found. Since no exact energy values were available at the time,

comparisons with the values obtained via the Hill determinant method are shown. The values obtained using the asymptotic expansion agree with the values obtained using the Hill determinant method and increase in accuracy as the energy level increases. In [124], an asymptotic expansion is presented for the energy values of potentials of the form $V(x) = \sum_{i=}^{N} a_i x^i + \sum_{j=1}^{M} c_j x^{-j}$. This method allows for an easier way to obtain analytically the coefficients for the leading terms in the WKB expansion, which normally would require computation of a considerably large number of complicated contour integrals. As an example of application, the first seven coefficients of the WKB expansion for the energy eigenvalues of the potentials $V(x) = x^4 + bx^2$ and $V(x) = x^6$ are presented. In [111], the WKB method and the Lanczos algorithm are used to calculate energy eigenvalues of the potential $V(x) = \frac{1}{2}x^2 + \lambda\, x^{2m}$ with m from two to six to a high accuracy. Using a starting energy value from a JWKB analysis, their shifted Lanczos algorithm is able to achieve 33 correct digits in three iterations or less for all energy states. In [130], the variational principle is used to calculate the first n energy eigenvalues using a Rayleigh-Ritz matrix for the perturbed Hamiltonian $\mathcal{H} = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}\Omega^2 x^2 + \epsilon[\lambda x^4 + \frac{1}{2}(\omega^2 - \Omega^2)x^2]$. Utilizing the non-linear parameter Ω, this method becomes applicable when the parameter $\omega^2 < 0$. Moreover, this method is able to find eigenvalues for several lower energy states even in deep double well potentials. In [33], a variational approach is used to obtain the energies of the ground state and the first excited state for potentials of the form $x^2 + \lambda V(x)$, where $V(x)$ is an even analytic function. A numerical study is presented for $V(x) = x^{2m}$ for $m = 2, \ldots, 6$ as well as $V(x) = x^2 + \lambda x^4 + \mu x^6$ and the numerical results obtained agree quite well with the values obtained using the Hill determinant method. In [51], an

approximate analytic expression for the energy eigenvalues for the anharmonic oscillator $V(x) = Ax^6 + Bx^2$ is introduced. These approximate solutions are derived from particular analytic solutions which are valid when certain relations between the parameters A and B are satisfied. In [75], exact solutions in the form of definite integrals are found for the anharmonic oscillator of the form $V(x) = \frac{1}{2}\omega^2 x^2 + \frac{1}{4}\lambda x^4 + \frac{1}{6}\eta x^6$. Exact analytical energy eigenvalues are derived when the coefficients ω, λ and η satisfy specific constraints.

The Hill determinant method as well as the Hill determinant method with a variational parameter have also shown great promises [4,39,43,54,148,171,197]. To create a Hill determinant matrix, one starts by substituting a suitable ansatz into the Schrödinger equation of the from $\psi(x) = e^{s(x)} \sum_{i=0}^{\infty} \gamma_i x^{2i+\delta}$, where $s(x)$ is an even polynomial function that depends on the potential $V(x)$ and $\delta = 0$ or 1 depending on the parity of the solution. With this substitution, one obtains a recurrence relation for the coefficients γ_i. By rewriting this recurrence relation in a matrix form and setting the determinant of this matrix to zero, one can create a sequence of approximations for the energy eigenvalues of the potential $V(x)$. In [97], the discretization of the Hamiltonian operator using a finite difference technique is discussed to solve this type of eigenvalue problem. The Riccati equation for the logarithmic derivative of the wavefunction using Padé approximants or the Turbiner method has also been used extensively. Further analysis of the Riccati equation solution leads to a better understanding of the overall nature of the wavefunction and thus its energy eigenvalues. In [71], a non-perturbative method utilizing the solution to the Riccati equation is proposed for finding energy eigenvalues. The method is applied to the potential $V(x) = x^2 + \lambda x^4$ and yields good estimates

for lower energy values. In [28], a method utilizing the solution to the Riccati equation for finding exact solutions to anharmonic oscillators is discussed. The method is applied to the potential $V(x) = x^2 + \lambda x^4$ and energy eigenvalues are computed for coupling constants ranging from $\lambda = 0.002$ to $\lambda = 20000$. In [72], a method is introduced based on rational approximations to the solution of the Riccati equation to obtain tight lower and upper bounds for the energy eigenvalues of anharmonic oscillators.

Recently [82], an asymptotic expansion for the energy eigenvalues of the potential $V(x) = \kappa\, x^{2q} + \omega\, x^2$, where $\kappa \in \mathbb{R}^+$, $\omega \in \mathbb{R}$ and $q \in \mathbb{N} \setminus \{1\}$ as the energy level n approaches infinity is derived using the WKB method and series reversion. In [179, 180], the potential $V(x) = ax^2 + \lambda x^4$ with $a < 0$ and $\lambda \geq 0$ is explored. Using asymptotic expansion of the Riccati equation solutions, an approximate solution is found which yields 9 to 10 significant digits for energy values. In [17], an asymptotic iteration method is used to calculate the energy eigenvalues of potentials of the form $V(x) = Ax^{2\alpha} + Bx^2$.

As can be seen by the numerous approaches which have been made to solve this problem, there is a beautiful diversity yet lack of uniformity in its resolution. While several of these methods yield excellent results for specific cases, it would be favorable to have one general method that could handle any anharmonic potential while being capable of computing efficiently approximations of eigenvalues to a high pre-determined accuracy.

The Sinc collocation method (SCM) has been used extensively during the last three decades to solve many problems in numerical analysis [9, 37, 57, 58, 107, 115, 153–155, 158]. Their applications include numerical integration, linear and non-linear ordinary differential equations, partial differential equations, in-

terpolation and approximations to function derivatives. Recently, combination of the SCM with the double exponential (DE) transformation has sparked great interest [164,168]. The double exponential transformation, introduced in [166] yields optimal accuracy for a given number of function evaluations when using the trapezoidal rule in numerical integration [121]. Since its derivation in 1974, many have studied its effectiveness in computing integrals [161,166].

In [84], we used the SCM and the DE transformation to solve efficiently singular Sturm-Liouville eigenvalue problems. In the present work, we use this method to compute energy eigenvalues of anharmonic oscillators to unprecedented accuracy. The double exponential Sinc collocation method (DESCM) starts by approximating the wave function as a series of weighted Sinc functions. By substituting this approximation in the Schrödinger equation and evaluating this expression at several collocation points spaced equally by a specified mesh size h, we obtain a generalized eigensystem which can be transformed into a regular eigenvalue problem. For multiple-well potentials, the existing expression for the optimal mesh size h turns out to be not very effective. In such a case, we introduce an alternate mesh size $\hat{h}$ by minimizing the trace of the resulting matrix using the principle of minimal sensitivity. After conducting an asymptotic study of this minimizing problem, we obtain the first order term in the asymptotic expansion of the alternate mesh size $\hat{h}$.

The proposed method has numerous advantages over the existing alternatives. It can be applied to a large set of anharmonic potentials and is insensitive to changes in the potential parameters. The method is now shown to be efficient and accurate when dealing with multiple-well potentials. In addition, the DESCM has a near-exponential convergence rate and the matrices generated

by the DESCM have useful symmetric properties which simplify considerably the computation of their eigenvalues.

4.2 General definitions and properties

The sinc function is defined by the following expression:

$$\operatorname{sinc}(z) = \frac{\sin(\pi z)}{\pi z}, \qquad z \in \mathbb{C}. \tag{4.1}$$

The Sinc function $S(j,h)(x)$ for $h \in \mathbb{R}^+$ and $j \in \mathbb{Z}$ is given by:

$$S(j,h)(x) = \operatorname{sinc}\left(\frac{x - jh}{h}\right), \qquad x \in \mathbb{C}. \tag{4.2}$$

The discrete orthogonality of Sinc functions is given by:

$$S(j,h)(kh) = \delta_{j,k} \qquad \text{for} \qquad j,k \in \mathbb{Z}, \tag{4.3}$$

where $\delta_{j,k}$ is the Kronecker's delta function.

Similarly to Fourier series, we can expand well-defined functions as series of Sinc functions. Such expansions are known as Sinc expansions or Whittaker Cardinal expansions.

Definition 4.2.1. *[155] Given any function $v(x)$ defined everywhere on the real line and any $h > 0$, the Sinc expansion of $v(x)$ is defined by the following series:*

$$C(v,h)(x) = \sum_{j=-\infty}^{\infty} v_{j,h} S(j,h)(x), \tag{4.4}$$

where $v_{j,h} = v(jh)$.

The non-symmetric truncated Sinc expansion of the function $v(x)$ is defined by the following series:

$$C_N(v,h)(x) = \sum_{j=-N}^{M} v_{j,h}\, S(j,h)(x) \qquad \text{for} \qquad N, M \in \mathbb{N}. \tag{4.5}$$

The symmetric truncated Sinc expansion is obtained by taking $M = N$ in the above equation.

In [155], a class of functions which are successfully approximated by a Sinc expansion is introduced. We present the definition for this class of functions bellow.

Definition 4.2.2. *[155] Let* $d > 0$ *and let* $\mathscr{D}_d$ *denote the strip of width* $2d$ *about the real axis:*

$$\mathscr{D}_d = \{z \in \mathbb{C} : |\,\Im(z)| < d\}. \tag{4.6}$$

For $\epsilon \in (0,1)$*, let* $\mathscr{D}_d(\epsilon)$ *denote the rectangle in the complex plane:*

$$\mathscr{D}_d(\epsilon) = \{z \in \mathbb{C} : |\,\Re(z)| < 1/\epsilon,\ |\,\Im(z)| < d(1-\epsilon)\}. \tag{4.7}$$

Let $\mathbf{B}_2(\mathscr{D}_d)$ *denote the family of all functions* g *that are analytic in* $\mathscr{D}_d$*, such that:*

$$\int_{-d}^{d} |\,g(x+iy)|\,dy \to 0 \quad \textit{as} \quad x \to \pm\infty \tag{4.8}$$

and

$$\mathscr{N}_2(g, \mathscr{D}_d) = \lim_{\epsilon \to 0} \left(\int_{\partial \mathscr{D}_d(\epsilon)} |\,g(z)|^2\,|dz| \right)^{1/2} < \infty. \tag{4.9}$$

The time independent Schrödinger equation is given by:

$$\mathcal{H}\,\psi(x) \;=\; E\,\psi(x), \tag{4.10}$$

where the Hamiltonian is given by the following linear operator:

$$\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x),$$

where $V(x)$ is the potential energy function.

In the case of anharmonic oscillators, the potential $V(x)$ is given by:

$$V(x) = \sum_{i=1}^{m} c_i x^{2i} \qquad \text{with} \qquad c_m > 0 \quad \text{and} \quad m \in \mathbb{N}\backslash\{1\}. \tag{4.11}$$

The time independent Schrödinger equation (4.10) can be written as the following boundary value problem:

$$-\psi''(x) + V(x)\psi(x) = E\psi(x) \qquad \text{with} \qquad \lim_{|x|\to\infty} \psi(x) = 0. \tag{4.12}$$

Equation (4.12) is similar to the Sturm-Liouville problem to which we applied successfully the DESCM [84].

As we stated in [84], Eggert et al. [56] demonstrate that applying an appropriate substitution to the boundary value problem (4.12), results in a symmetric discretized system when using Sinc expansion approximations. The change of variable they propose is given by:

$$v(x) = \left(\sqrt{(\phi^{-1})'}\,\psi\right) \circ \phi(x) \qquad \Longrightarrow \qquad \psi(x) = \frac{v \circ \phi^{-1}(x)}{\sqrt{(\phi^{-1}(x))'}}, \tag{4.13}$$

where $\phi^{-1}(x)$ a conformal map of a simply connected domain in the complex plane with boundary points $a \neq b$ such that $\phi^{-1}(a) = -\infty$ and $\phi^{-1}(b) = \infty$.

Applying the substitution (4.13) to (4.12), we obtain:

$$\hat{\mathcal{H}}\, v(x) = -v''(x) + \tilde{V}(x)v(x) \;=\; E(\phi'(x))^2 v(x), \tag{4.14}$$

where:

$$\tilde{V}(x) = -\sqrt{\phi'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\phi'(x)}\frac{\mathrm{d}}{\mathrm{d}x}(\sqrt{\phi'(x)})\right)+(\phi'(x))^2 V(\phi(x)) \quad \text{and} \quad \lim_{|x|\to\infty} v(x) = 0. \tag{4.15}$$

4.3 The double exponential Sinc collocation method (DESCM)

A function $\omega(x)$ decays double exponentially at infinities if there exist positive constants A, B, γ such that:

$$|\,\omega(x)| \leq A\exp(-B\exp(\gamma|\,x|)) \qquad \text{for} \qquad x \in \mathbb{R}. \tag{4.16}$$

The double exponential transformation is a conformal mapping $\phi(x)$ which allows for the solution of (4.14) to have double exponential decay at both infinities.

To implement the DESCM, we begin by approximating the solution of (4.14) by a truncated Sinc expansion (4.5).

Inserting (4.5) into (4.14), we obtain the following system of equations:

$$\hat{\mathcal{H}}\, C_N(b,h)(x_k) = \sum_{j=-N}^{N} \left[-\frac{\mathrm{d}^2}{\mathrm{d}x_k^2} S(j,h)(x_k) + \tilde{V}(x_k) S(j,h)(x_k) \right] v_{j,h} \tag{4.17}$$

$$= \mathcal{E} \sum_{j=-N}^{N} S(j,h)(x_k)(\phi'(x_k))^2 v_{j,h} \qquad \text{for} \qquad k = -N, \ldots, N, \tag{4.18}$$

where the collocation points $x_k = kh$ and $\mathcal{E}$ is an approximation of the eigenvalue E in (4.14).

The above equation can be re-written as follows:

$$\hat{\mathcal{H}}\, C_N(v,h)(x_k) = \sum_{j=-N}^{N} \left[-\frac{1}{h^2}\, \delta_{j,k}^{(2)} + \tilde{V}(kh)\, \delta_{j,k}^{(0)} \right] v_{j,h}$$

$$= \mathcal{E} \sum_{j=-N}^{N} \delta_{j,k}^{(0)} (\phi'(kh))^2 v_{j,h} \quad \text{for} \quad k = -N, \ldots, N, \tag{4.19}$$

where $\delta_{j,k}^{(l)}$ are given by [154]:

$$\delta_{j,k}^{(l)} = h^l \left(\frac{d}{dx} \right)^l S(j,h)(x) \bigg|_{x=kh}. \tag{4.20}$$

Equation (4.19) can be represented in matrix form as follows:

$$\hat{\mathcal{H}}\, \mathbf{C}_N(v,h) = \mathbf{H}\mathbf{v} \;=\; \mathcal{E}\mathbf{D}^2\mathbf{v} \quad \Longrightarrow \quad (\mathbf{H} - \mathcal{E}\mathbf{D}^2)\mathbf{v} \;=\; 0, \tag{4.21}$$

where:

$$\mathbf{v} = (v_{-N,h}, \ldots, v_{N,h})^T \qquad \text{and} \qquad \mathbf{C}_N(v,h) = (C_N(v,h)(-Nh), \ldots, C_N(v,h)(Nh))^T.$$

$\mathbf{H}$ is a $(2N+1)\times(2N+1)$ matrix with entries $H_{j,k}$ given by:

$$H_{j,k} = -\frac{1}{h^2}\,\delta^{(2)}_{j,k} + \tilde{V}(kh)\,\delta^{(0)}_{j,k} \qquad \text{with} \qquad -N \le j,k \le N, \tag{4.22}$$

and $\mathbf{D}^2$ is a $(2N+1)\times(2N+1)$ diagonal matrix with entries $D^2_{j,k}$ given by :

$$D^2_{j,k} = (\phi'(kh))^2\,\delta^{(0)}_{j,k} \qquad \text{with} \qquad -N \le j,k \le N. \tag{4.23}$$

To obtain nontrivial solutions for (4.21), we have to set:

$$\det(\mathbf{H} - \mathcal{E}\mathbf{D}^2) = 0. \tag{4.24}$$

To find an approximation of the eigenvalues of equation (4.14), one simply has to solve the above generalized eigenvalue problem. The matrix $\mathbf{D}^2$ is symmetric positive definite and the matrix $\mathbf{H}$ is symmetric. If there exits a constant $\delta > 0$ such that $\tilde{V}(x) \ge \delta^{-1}$, then the matrix $\mathbf{H}$ is symmetric positive definite.

In [84, Theorem 3.2], we present the convergence analysis of DESCM which we state here in the case of the transformed Schrödinger equation (4.14). The proof of the Theorem is given in [84].

Theorem 4.3.1. *[84, Theorem 3.2] Let E and $v(x)$ be an eigenpair of the transformed Schrödinger equation:*

$$-v''(x) + \tilde{V}(x)v(x) = E(\phi'(x))^2 v(x), \tag{4.25}$$

where:

$$\tilde{V}(x) = -\sqrt{\phi'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\phi'(x)}\frac{\mathrm{d}}{\mathrm{d}x}(\sqrt{\phi'(x)})\right)+(\phi'(x))^2 V(\phi(x)) \quad \textit{and} \quad \lim_{|x|\to\infty} v(x) = 0. \tag{4.26}$$

Assume there exist positive constants A, B, γ *such that:*

$$|v(x)| \leq A\exp(-B\exp(\gamma|x|)) \qquad \textit{for all} \qquad x \in \mathbb{R}, \tag{4.27}$$

and that $v \in \mathbf{B}_2(\mathscr{D}_d)$ *with* $d \leq \dfrac{\pi}{2\gamma}$.

If there is a constant $\delta > 0$ *such that* $\tilde{V}(x) \geq \delta^{-1}$ *and the selection of the optimal mesh size* h *is such that:*

$$h = \frac{W(\pi d\gamma N/B)}{\gamma N}, \tag{4.28}$$

where $W(x)$ *is the Lambert W function.*

Then, there is an eigenvalue $\mathcal{E}$ *of the generalized eigenvalue problem satisfying:*

$$|\mathcal{E} - E| \leq \vartheta_{v,d}\sqrt{\delta E}\left(\frac{N^{5/2}}{\log(N)^2}\right)\exp\left(-\frac{\pi d\gamma N}{\log(\pi d\gamma N/B)}\right) \quad \textit{as} \quad N \to \infty, \tag{4.29}$$

where $\vartheta_{v,d}$ *is a constant that depends on* v *and* d.

As we can see from the results obtained in Theorem 4.3.1, $|\mathcal{E} - E| \to 0$ as $N \to \infty$ for all energy eigenvalues E.

4.4 Anharmonic oscillators

To implement the DE transformation, we choose a function ϕ which would result in the solution of (4.14) to decay doubly exponentially. Since the anharmonic potential is analytic in $\mathbb{C}$ and grows to infinity as $x \to \pm\infty$, the wave function is also analytic in $\mathbb{C}$ and normalizable over $\mathbb{R}$.

To find the decay rate of the solution to equation (4.12) with the anharmonic oscillator potential, we will use the WKB method. Substituting the ansatz $\psi(x) = e^{S(x)}$ into equation (4.12) and simplifying, we obtain:

$$S''(x) + (S'(x))^2 - \sum_{i=1}^{m} c_i x^{2i} + E = 0. \tag{4.30}$$

Since $m > 1$, we have $S''(x) = o\left(S'(x)^2\right)$ as $|x| \to \infty$. Hence:

$$(S'(x))^2 \sim c_m x^{2m} \qquad \text{as} \qquad |x| \to \infty. \tag{4.31}$$

Using the initial condition $\lim_{|x|\to\infty} \psi(x) = 0$, we obtain:

$$S(x) \sim -\frac{\sqrt{c_m}\,|x|^{m+1}}{m+1} \qquad \text{as} \qquad |x| \to \infty. \tag{4.32}$$

To find the second order term, we make the substitution:

$$S(x) = -\frac{\sqrt{c_m}\,|x|^{m+1}}{m+1} + C(x), \tag{4.33}$$

in equation (4.30), where $C(x) = o\left(|x|^{m+1}\right)$ as $|x| \to \infty$.

After simplifying and keeping only the higher order terms, we obtain:

$$C'(x) \sim -\frac{m}{2x} \qquad \text{as} \qquad |x| \to \infty. \tag{4.34}$$

Solving for $C(x)$, we obtain:

$$C(x) \sim \ln\left(|x|^{-m/2}\right) \qquad \text{as} \qquad |x| \to \infty. \tag{4.35}$$

From (4.32) and (4.35), it follows that $\psi(x)$ has the following decay rate at both infinities:

$$\psi(x) = \mathcal{O}\left(|x|^{-m/2} \exp\left(-\frac{\sqrt{c_m}\,|x|^{m+1}}{m+1}\right)\right) \qquad \text{as} \qquad |x| \to \infty. \tag{4.36}$$

Away from both infinities, the wave function $\psi(x)$ will undergo oscillatory behavior.

As can be seen from (4.36), the wave function $\psi(x)$ decays only single exponentially at infinities.

By taking $\phi(x) = \sinh(x)$, we have:

$$\begin{aligned} |v(x)| &= \left|\frac{\psi \circ \phi(x)}{\sqrt{\phi'(x)}}\right| \\ &\leq A|\sinh(x)|^{-m/2}|\cosh(x)|^{-1/2} \exp\left(-\frac{\sqrt{c_m}|\sinh(x)|^{m+1}}{m+1}\right) \\ &\leq A \exp\left(-\frac{\sqrt{c_m}}{(m+1)2^{m+1}} \exp((m+1)|x|)\right), \end{aligned} \tag{4.37}$$

for some positive constant A.

From (4.37), it follow that the optimal mesh size according to Theo-

rem 4.3.1 is given by:

$$h = \frac{W\left(\frac{2^m \pi^2 (m+1)N}{\sqrt{c_m}}\right)}{(m+1)N}. \tag{4.38}$$

As will be illustrated in our numerical study, the optimal mesh size h given by (4.38) does not prove effective when dealing with multiple-well potentials. In this case, we use the principle of minimal sensitivity [9] to obtain an alternate mesh size, which we will denote by $\hat{h}$.

First, we start by simplifying the eigensystem (4.21) as follows. Applying a Cholesky factorization to the symmetric positive diagonal matrix $\mathbf{D}^2$, leads to:

$$\mathbf{D}^2 = \mathbf{D}\mathbf{D}^T = \mathbf{D}\mathbf{D}. \tag{4.39}$$

Using the above equation, we can re-write the eigensystem (4.21) as follows:

$$(\mathbf{D}^{-1}\mathbf{H}\mathbf{D}^{-1} - \mathcal{E}\,\mathbf{I})\mathbf{z} = 0 \qquad \text{and} \qquad \mathbf{z} = \mathbf{D}\mathbf{v}. \tag{4.40}$$

The inverse matrix $\mathbf{D}^{-1}$ exists since $\mathbf{D}^2$ is a diagonal positive definite matrix.

Let us denote the new matrix in (4.40) by $\mathbf{K} = \mathbf{D}^{-1}\mathbf{H}\mathbf{D}^{-1}$. Therefore, $\mathbf{K}$ is a $(2N+1) \times (2N+1)$ matrix with entries $K_{j,k}$ given by:

$$K_{j,k} = -\left(\frac{1}{h^2 \phi'(jh)\phi'(kh)}\right)\delta^{(2)}_{j,k} + \left(\frac{\tilde{V}(kh)}{(\phi'(kh))^2}\right)\delta^{(0)}_{j,k} \quad \text{with} \quad -N \le j,k \le N, \tag{4.41}$$

where $\phi(x) = \sinh(x)$ and $\tilde{V}(x)$ is given by:

$$\tilde{V}(x) \;=\; \frac{1}{4} - \frac{3}{4}\operatorname{sech}^2(x) + \cosh^2(x)\sum_{i=1}^{m} c_i \sinh^{2i}(x). \tag{4.42}$$

Denoting the trace of a matrix by $\mathrm{Tr}(\cdot)$, we have:

$$\mathrm{Tr}(\mathbf{K})(h) = \sum_{i=0}^{2N} \mathcal{E}_i(h), \tag{4.43}$$

where $\{\mathcal{E}_i(h)\}_{i=0,\ldots,2N}$ are the $2N+1$ eigenvalues of the matrix $\mathbf{K}$ or equivalently the generalized eigenvalues of the matrices $\mathbf{H}$ and $\mathbf{D}^2$. Note that the eigenvalues depend strongly on the mesh size h. Since our goal is to obtain the best approximations to these energy eigenvalues, by the principle of minimal sensitivity [9], it seems logical to minimize their sum with respect to h. In other words, this alternate mesh size is given as the solution of the following optimization problem:

$$\hat{h} = \arg\min_{h\in\mathbb{R}^+} \{\mathrm{Tr}(\mathbf{K})(h)\}. \tag{4.44}$$

As an example, in Figure 4.1, we plot $\mathrm{Tr}(\mathbf{K})(h)$ with $N = 20$ for the potentials in (4.64) along with the absolute error obtained when approximating energy eigenvalues.

To find this alternate mesh size, one would need to solve the minimization problem in (4.44). To achieve this goal, we require the following theorem establishing the existence of such a minimum.

Theorem 4.4.1. *If* $\mathbf{K}$ *is a matrix with components defined by equation* (4.41)*,* $\phi(x)$ *is the inverse function of the conformal map* $\phi^{-1}(x)$ *and* $(V(x), \phi(x)) \in \mathcal{X}$ *where* $\mathcal{X}$ *is defined as the following function space:*

$$\mathcal{X} = \left\{ (V(x),\phi(x)) \in C(\mathbb{R}) \times C^3(\mathbb{R}) : \lim_{|x|\to\infty} \frac{\tilde{V}(x)}{(\phi'(x))^2} = \infty \quad \textit{and} \quad \phi'(x) > 0,\ \forall x \in \mathbb{R}\cup\{\pm\infty\} \right\}, \tag{4.45}$$

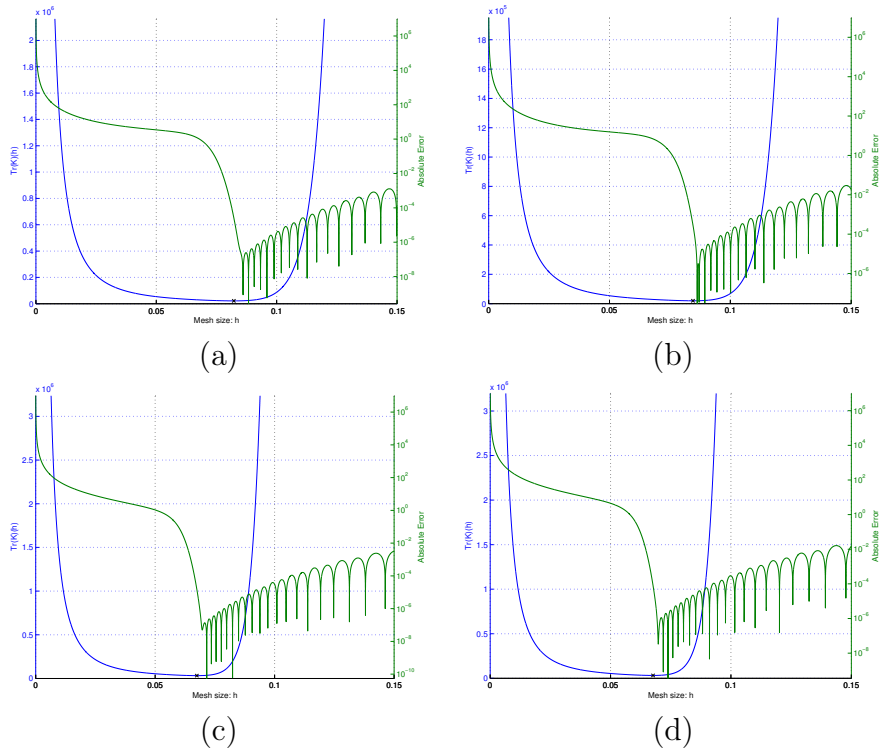

Figure 4.1: Trace and absolute error vs. h for the potentials $V_i(x)$ for $i = 1, 2, 3, 4$ given by equation (4.64) with $\phi(x) = \sinh(x)$. Figure (a) shows the results for the potential $V_1(x) = x^2 - 4x^4 + x^6$ with exact eigenvalue $E_0 = -2$. Figure (b) shows the results for the potential $V_2(x) = 4x^2 - 6x^4 + x^6$ with exact eigenvalue $E_1 = -9$. Figure (c) shows the results for the potential $V_3(x) = (105/64)x^2 - (43/8)x^4 + x^6 - x^8 + x^{10}$ with exact eigenvalue $E_0 = 3/8$. Figure (d) shows the results for the potential $V_4(x) = (169/64)x^2 - (59/8)x^4 + x^6 - x^8 + x^{10}$ with exact eigenvalue $E_1 = 9/8$.

then for $N \geq 1$, $\exists\, \hat{h} \in (0, \infty)$ *such that* $\hat{h} = \arg\min_{h \in \mathbb{R}^+} \{\mathrm{Tr}(\mathbf{K})(h)\}$.

Proof. The trace of the matrix $\mathbf{K}$ is given by:

$$\mathrm{Tr}(\mathbf{K})(h) = \frac{\pi^2}{3h^2} \sum_{k=-N}^{N} \frac{1}{(\phi'(kh))^2} + \sum_{k=-N}^{N} \frac{\tilde{V}(kh)}{(\phi'(kh))^2}. \tag{4.46}$$

The function $\mathrm{Tr}(\mathbf{K})(h)$ is continuous on the interval $(0, \infty)$ because it is composed of continuous functions and $\phi'(x) > 0$ for all $x \in \mathbb{R}$ by assump-

tion. In addition, the function $\tilde{V}(x)$ is bounded when $x = 0$ using the same assumption.

Taking the limit as $h \to 0^+$, we obtain:

$$\begin{aligned}\lim_{h\to 0^+} \mathrm{Tr}(\mathbf{K})(h) &= \lim_{h\to 0^+} \frac{\pi^2}{3h^2} \sum_{k=-N}^{N} \frac{1}{(\phi'(kh))^2} + \lim_{h\to 0^+} \sum_{k=-N}^{N} \frac{\tilde{V}(kh)}{(\phi'(kh))^2} \\ &= \infty \times \frac{(2N+1)}{(\phi'(0))^2} + \frac{(2N+1)\tilde{V}(0)}{(\phi'(0))^2} \\ &= \infty. \end{aligned} \tag{4.47}$$

Taking the limit as $h \to \infty$, we obtain:

$$\begin{aligned}\lim_{h\to \infty} \mathrm{Tr}(\mathbf{K})(h) &= \lim_{h\to \infty} \sum_{k=-N}^{N} \left(\frac{\pi^2}{3h^2} \frac{1}{(\phi'(kh))^2} \right) + \lim_{h\to \infty} \sum_{k=-N}^{N} \frac{\tilde{V}(kh)}{(\phi'(kh))^2} \\ &= 0 + \frac{\tilde{V}(0)}{\rho(\phi(0))(\phi'(0))^2} + N \times \left(\lim_{x\to\infty} \frac{\tilde{V}(x)}{(\phi'(x))^2} + \lim_{x\to-\infty} \frac{\tilde{V}(x)}{(\phi'(x))^2} \right) \\ &= \infty. \end{aligned} \tag{4.48}$$

Since:

$$\lim_{h\to 0^+} \mathrm{Tr}(\mathbf{K})(h) = \lim_{h\to \infty} \mathrm{Tr}(\mathbf{K})(h) = \infty,$$

and the function $\mathrm{Tr}(\mathbf{K})(h)$ is continuous on the interval $(0, \infty)$, by the Weierstrass extreme value theorem, $\exists\, \hat{h} \in (0, \infty)$ such that $\hat{h} = \arg\min_{h\in\mathbb{R}^+} \{\mathrm{Tr}(\mathbf{K})(h)\}$.

□

Solving the optimization problem in equation (4.44) at every iteration certainly adds to the complexity of the DESINC algorithm. In the hopes of reducing the computational cost, we present the following theorem which pro-

vides an asymptotic estimate of $\hat{h}$ as $N \to \infty$.

Theorem 4.4.2. *Let* $\mathbf{K}$ *denote the matrix with components defined by equation* (4.41). *Let* $\hat{h}$ *denote the solution to the optimization problem* $\hat{h} = \arg\min_{h \in \mathbb{R}^+} \{\mathrm{Tr}(\mathbf{K})(h)\}$. *Then* $\hat{h}$ *is asymptotic to the following function:*

$$\hat{h} \sim \frac{3W\left(\frac{2m}{3}\left(\frac{2^m \pi N}{\sqrt{c_m}}\right)^{2/3}\right)}{2mN} \qquad as \qquad N \to \infty, \tag{4.49}$$

where $W(x)$ *is the Lambert W function.*

Proof. The trace of the matrix $\mathbf{K}$ is given by:

$$\mathrm{Tr}(\mathbf{K})(h) = \sum_{k=-N}^{N} \left(\frac{\pi^2}{3h^2}\mathrm{sech}^2(kh) + \frac{\mathrm{sech}^2(kh)}{4} - \frac{3}{4}\mathrm{sech}^4(kh) + \sum_{i=1}^{m} c_i \sinh^{2i}(kh) \right). \tag{4.50}$$

In order to find an asymptotic representation of the trace, we will use the Euler-Maclaurin formula [15, 47, 117]:

$$\sum_{n=a}^{b} f(n) \sim \int_a^b f(x)dx + \frac{f(b)+f(a)}{2} + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}\left(f^{(2k-1)}(b) - f^{(2k-1)}(a)\right), \tag{4.51}$$

where B_{2k} are the Bernoulli numbers.

We start by applying equation (4.51) to the function $f(k)$ which is given by:

$$f(k) = \frac{\pi^2}{3h^2}\mathrm{sech}^2(kh) + \frac{\mathrm{sech}^2(kh)}{4} - \frac{3}{4}\mathrm{sech}^4(kh), \tag{4.52}$$

as $N \to \infty$, $h \to 0$ and $Nh \to \infty$, and we obtain:

$$\sum_{k=-N}^{N} f(k) \sim \frac{2\pi^2}{3h^3} - \frac{1}{2h} + e^{-2Nh}\left(-\frac{4\pi^2}{3}\sum_{i=0}^{\infty}\frac{B_{2i}4^i}{(2i)!}h^{2i-3} + \frac{4\pi^2}{3h^2} + 1 - \sum_{i=0}^{\infty}\frac{B_{2i}4^i}{(2i)!}h^{2i-1}\right). \tag{4.53}$$

Hence:

$$\sum_{k=-N}^{N}\left(\frac{\pi^2}{3h^2}\operatorname{sech}^2(kh) + \frac{\operatorname{sech}^2(kh)}{4} - \frac{3}{4}\operatorname{sech}^4(kh)\right) = \frac{2\pi^2}{3h^3} + \mathcal{O}\left(\frac{1}{h}\right). \tag{4.54}$$

Then, we apply (4.51) to the function $g(k)$ which is given by:

$$g(k) = \sum_{i=1}^{m} c_i \sinh^{2i}(kh), \tag{4.55}$$

as $N \to \infty$, $h \to 0$ and $Nh \to \infty$, and we obtain:

$$\sum_{k=-N}^{N}\left(\sum_{i=1}^{m} c_i \sinh^{2i}(kh)\right) \sim \frac{c_m e^{2mNh}}{2^{2m}}\left(\frac{1}{mh} + 1 + \sum_{i=1}^{\infty}\frac{4^i B_{2i}}{(2i)!}(mh)^{2i-1}\right). \tag{4.56}$$

Hence:

$$\sum_{k=-N}^{N}\left(\sum_{i=1}^{m} c_i \sinh^{2i}(kh)\right) = \frac{c_m e^{2mNh}}{2^{2m}mh} + \mathcal{O}\left(e^{2mNh}\right). \tag{4.57}$$

Combining (4.54) with (4.57), we obtain:

$$\operatorname{Tr}(\mathbf{K})(h) \sim \frac{2\pi^2}{3h^3} + \frac{c_m e^{2mNh}}{2^{2m}mh} \qquad \text{as} \qquad N \to \infty,\ h \to 0,\ Nh \to \infty. \tag{4.58}$$

Taking the derivative with respect to h, simplifying and keeping only the

higher order terms, we obtain:

$$\frac{d}{dh}\mathrm{Tr}(\mathbf{K})(h) \sim -\frac{2\pi^2}{h^4} + \frac{2Nc_m e^{2mNh}}{2^{2m}h} \qquad \text{as} \qquad N \to \infty,\, h \to 0,\, Nh \to \infty. \tag{4.59}$$

Setting this equation to zero and solving for h, we obtain the desired result (4.49). □

Since the wave function has the following decay rate:

$$|v(x)| \leq A \exp\left(-B \exp(\gamma|x|)\right), \tag{4.60}$$

where:

$$B = \frac{\sqrt{c_m}}{(m+1)2^{m+1}} \qquad \text{and} \qquad \gamma = m+1, \tag{4.61}$$

and $v \in \mathbf{B}_2(\mathscr{D}_d)$ with $d = \dfrac{\pi}{2\gamma}$, we can rewrite equation (4.49) in terms of the parameters B, γ, d and we obtain:

$$\hat{h} \sim \frac{W\left(\tilde{\gamma}\left(\dfrac{dN}{B}\right)^{2/3}\right)}{\tilde{\gamma}N} \qquad \text{where} \qquad \tilde{\gamma} = \frac{2(\gamma-1)}{3}. \tag{4.62}$$

To illustrate the efficiency of the asymptotic estimate, we present in Figure 4.2 the difference between $\hat{h}$ and its asymptotic estimate (4.62) for the three well potential $V_1(x) = x^2 - 4x^4 + x^6$ with exact eigenvalue $E_0 = -2$, the five well potential $V(x) = T_{10}(x) - 1$ and the ten well potential $V(x) = T_{20}(x) - 1$ respectively. The function $T_n(x)$ corresponds to the n^{th} Chebyshev polynomial. As can be seen, the asymptotic estimate agrees quite well with the value obtained by solving the optimisation problem in (4.44) but diminishes slightly

in accuracy as the number of wells increases.

By construction, we already know that $\mathbf{K}$ is a symmetric matrix. However, without loss of generality, we can also assume the matrix $\mathbf{K}$ to be positive definite by the following demonstration.

Given a potential of the form in (4.11), it is possible to find a constant $\Omega > 0$ such that $\tilde{V}(x) > -\Omega \cosh^2(x)$ for all $x \in \mathbb{R}$. Consequently, we can rewrite (4.14) as follows:

$$\begin{aligned}
&-v''(x) + \tilde{V}(x)v(x) = E\cosh^2(x)v(x) \\
&\qquad \implies -v''(x) + \tilde{V}(x)v(x) + \Omega\cosh^2(x)v(x) = E\cosh^2(x)v(x) + \Omega\cosh^2(x)v(x) \\
&\qquad \implies -v''(x) + (\tilde{V}(x) + \Omega\cosh^2(x))v(x) = (\Omega + E)\cosh^2(x)v(x) \\
&\qquad \implies -v''(x) + \hat{V}(x)v(x) = \hat{E}\cosh^2(x)v(x), \qquad (4.63)
\end{aligned}$$

where $\hat{V}(x) = \tilde{V}(x) + \Omega\cosh^2(x) > 0$ and $\hat{E} = \Omega + E$.

Since $\hat{V}(x) > 0$ for all $x \in \mathbb{R}$, the matrix $\mathbf{H}$ resulting from the DESCM is positive definite. Consequently, the matrix $\mathbf{K}$ is also positive definite. All the assumptions of Theorem 4.3.1 are satisfied, hence the eigenvalues of (4.40) converge to the eigenvalues of (4.12).

4.5 Numerical discussion

In this section, we present numerical results for the energy values of anharmonic oscillator potentials.

All calculations are performed using the programming language Julia [30] in double precision. The eigenvalue solvers in Julia utilize the linear algebra

package *LAPACK* [13]. Unless otherwise stated, the mesh size h (4.38) is used in the calculations.

The optimization problem in (4.44) is solved using the optimization Julia package *Optim* is used [187]. The matrix $\mathbf{K}$ is constructed using (4.41).

In [39], Chaudhuri et al. presented several potentials which have known analytic solutions for energy levels calculated using supersymmetric quantum mechanics. These are given by:

$$\begin{aligned} V_1(x) &= x^2 - 4x^4 + x^6 && \Rightarrow \quad E_0 = -2 \\ V_2(x) &= 4x^2 - 6x^4 + x^6 && \Rightarrow \quad E_1 = -9 \\ V_3(x) &= (105/64)x^2 - (43/8)x^4 + x^6 - x^8 + x^{10} && \Rightarrow \quad E_0 = 3/8 \\ V_4(x) &= (169/64)x^2 - (59/8)x^4 + x^6 - x^8 + x^{10} && \Rightarrow \quad E_1 = 9/8. \end{aligned} \tag{4.64}$$

Using these exact values, we present Figure 4.3 to illustrate the convergence of the DESCM.

Figure 4.3 shows the absolute error between the approximations obtained for the eigenvalues using the proposed method and the exact values given in (4.64). The absolute error is defined by:

$$\text{Absolute error} = |\mathcal{E}_l(N) - \text{Exact value}| \qquad \text{for} \qquad l = 0, 1. \tag{4.65}$$

As can be seen from Figure 4.3, the approximations obtained using DESCM converge quite well.

In Tables 4.1 and 4.2, we present approximations of energies for the ground state and first two excited states for two different potentials with unknown energy eigenvalues. There appears to be convergence in all cases.

Tables 4.3, 4.4, 4.5, and 4.6 display the ground state energy for various potentials as well as an approximation to the absolute error. In these tables, the approximation to the absolute error is given by:

$$\epsilon_n(N) = |\mathcal{E}_n(N-1) - \mathcal{E}_n(N)| \qquad \text{for} \qquad N = 2, 3, 4, \ldots \quad \text{and} \quad n = 0, 1, 2, \ldots. \tag{4.66}$$

Table 4.3 displays values obtained for the potential $V(x) = c_1x^2 + c_2x^4$ for different values of c_1 and c_2. Table 4.4 displays values obtained for the potential $V(x) = c_1x^2 + c_2x^4 + c_3x^6$ for different values of c_1, c_2 and c_3. Table 4.5 displays values obtained for the potential $V(x) = c_1x^2 + c_2x^4 + c_3x^6 + c_4x^8$ for different values of c_1, c_2, c_3 and c_4. Table 4.6 displays values obtained for the potential $V(x) = c_1x^2 + c_2x^4 + c_3x^6 + c_4x^8 + c_5x^{10}$ for different values of c_1, c_2, c_3, c_4 and c_5.

In all four tables, we use $\epsilon_0(N) < 5 \times 10^{-12}$ as a stopping criterion and the numbers between parentheses represent powers of ten.

In general, the DESINC method performs well when using the optimal mesh size h for low oscillatory potentials. However, as the number of oscillations increase in the potential, the mesh size h performs significantly less than $\hat{h}$. To illustrate this claim, we present in Figure 4.4 three potentials with three, five and ten wells respectively. The first row in Figure 4.4 illustrates the mesh sizes used and the convergence of the DESINC method for the three well potential $V_2(x) = 4x^2 - 6x^4 + x^6$ in (4.64) with exact eigenvalue $E_1 = -9$. The second row in Figure 4.4 displays the mesh sizes used and the convergence of the DESINC method for the five well potential $V(x) = T_{10}(x) - 1$, where $T_{10}(x)$ is the 10^{th} Chebyshev polynomial. Finally the third row in Figure 4.4

displays the mesh sizes used and the convergence of the DESINC method for the ten well potential $V(x) = T_{20}(x) - 1$, where $T_{20}(x)$ is the 20^{th} Chebyshev polynomial.

We would like to mention that even though the asymptotic estimate obtained in Theorem 4.4.2 agrees quite well in absolute error with the mesh size $\hat{h}$, it still under-performs in the case of multiple-well potentials compared to $\hat{h}$ obtained from the minimization problem (4.44). This would indicate that more terms might be needed in the asymptotic expansion of the trace to improve the accuracy in lower orders of N. Moreover, this numerical result also reinforces the idea that the choice of the mesh size is crucial for convergence when dealing with potentials with multiple wells.

In Figure 4.5, we implement the algorithm with the mesh size $\hat{h}$ for the ten well potential:

$$V(x) = T_{20}(x) - 1, \tag{4.67}$$

for $N = 1, 2, \ldots, 1000$. Using the stopping criterion $\epsilon_n(N) < 5 \times 10^{-12}$, we are able to find an approximation to 1353 eigenvalues of this ten well potential.

In [184], Weniger uses a Rayleigh-Schrödinger perturbation series and sequence transformations to evaluate the ground state of the potential $V(x) = x^2 + x^4$ to high accuracy. Weniger uses the exact rational arithmetics of Maple with an accuracy of 300 decimal digits to obtain the following value:

$$E_0 \approx 1.392\,351\,641\,530\,291\,855\,657\,507\,876\,609\,934\,184\,600\,066\,711\,9. \tag{4.68}$$

We used Maple16™ to implement the algorithm for the same potential

with an accuracy of 100 correct digits and we obtain:

$$E_0 \approx 1.392\ 351\ 641\ 530\ 291\ 855\ 657\ 507\ 876\ 609\ 934\ 184\ 600\ 066\ 711\ 220\ 834$$
$$088\ 906\ 349\ 323\ 877\ 567\ 431\ 875\ 646\ 528\ 590\ 973\ 563\ 467\ 791\ 759\ 121, \tag{4.69}$$

which is in excellent agreement with Weniger's value.

4.6 Conclusion

Various methods have been used to calculate the energy eigenvalues of quantum anharmonic oscillators given a specific set of parameters. While several of these methods yield excellent results for specific cases, there is a beautiful diversity yet lack of uniformity in the resolution of this problem. In this work, we present a method based on the DESCM where the wave function of a transformed Schrödinger equation (4.14) is approximated by as a Sinc expansion. By summing over $2N+1$ collocation points, we construct a symmetric positive definite matrices $\mathbf{K}$ whose eigenvalues are approximations to the energy eigenvalues of (4.10). The DESCM method has a convergence rate of $\mathcal{O}\left(\left(\frac{N^{5/2}}{\log(N)^2}\right)\exp\left(-\kappa\frac{N}{\log(N)}\right)\right)$. The convergence is improved for potential with multiple wells by using the alternate mesh size $\hat{h}$ obtained by minimizing the trace of the discretized Hamiltonian.

The numerical results obtained for a number of different potentials including potentials with multiple wells, show clearly the efficiency and accuracy of the proposed method.

4.7 Tables and Figures

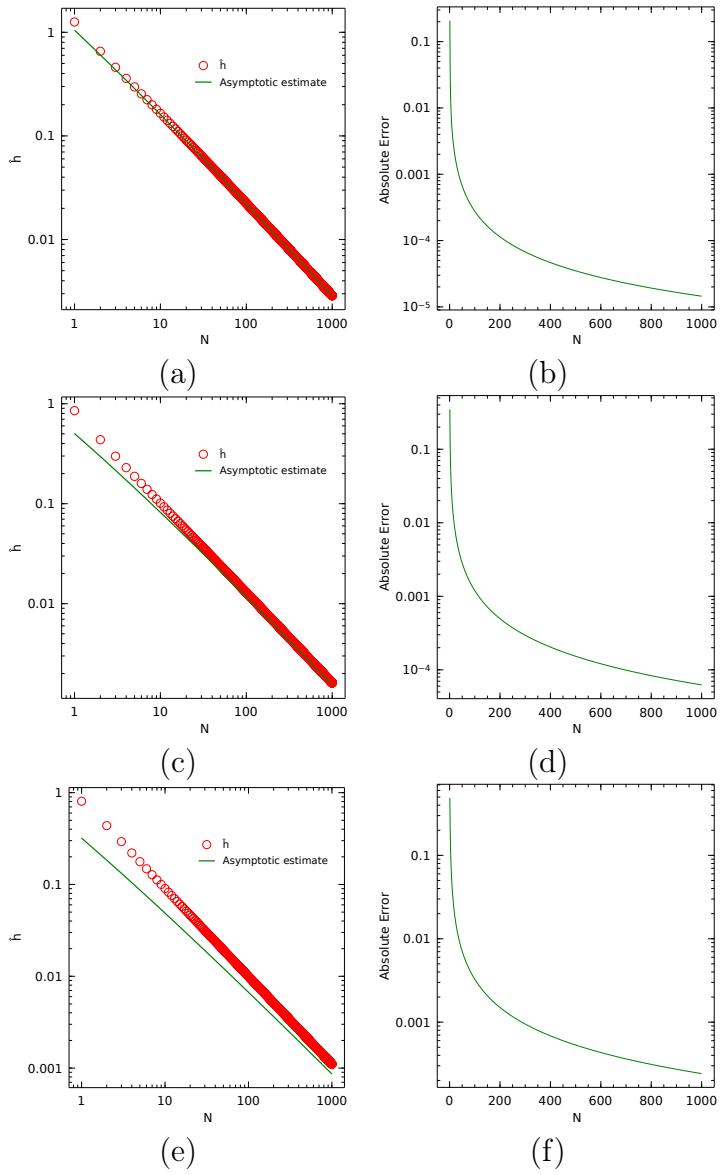

Figure 4.2: Figures (a), (c) and (e) displays both the alternate mesh size $\hat{h}$ and its asymptotic estimate given by (4.62) while figures (b), (d) and (f) displays the absolute error between the alternate mesh size $\hat{h}$ and its asymptotic estimate for the three well potential $V_1(x) = x^2 - 4x^4 + x^6$ with exact eigenvalue $E_0 = -2$, the five well potential $V(x) = T_{10}(x) - 1$ and the ten well potential $V(x) = T_{20}(x) - 1$ respectively.

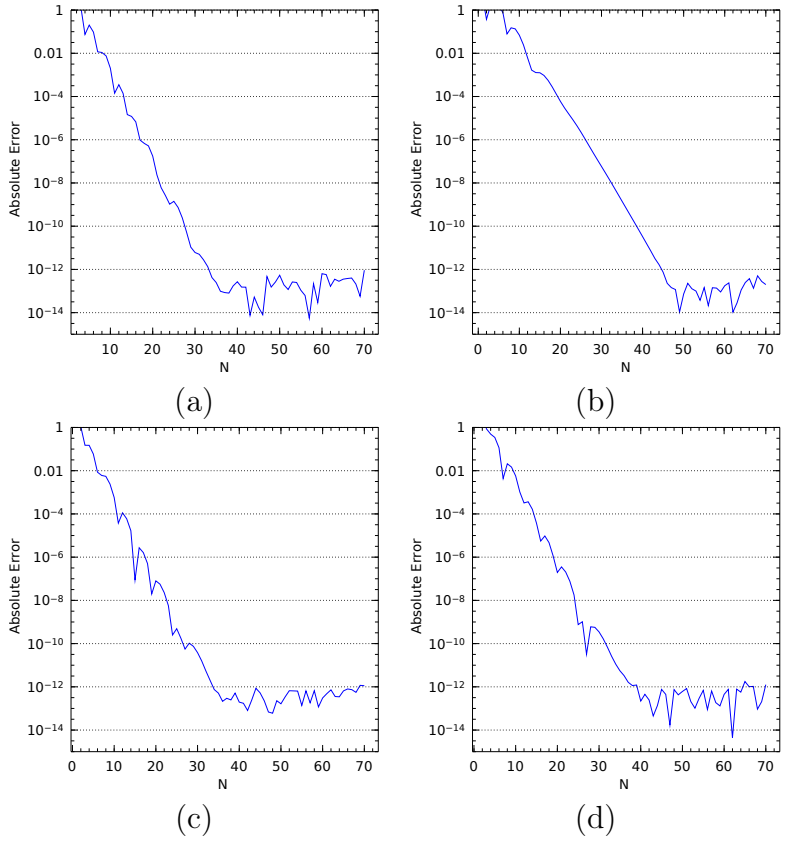

Figure 4.3: Absolute error between the approximations obtained for the eigenvalues using the proposed method and the exact values for the potentials $V_i(x)$ for $i = 1, 2, 3, 4$ given by (4.64) with $\phi(x) = \sinh(x)$.
(a) $V_1(x) = x^2 - 4x^4 + x^6$ with exact eigenvalue $E_0 = -2$. (b) $V_2(x) = 4x^2 - 6x^4 + x^6$ with exact eigenvalue $E_1 = -9$. (c) $V_3(x) = (105/64)x^2 - (43/8)x^4 + x^6 - x^8 + x^{10}$ with exact eigenvalue $E_0 = 3/8$. (d) $V_4(x) = (169/64)x^2 - (59/8)x^4 + x^6 - x^8 + x^{10}$ with exact eigenvalue $E_1 = 9/8$.

Table 4.1: Energies for the ground state and first two excited states for $V(x) = -x^2 + 3x^4 - 2x^6 + 0.1x^{10}$.

N	$\mathcal{E}_0(N)$	$\mathcal{E}_1(N)$	$\mathcal{E}_2(N)$
5	-0.183054938746611	0.441479870018253	2.620487757023682
10	-0.0976947154532108	0.670920848438211	3.112803149372351
15	-0.0962838618463357	0.672983395806946	3.110900059783247
20	-0.0962939179110841	0.672989564944146	3.111020042497232
25	-0.0962917320927764	0.672993682058299	3.111022843861247
30	-0.0962919468261398	0.672993241672601	3.111022328272051
35	-0.0962919458832259	0.672993243476173	3.111022329656410
40	-0.0962919462260392	0.672993242754209	3.111022328736961
45	-0.0962919462302011	0.672993242746560	3.111022328725989
50	-0.0962919462309655	0.672993242745170	3.111022328724715

Table 4.2: Energies for the ground state and first two excited states for $V(x) = x^2 + 100x^8$.

N	$\mathcal{E}_0(N)$	$\mathcal{E}_1(N)$	$\mathcal{E}_2(N)$
3	3.18583889990311	12.1774056576440	25.9667305118017
6	3.18865215097014	12.1950090976147	26.0334131709351
9	3.18865434610824	12.1950219328947	26.0334583310462
12	3.18865434649856	12.1950219336715	26.0334583214430
15	3.18865434649231	12.1950219336306	26.0334583212540
18	3.18865434649241	12.1950219336298	26.0334583212524
21	3.18865434649213	12.1950219336305	26.0334583212523
24	3.18865434649426	12.1950219336305	26.0334583212539
27	3.18865434649200	12.1950219336299	26.0334583212526
30	3.18865434649236	12.1950219336314	26.0334583212516

Table 4.3: The ground state energy for $V(x) = c_1x^2 + c_2x^4$.

c_1	c_2	N	$\mathcal{E}_0(N)$	$\epsilon_0(N)$
0.1	0.1	20	5.6694532770815997(-1)	1.6(-12)
0.1	1	18	1.0962243662319233(0)	2.3(-12)
1	1	17	1.3923516415352821(0)	2.5(-12)
1	10	17	2.4491740721179220(0)	8.8(-14)
10	10	15	3.7029004216662731(0)	4.0(-13)
-0.1	0.1	21	4.1046961591503783(-1)	2.6(-12)
-0.1	1	18	1.0238094432848113(0)	4.7(-13)
-1	1	19	6.5765300518294945(-1)	5.4(-14)
-1	10	17	2.1128778980507850(0)	7.1(-13)
-10	10	19	9.0479065692642441(-2)	1.7(-12)

Table 4.4: The ground state energy for $V(x) = c_1x^2 + c_2x^4 + c_3x^6$.

c_1	c_2	c_3	N	$\mathcal{E}_0(N)$	$\epsilon_0(N)$
0.1	0.1	0.1	23	7.6469531499643029(-1)	4.2(-13)
1	1	1	20	1.6148940820343036(0)	1.6(-12)
0.1	1	10	19	2.1277742176946535(0)	3.7(-12)
1	10	10	17	2.7940871778594101(0)	3.3(-12)
10	10	10	16	3.8948206179865981(0)	2.5(-12)
-0.1	0.1	0.1	23	6.6383017274207901(-1)	2.0(-12)
1	-1	1	23	1.2022669303165900(0)	8.0(-13)
-0.1	-1	10	20	1.9385567907196897(0)	2.7(-13)
-1	10	10	17	2.5157308558338656(0)	2.3(-12)
10	-10	10	20	2.9588710692969618(0)	1.9(-12)

Table 4.5: The ground state energy for $V(x) = c_1x^2 + c_2x^4 + c_3x^6 + c_4x^8$.

c_1	c_2	c_3	c_4	N	$\mathcal{E}_0(N)$	$\epsilon_0(N)$
0.1	0.1	0.1	0.1	23	9.2287072386834434(-1)	3.0(-13)
0.1	1	10	10	21	2.3988345516957166(0)	2.2(-12)
1	1	10	10	21	2.5285749972092857(0)	2.2(-12)
1	10	10	10	20	2.9458972541841404(0)	9.8(-13)
10	10	10	10	19	3.9840271957255702(0)	3.1(-12)
-0.1	0.1	-0.1	0.1	27	6.9423980434904176(-1)	1.6(-12)
0.1	-1	10	10	22	2.2867765902246440(0)	1.0(-12)
-1	-1	10	10	22	2.1181378732419969(0)	1.4(-12)
1	10	-10	10	23	2.3756889547019138(0)	3.9(-12)
-10	-10	-10	10	35	-9.7139097706403668(0)	4.8(-12)

Table 4.6: The ground state energy for $V(x) = c_1x^2 + c_2x^4 + c_3x^6 + c_4x^8 + c_5x^{10}$.

c_1	c_2	c_3	c_4	c_5	N	$\mathcal{E}_0(N)$	$\epsilon_0(N)$
0.1	0.1	0.1	0.1	0.1	27	1.0520482472987258(0)	4.9(-12)
0.1	0.1	1	1	1	24	1.5773348519927783(0)	2.6(-12)
1	1	1	10	10	23	2.4237300030396556(0)	3.1(-12)
1	10	10	10	10	21	3.0275420892666491(0)	7.4(-13)
10	10	10	10	10	21	4.0329202866021152(0)	1.6(-12)
-0.1	-0.1	0.1	0.1	0.1	29	9.2562395524222385(-1)	2.4(-12)
0.1	0.1	-1	-1	1	33	8.6187455263857027(-1)	4.4(-12)
-1	1	1	-10	10	35	1.3353894631528094(0)	4.6(-12)
1	-10	-10	10	10	28	1.0275704201029547(0)	2.8(-12)
-10	-10	-10	-10	10	52	-2.2446238129792420(1)	2.7(-12)

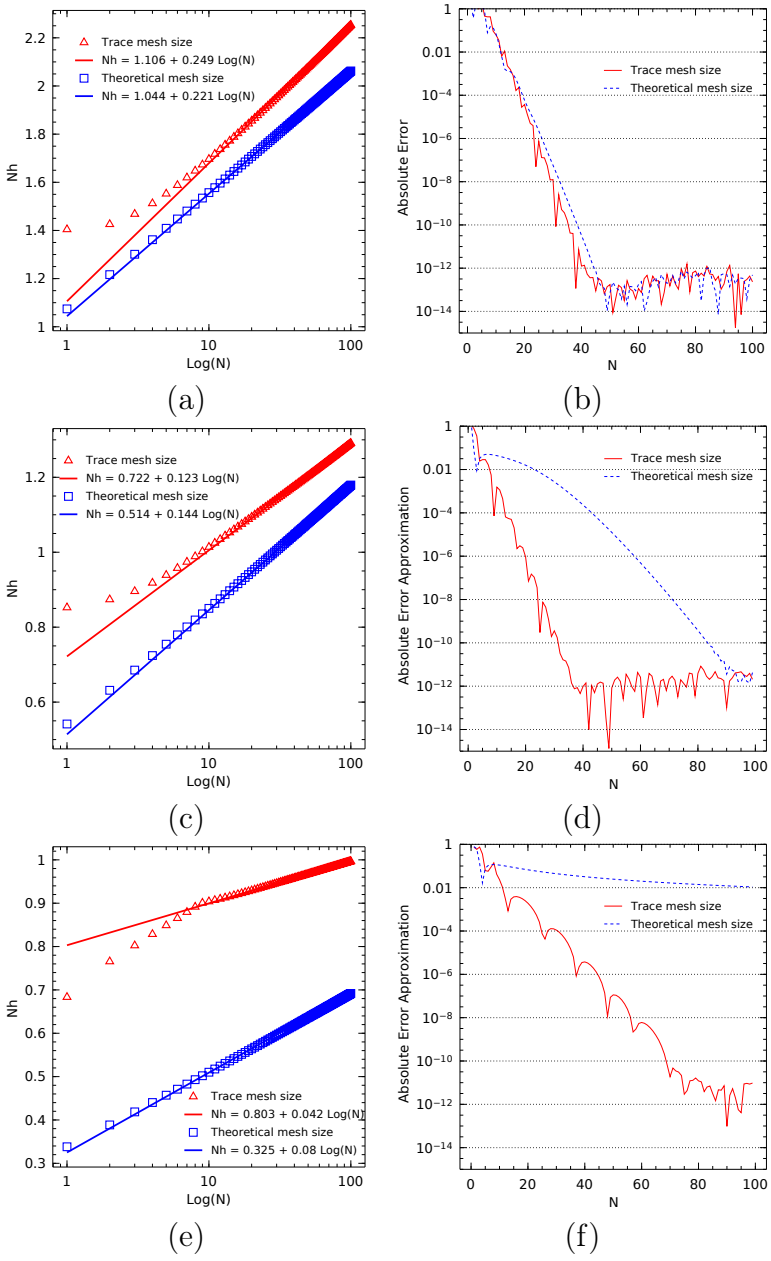

Figure 4.4: Figures (a), (c) and (e) display both the optimal and alternate mesh sizes used when evaluating the absolute error of the DESINC method in figure (b), (d) and (f) for the potentials $V_2(x) = 4x^2 - 6x^4 + x^6$ with exact eigenvalue $E_1 = -9$, $V(x) = T_{10}(x) - 1$ and $V(x) = T_{20}(x) - 1$ respectively.

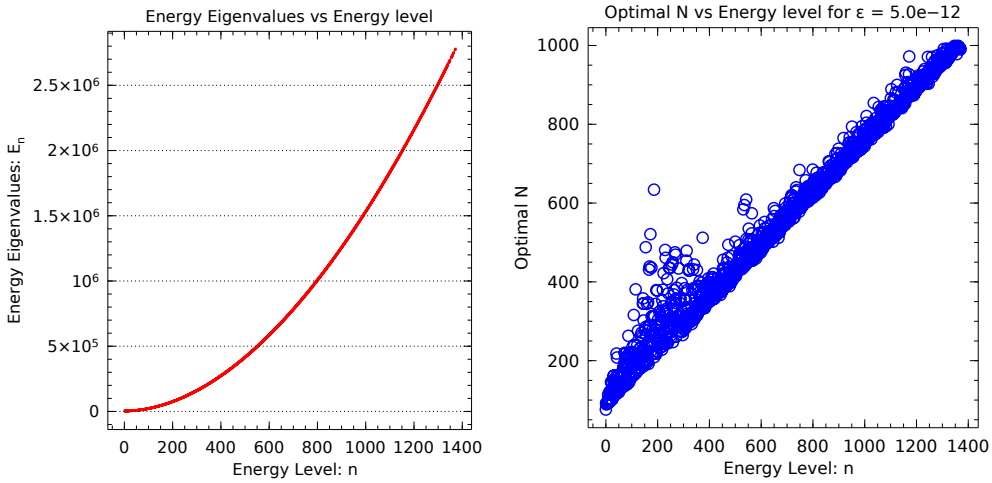

Figure 4.5: Figure (a) displays an approximation for 1353 eigenvalues that achieved a approximate absolute error less than 5×10^{-12} for the ten well potential $V(x) = T_{20}(x) - 1$ as shown in equation (4.67) with $\phi(x) = \sinh(x)$. Figure (b) displays the value of N needed for each eigenvalue in figure (a) to achieve an approximate absolute error less than 5×10^{-12}.

Chapter 5

Centrosymmetric Matrices in the Sinc Collocation Method for Sturm-Liouville Problems

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Abstract.

Recently, we used the Sinc collocation method with the double exponential transformation to compute eigenvalues for singular Sturm-Liouville problems. In this work, we show that the computation complexity of the eigenvalues of such a differential eigenvalue problem can be considerably reduced when its operator commutes with the parity operator. In this case, the matrices resulting from the Sinc collocation method are centrosymmetric. Utilizing

well known properties of centrosymmetric matrices, we transform the problem of solving one large eigensystem into solving two smaller eigensystems. We show that only $\frac{1}{N+1}$ of all components need to be computed and stored in order to obtain all eigenvalues, where $2N+1$ corresponds to the dimension of the eigensystem. We applied our result to the Schrödinger equation with the anharmonic potential and the numerical results section clearly illustrates the substantial gain in efficiency and accuracy when using the proposed algorithm.

5.1 Introduction

The following chapter follows from our published work in [81]. In science and engineering, differential eigenvalue problems occur abundantly. Differential eigenvalue problems can arise when partial differential equations are solved using the method of separation of variables. Consequently, they also play an important role in Sturm-Liouville (SL) differential eigenvalue problems [193]. For example, the solution of the wave equation in a bounded domain can be expressed as a sum of standing waves. The frequencies of these standing waves are precisely the eigenvalues of its corresponding Sturm-Liouville problem. Similarly, in quantum mechanics, the energy eigenvalues associated with a Hamiltonian operator are modelled using the time-independent Schrödinger equation which is in fact a special case of the Sturm-Liouville differential eigenvalue problem.

Recently, collocation and spectral methods have shown great promise for solving singular Sturm-Liouville differential eigenvalue problems [16,38]. More specifically, the Sinc collocation method (SCM) [94,172,173] has been shown to

yield exponential convergence. During the last three decades the SCM has been used extensively to solve many problems in numerical analysis. The applications include numerical integration, linear and non-linear ordinary differential equations, partial differential equations, interpolation and approximations to functions [155, 158]. The SCM applied to Sturm-Liouville problems consists of expanding the solution of a SL problem using a basis of Sinc functions. By evaluating the resulting approximation at the Sinc collocation points separated by a fixed mesh size h, one obtains a matrix eigenvalue problem or generalized matrix eigenvalue problem for which the eigenvalues are approximations to the eigenvalues of the SL operator. In [84], we used the double exponential Sinc collocation method (DESCM) to compute the eigenvalues of singular Sturm-Liouville boundary value problems. The DESCM leads to a generalized eigenvalue problem where the matrices are symmetric and positive-definite. In addition, we demonstrate that the convergence of the DESCM is of the rate $\mathcal{O}\left(\frac{N^{5/2}}{\log(N)^2}e^{-\kappa N/\log(N)}\right)$ for some $\kappa > 0$ as $N \to \infty$, where $2N+1$ is the dimension of the resulting generalized eigenvalue system. The DESCM was also applied successfully to the Schrödinger equation with the anharmonic oscillators [83].

In the present contribution, we show how the parity symmetry of the Sturm-Liouville operator can be conserved and exploited when converting the differential eigenvalue problem into a matrix eigenvalue problem. Indeed, given certain parity assumptions, the matrices resulting from the DESINC method are not only symmetric and positive definite; they are also centrosymmetric. The study of centrosymmetry has a long history [36,44,48,88,101,123,127,144, 159,182]. However, the last two decades has stemmed much research focused on

the properties and applications of centrosymmetric matrices ranging from iterative methods for solving linear equations to least-squares problems to inverse eigenvalue problems [1, 14, 59, 66, 102, 104–106, 116, 169, 174, 176, 177, 194–196].

Using the eigenspectrum properties of symmetric centrosymmetric matrices presented in [36], we apply the DESCM algorithm to Sturm-Liouville eigenvalue problems and demonstrate that solving the resulting generalized eigensystem of dimension $(2N+1) \times (2N+1)$ is equivalent to solving two smaller eigensystems of dimension $N \times N$ and $(N+1) \times (N+1)$. Moreover, we also demonstrate that only $\frac{1}{N+1}$ of all components need to be stored at every iteration in order to obtain all generalized eigenvalues. To illustrate the gain in efficiency obtained by this method, we apply the DESCM method to the time independent Schrödinger equation with an anharmonic potential. Furthermore, it is worth mentioning that research concerning inverse eigenvalue problems where the matrices are assumed centrosymmetric has been the subject of much research recently [177, 195]. Consequently, the combination of these results and our findings could lead to a general approach for solving inverse Sturm-Liouville problems.

All calculations are performed using the programming language Julia and all the codes are available upon request.

5.2 Definitions and basic properties

The sinc function valid for all $z \in \mathbb{C}$ is defined by the following expression:

$$\operatorname{sinc}(z) = \begin{cases} \dfrac{\sin(\pi z)}{\pi z} & \text{for} \quad z \neq 0 \\ 1 & \text{for} \quad z = 0. \end{cases} \tag{5.1}$$

For $j \in \mathbb{Z}$ and h a positive number, we define the Sinc function $S(j,h)(x)$ by:

$$S(j,h)(x) = \operatorname{sinc}\left(\frac{x - jh}{h}\right) \quad \text{for} \quad x \in \mathbb{C}. \tag{5.2}$$

The Sinc function defined in (5.2) form an interpolatory set of functions with the discrete orthogonality property:

$$S(j,h)(kh) = \delta_{j,k} \qquad \text{for} \qquad j,k \in \mathbb{Z}, \tag{5.3}$$

where $\delta_{j,k}$ is the Kronecker delta function.

Definition 5.2.1. *[155] Given any function v defined everywhere on the real line and any $h > 0$, the symmetric truncated Sinc expansion of v is defined by the following series:*

$$C_N(v,h)(x) = \sum_{j=-N}^{N} v_{j,h}\, S(j,h)(x), \tag{5.4}$$

where $v_{j,h} = v(jh)$.

The Sturm-Liouville (SL) equation in Liouville form is defined as follows:

$$\begin{aligned} Lu(x) = -u''(x) + q(x)u(x) \;&=\; \lambda\rho(x)u(x) \\ a < x < b \qquad\qquad & u(a) = u(b) = 0, \end{aligned} \tag{5.5}$$

where $-\infty \leq a < b \leq \infty$. Moreover, we assume that the function $q(x)$ is non-negative and the weight function $\rho(x)$ is positive. The values λ are known as the eigenvalues of the SL equation.

In [84], we applied the DESCM to obtain an approximation to the eigenvalues λ of equation (5.5). We initially applied Eggert et al.'s transformation to equation (3.13) since it was shown that the proposed change of variable results in a symmetric discretized system when using the Sinc collocation method [56]. The proposed change of variable is of the form [56, Defintion 2.1]:

$$v(x) = \left(\sqrt{(\phi^{-1})'}\, u\right) \circ \phi(x) \qquad \Longrightarrow \qquad u(x) = \frac{v \circ \phi^{-1}(x)}{\sqrt{(\phi^{-1}(x))'}}, \tag{5.6}$$

where $\phi^{-1}(x)$ is a conformal map of a simply connected domain in the complex plane with boundary points $a \neq b$ such that $\phi^{-1}(a) = -\infty$ and $\phi^{-1}(b) = \infty$.

Applying the change of variable (5.6) into equation (3.13), one obtains [56]:

$$\mathcal{L}\, v(x) = -v''(x) + \tilde{q}(x)v(x) = \lambda\rho(\phi(x))(\phi'(x))^2 v(x) \quad \text{with} \quad \lim_{|x|\to\infty} v(x) = 0, \tag{5.7}$$

where:

$$\tilde{q}(x) = -\sqrt{\phi'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\phi'(x)}\frac{\mathrm{d}}{\mathrm{d}x}(\sqrt{\phi'(x)})\right) + (\phi'(x))^2 q(\phi(x)). \tag{5.8}$$

To implement the double exponential transformation, we use a conformal mapping $\phi(x)$ such that the solution to equation (5.7) decays double exponentially. In other words, we need to find a function $\phi(x)$ such that:

$$|v(x)| \leq A \exp\left(-B \exp\left(\gamma |x|\right)\right), \tag{5.9}$$

for some positive constants A, B, γ. Examples of such mappings are given in [84, 121].

Applying the SCM method, we obtain the following generalized eigenvalue problem:

$$\mathcal{L}\, \mathbf{C}_M(v,h) = \mathbf{A}\mathbf{v} \;=\; \mu \mathbf{D}^2 \mathbf{v} \quad \Longrightarrow \quad (\mathbf{A} - \mu \mathbf{D}^2)\mathbf{v} \;=\; 0, \tag{5.10}$$

where the vectors $\mathbf{v}$ and $\mathbf{C}_M(v,h)$ are given by:

$$\mathbf{v} = (v_{-N,h}, \ldots, v_{N,h})^T \qquad \text{and} \qquad \mathbf{C}_N(v,h) = (C_N(v,h)(-Nh), \ldots, C_N(v,h)(Nh))^T, \tag{5.11}$$

and μ are approximations of the eigenvalues λ of equation (5.7). For more details on the application of the SCM, we refer the readers to [84].

As in [157], we let $\delta_{j,k}^{(l)}$ denote the l^{th} Sinc differentiation matrix with unit mesh size:

$$\delta_{j,k}^{(l)} = h^l \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l S(j,h)(x)\bigg|_{x=kh}. \tag{5.12}$$

The entries $A_{j,k}$ of the $(2N+1) \times (2N+1)$ matrix $\mathbf{A}$ are then given by:

$$A_{j,k} = -\frac{1}{h^2}\, \delta_{j,k}^{(2)} + \tilde{q}(kh)\, \delta_{j,k}^{(0)} \qquad \text{with} \qquad -N \leq j,k \leq N, \tag{5.13}$$

and the entries $D^2_{j,k}$ of the $(2N+1)\times(2N+1)$ diagonal matrix $\mathbf{D}^2$ are given by:

$$D^2_{j,k} = (\phi'(kh))^2\rho(\phi(kh))\,\delta^{(0)}_{j,k} \qquad \text{with} \qquad -N \leq j,k \leq N. \tag{5.14}$$

As previously mentioned, Eggert et al.'s transformation leads to matrices $\mathbf{A}$ and $\mathbf{D}^2$ which are symmetric and positive definite. However, as will be illustrated in the next section, given certain parity assumptions, these matrices yield even more symmetry.

5.3 Centrosymmetric properties of the matrices A and $\mathbf{D}^2$

In this section, we present some properties of the matrix $\mathbf{A}$ and $\mathbf{D}^2$ that will be beneficial in the computation of their eigenvalues. The matrices $\mathbf{A}$ and $\mathbf{D}^2$ are symmetric positive definite matrices when equation (5.7) is discretized using the Sinc collocation method. Additionally, given certain parity assumptions on the functions $q(x)$, $\phi(x)$ and $\rho(x)$ in equation (5.7), the matrices $\mathbf{A}$ and $\mathbf{D}^2$ will also be centrosymmetric.

Definition 5.3.1. *[34, Section 5.10] Let $\mathcal{J}$ denote the parity operator defined by:*

$$\mathcal{J}f(x) = f(-x), \tag{5.15}$$

where $f(x)$ is a well defined function being acted upon by $\mathcal{J}$.

Definition 5.3.2. *An operator $\mathcal{B}$ is said to commute with the parity operator*

$\mathcal{J}$ if it satisfies the following relation:

$$\mathcal{B}\mathcal{J}f(x) = \mathcal{J}\mathcal{B}f(x). \tag{5.16}$$

Equivalently, we can say that the the commutator between $\mathcal{B}$ and $\mathcal{J}$ is zero, that is:

$$[\mathcal{B}, \mathcal{J}] = \mathcal{B}\mathcal{J} - \mathcal{J}\mathcal{B} = 0. \tag{5.17}$$

Definition 5.3.3. *[182, Definition 5] An exchange matrix denoted by* $\mathbf{J}$ *is a square matrix with ones along the anti-diagonal and zeros everywhere else:*

$$\mathbf{J} = \begin{pmatrix} 0 & & 1 \\ & \iddots & \\ 1 & & 0 \end{pmatrix}. \tag{5.18}$$

Definition 5.3.4. *[182, Definition 2] Let* $\mathbf{B}$ *be a matrix of dimension* $(2N+1)\times(2N+1)$ *with components* $B_{j,k}$ *for* $-N \leq j,k \leq N$. $\mathbf{B}$ *is centrosymmetric if and only if* $\mathbf{B}$ *satisfies the following property:*

$$\mathbf{BJ} = \mathbf{JB}, \tag{5.19}$$

where $\mathbf{J}$ *is an exchange matrix of dimension* $(2N+1)\times(2N+1)$. *Writing equation* (5.19) *in a component wise form, we have the following relation:*

$$B_{-j,-k} = B_{j,k} \quad for \quad -N \leq j,k \leq N. \tag{5.20}$$

We now present the following theorem establishing the connection between

symmetries of the Sturm-Liouville operator and its resulting matrix approximation.

Theorem 5.3.5. *Let $\mathcal{L}$ denote the operator of the transformed Sturm-Liouville problem in equation* (5.7)*:*

$$\mathcal{L} = \frac{1}{\rho(\phi(x))(\phi'(x))^2}\left(-\frac{d^2}{dx^2} + \tilde{q}(x)\right). \tag{5.21}$$

If the commutator $[\mathcal{L}, \mathcal{J}] = 0$, where $\mathcal{J}$ is the parity operator, then the matrices $\mathbf{A}$ and $\mathbf{D}^2$ defined by equations (5.13) *and* (5.14) *resulting from the DESCM are centrosymmetric.*

Proof The commutator $[\mathcal{L}, \mathcal{J}] = 0$ if and only if $q(x)$ and $\rho(x)$ are even functions and $\phi(x)$ is an odd function.

If $\phi(x)$ is an odd function, then $\phi'(x)$ is even, $\phi''(x)$ is odd and $\phi'''(x)$ is even. From this and equation (5.8), it follows that $\tilde{q}(x)$ is even.

In order to show that the resulting matrices $\mathbf{A}$ and $\mathbf{D}^2$ are centrosymmetric, we demonstrate that both these matrices satisfy equation (5.20). Before doing so, it is important to notice that the l^{th} Sinc differentiation matrices defined in equation (5.12) have the following symmetric properties:

$$\delta^{(l)}_{-j,-k} = h^l \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l S(-j,h)(x)\bigg|_{x=-kh} = \begin{cases} \delta^{(l)}_{j,k} & \text{if} \quad l \text{ is even} \\ -\delta^{(l)}_{j,k} & \text{if} \quad l \text{ is odd.} \end{cases} \tag{5.22}$$

Hence, the l^{th} Sinc differentiation matrices are centrosymmetric if l is even. It is worth noting that when l is odd, the Sinc differentiation matrices are skew-centrosymmetric [176]. Consequently, investigating the form for the compo-

nents of the matrix $\mathbf{A}$ in equation (5.13), we obtain:

$$\begin{aligned} A_{-j,-k} &= -\frac{1}{h^2}\,\delta^{(2)}_{-j,-k} + \tilde{q}(-kh)\,\delta^{(0)}_{-j,-k} \\ &= -\frac{1}{h^2}\,\delta^{(2)}_{j,k} + \tilde{q}(kh)\,\delta^{(0)}_{j,k} \\ &= A_{j,k}. \end{aligned} \tag{5.23}$$

Similarly, investigating the form for the components of the matrix $\mathbf{D}^2$ in equation (5.14), we obtain:

$$\begin{aligned} D^2_{-j,-k} &= (\phi'(-kh))^2 \rho(\phi(-kh))\,\delta^{(0)}_{-j,-k} \\ &= (\phi'(kh))^2 \rho(\phi(kh))\,\delta^{(0)}_{j,k} \\ &= D^2_{j,k}. \end{aligned} \tag{5.24}$$

Both matrices $\mathbf{A}$ and $\mathbf{D}^2$ satisfy equation (5.20). From this it follows that $\mathbf{A}$ and $\mathbf{D}^2$ are centrosymmetric.

Theorem 5.3.5 illustrates that Sinc basis functions preserve the parity property of the Sturm-Liouville operator when discretized. Hence, when the matrices $\mathbf{A}$ and $\mathbf{D}^2$ are symmetric centrosymmetric positive definite matrices, we can utilize these symmetries when solving for their generalized eigenvalues. In [36], Cantoni et al. proved several properties of symmetric centrosymmetric matrices. In the following, we will utilize some of these properties to facilitate our task of obtaining approximations to the generalized eigenvalues of the matrices $\mathbf{A}$ and $\mathbf{D}^2$. The following lemma will demonstrate the internal block structure of symmetric centrosymmetric matrices.

Lemma 5.3.6. *[36, Lemma 2] If* $\mathbf{H}$ *is a square symmetric centrosymmetric*

matrix of dimension $(2N+1)\times(2N+1)$*, then* $\mathbf{H}$ *can be written as:*

$$\mathbf{H} = \begin{bmatrix} \mathbf{S} & \mathbf{x} & \mathbf{C^T} \\ \mathbf{x^T} & a & \mathbf{x^T J} \\ \mathbf{C} & \mathbf{Jx} & \mathbf{JS\,J} \end{bmatrix}, \tag{5.25}$$

where $\mathbf{S}, \mathbf{C}$ *are matrices of size* $N\times N$*,* $\mathbf{J}$ *is the exchange matrix of size* $N\times N$*,* $\mathbf{x}$ *is a column vector of length* N *and* a *is a scalar. In addition,* $\mathbf{S^T} = \mathbf{S}$ *and* $\mathbf{C^T} = \mathbf{JCJ}$*.*

The next lemma simplifies the calculation needed to solve for these eigenvalues.

Lemma 5.3.7. *[36, Lemma 3] Let* $\mathbf{H}$ *be a square symmetric centrosymmetric matrix as defined in lemma 5.3.6 and let* $\mathbf{V}$ *be a square matrix of dimension* $(2N+1)\times(2N+1)$ *defined by:*

$$\mathbf{V} = \begin{bmatrix} \mathbf{S-JC} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & a & \sqrt{2}\,\mathbf{x^T} \\ \mathbf{0} & \sqrt{2}\,\mathbf{x} & \mathbf{S+JC} \end{bmatrix}, \tag{5.26}$$

then $\mathbf{H}$ *and* $\mathbf{V}$ *are orthogonally similar. That is, the matrices* $\mathbf{H}$ *and* $\mathbf{V}$ *have the same Jordan normal form and thus the same eigenvalue spectrum.*

Cantoni et al. use Lemmas 5.3.6 and 5.3.7 to prove the following theorem concerning a standard eigenvalue problem where the matrix is centrosymmetric.

Theorem 5.3.8. *[36, Theorem 2] Let* $\mathbf{H}$ *be a square symmetric centrosymmetric matrix as defined in Lemma 5.3.6, then solving the eigenvalue problem*

$\det(\mathbf{H} - \lambda\mathbf{I}) = 0$ *is equivalent to solving two smaller eigenvalue problems:*

$$\det(\mathbf{S} - \mathbf{JC} - \lambda\mathbf{I}) = 0 \quad \textit{and} \quad \det\left(\begin{bmatrix} a & \sqrt{2}\,\mathbf{x}^{\mathbf{T}} \\ \sqrt{2}\,\mathbf{x} & \mathbf{S} + \mathbf{JC} \end{bmatrix} - \lambda \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}\right) = 0. \tag{5.27}$$

Since our problem consists of solving a generalized eigenvalue problem where one matrix is a full symmetric centrosymmetric and the other is a diagonal centrosymmetric matrix, we propose the following theorem.

Theorem 5.3.9. *Let* $\mathbf{H}$ *and* $\mathbf{W}$ *be square symmetric centrosymmetric matrices of the same size, such that:*

$$\mathbf{H} = \begin{bmatrix} \mathbf{S} & \mathbf{x} & \mathbf{C}^{\mathbf{T}} \\ \mathbf{x}^{\mathbf{T}} & a & \mathbf{x}^{\mathbf{T}}\mathbf{J} \\ \mathbf{C} & \mathbf{J}\mathbf{x} & \mathbf{J}\mathbf{S}\,\mathbf{J} \end{bmatrix} \quad \textit{and} \quad \mathbf{W} = \begin{bmatrix} \operatorname{diag}(\mathbf{w}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & w & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{J}\operatorname{diag}(\mathbf{w})\mathbf{J} \end{bmatrix}, \tag{5.28}$$

then solving the generalized eigenvalue problem $\det(\mathbf{H} - \lambda\mathbf{W}) = 0$ *is equivalent to solving two smaller generalized eigenvalue problems:*

$$\det(\mathbf{S} - \mathbf{JC} - \lambda\operatorname{diag}(\mathbf{w})) = 0 \quad \textit{and} \quad \det\left(\begin{bmatrix} a & \sqrt{2}\,\mathbf{x}^{\mathbf{T}} \\ \sqrt{2}\,\mathbf{x} & \mathbf{S} + \mathbf{JC} \end{bmatrix} - \lambda \begin{bmatrix} w & \mathbf{0} \\ \mathbf{0} & \operatorname{diag}(\mathbf{w}) \end{bmatrix}\right) = 0. \tag{5.29}$$

Proof This proof relies on the unitary transformation matrix presented in [36, Lemma 3]:

$$\mathbf{K} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{I} & \mathbf{0} & -\mathbf{J} \\ \mathbf{0} & \sqrt{2} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{J} \end{bmatrix}, \tag{5.30}$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{J}$ is the exchange matrix.

It is easy to verify that:

$$\mathbf{KHK^T} = \mathbf{V}, \tag{5.31}$$

where $\mathbf{V}$ is the matrix in lemma 5.3.7.

This result is analogous for the matrix $\mathbf{W}$ with a change in notation. Hence:

$$\begin{aligned}
0 &= \det(\mathbf{H} - \lambda\mathbf{W}) \\
&= \det(\mathbf{K}) \det(\mathbf{H} - \lambda\mathbf{W}) \det(\mathbf{K^T}) \\
&= \det(\mathbf{KHK^T} - \lambda\mathbf{KWK^T}) \\
&= \det\left(\begin{bmatrix} \mathbf{S} - \mathbf{JC} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & a & \sqrt{2}\,\mathbf{x^T} \\ \mathbf{0} & \sqrt{2}\,\mathbf{x} & \mathbf{S} + \mathbf{JC} \end{bmatrix} - \lambda \begin{bmatrix} \mathrm{diag}\,(\mathbf{w}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & w & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathrm{diag}\,(\mathbf{w}) \end{bmatrix}\right) \\
&= \det(\mathbf{S} - \mathbf{JC} - \lambda \mathrm{diag}\,(\mathbf{w})) \det\left(\begin{bmatrix} a & \sqrt{2}\,\mathbf{x^T} \\ \sqrt{2}\,\mathbf{x} & \mathbf{S} + \mathbf{JC} \end{bmatrix} - \lambda \begin{bmatrix} w & \mathbf{0} \\ \mathbf{0} & \mathrm{diag}\,(\mathbf{w}) \end{bmatrix}\right),
\end{aligned} \tag{5.32}$$

from which the result follows.

Theorem 5.3.9 is very useful when N is large since it is less costly to solve two symmetric generalized eigensystems of dimensions $N \times N$ and $(N+1) \times (N+1)$ rather than one symmetric eigensystem of dimension $(2N+1) \times (2N+1)$. Additionally, Lemma 5.3.6 also has large ramifications when it comes to saving storage space. As is discussed in [157], the l^{th} Sinc differentiation matrices are symmetric Toeplitz matrices. Therefore, for a symmetric Toeplitz matrix of dimension $(2N+1) \times (2N+1)$, only $2N+1$ elements need to be

stored. Investigating the definition of the matrix $\mathbf{A}$ in equation (5.13), we can see that $\mathbf{A}$ is defined as a sum of a symmetric Toeplitz matrix and a diagonal matrix. Moreover, from Lemma 5.3.6 and theorem 5.3.9, using only the antidiagonal and anti-upper triangular half of matrix $\mathbf{C}$, the vector $\mathbf{x}$, the scalar a, the diagonal and lower triangular half of the matrix $\mathbf{S}$, the vector $\mathbf{w}$ and the scalar w, we can create all the elements needed to solve for the generalized eigenvalues of the matrices $\mathbf{A}$ and $\mathbf{D}^2$. Hence, the ratio of elements needed to be computed and stored at each iteration N in order to solve for these eigenvalues is given by:

$$\text{Proportion of Entries Needed } = \frac{(2N+N+1)+(N+1)}{(2N+1)^2+(2N+1)} = \frac{1}{N+1}. \tag{5.33}$$

Thus, only $\frac{1}{N+1}$ of the entries need to be generated and stored at every iteration to obtain all of the generalized eigenvalues.

In the following section, we will illustrate the gain in efficiency of these results by applying the DESCM to the Schrödinger equation with an anharmonic oscillator.

5.4 The anharmonic oscillator

The time independent Schrödinger equation is given by:

$$\mathcal{H}\,\psi(x) \;=\; E\,\psi(x) \qquad \text{with} \qquad \lim_{|x|\to\infty} \psi(x) = 0. \tag{5.34}$$

In equation (5.34), the Hamiltonian is given by the following linear opera-

tor:

$$\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x),$$

where $V(x)$ is the potential energy function and E is the energy eigenvalue of the Hamiltonian operator $\mathcal{H}$. In our case, we are treating the anharmonic oscillator potential $V(x)$ defined by:

$$V(x) = \sum_{i=1}^{m} c_i x^{2i} \qquad \text{with} \qquad c_m > 0 \quad \text{and} \quad m \in \mathbb{N}\backslash\{1\}. \tag{5.35}$$

In [83], we successfully applied the DESCM to time independent Schrödinger equation with an anharmonic potential. As we can see, the time independent Schrödinger equation (5.34) is a special case of the Sturm-Liouville equation with $q(x) = V(x)$ and $\rho(x) = 1$. Applying Eggert et al.'s transformation and the DESCM with $\phi(x) = \sinh(x)$, we arrived at the following generalized eigenvalue problem:

$$\det(\mathbf{A} - \mathcal{E}\mathbf{D}^2) = 0, \tag{5.36}$$

where $\mathcal{E}$ are approximations of the energy eigenvalues E.

The matrices $\mathbf{A}$ and $\mathbf{D}^2$ defined by equation (5.13) and (5.14) are given by:

$$A_{j,k} = -\left(\frac{1}{h^2}\right)\delta^{(2)}_{j,k} + \tilde{V}(kh)\delta^{(0)}_{j,k} \quad \text{with} \quad -N \leq j,k \leq N, \tag{5.37}$$

where:

$$\tilde{V}(x) = \frac{1}{4} - \frac{3}{4}\operatorname{sech}^2(x) + \cosh^2(x)\sum_{i=1}^{m} c_i \sinh^{2i}(x), \tag{5.38}$$

and:

$$D^2_{j,k} = \cosh^2(kh)\,\delta^{(0)}_{j,k} \qquad \text{with} \qquad -N \leq j,k \leq N. \tag{5.39}$$

Since the anharmonic potential $V(x)$ defined in (5.35) is an even function, the function $\rho(x) = 1$ is an even function and the conformal map $\phi(x) = \sinh(x)$ is an odd function, we know that theorem 5.3.5 applies. Hence, the matrices $\mathbf{A}$ and $\mathbf{D}^2$ are symmetric centrosymmetric.

5.5 Numerical Discussion

In this section, we test the computational efficiency of the results obtained in theorem 5.3.9. All calculations are performed using the programming language Julia in double precision. The eigenvalue solvers in Julia use the linear algebra package *LAPACK*.

In [39], Chaudhuri et al. presented several potentials with known analytic solutions for energy levels calculated using supersymmetric quantum mechanics, namely:

$$\begin{aligned}
V_1(x) &= x^2 - 4x^4 + x^6 && \Rightarrow && E_0 = -2 \\
V_2(x) &= 4x^2 - 6x^4 + x^6 && \Rightarrow && E_1 = -9 \\
V_3(x) &= (105/64)x^2 - (43/8)x^4 + x^6 - x^8 + x^{10} && \Rightarrow && E_0 = 3/8 \\
V_4(x) &= (169/64)x^2 - (59/8)x^4 + x^6 - x^8 + x^{10} && \Rightarrow && E_1 = 9/8.
\end{aligned} \tag{5.40}$$

Figure 5.1 presents the absolute error between our approximation and the

exact values given in (5.40). The absolute error is defined by:

$$\text{Absolute error} = |\mathcal{E}_l(N) - \text{Exact value}| \qquad \text{for} \qquad l = 0, 1. \tag{5.41}$$

The optimal mesh size obtained in [83]:

$$h = \frac{W\left(\frac{2^m \pi^2 (m+1)N}{\sqrt{c_m}}\right)}{(m+1)N}, \tag{5.42}$$

where $W(x)$ is the Lambert W function, is used in the calculation.

As can be seen from Figure 5.1, using the centrosymmetric property improves the convergence rate of the DESCM significantly.

5.6 Conclusion

Sturm-Liouville eigenvalue problems are abundant in scientific and engineering problems. In certain applications, these problems possess a symmetry structure which results in the Sturm-Liouville operator to be commutative with the parity operator. As was proven in theorem 5.3.5, applying the DESCM will preserve this symmetry and results in a generalized eigenvalue problem where the matrices are symmetric centrosymmetric. The centrosymmetric property leads to a substantial reduction in the computational cost when computing the eigenvalues by splitting the original eigenvalue problem of dimension $(2N + 1) \times (2N + 1)$ into two smaller generalized eigensystems of dimension $N \times N$ and $(N + 1) \times (N + 1)$. Moreover, due to the internal block structure of the matrices obtained using the DESCM, we have shown that

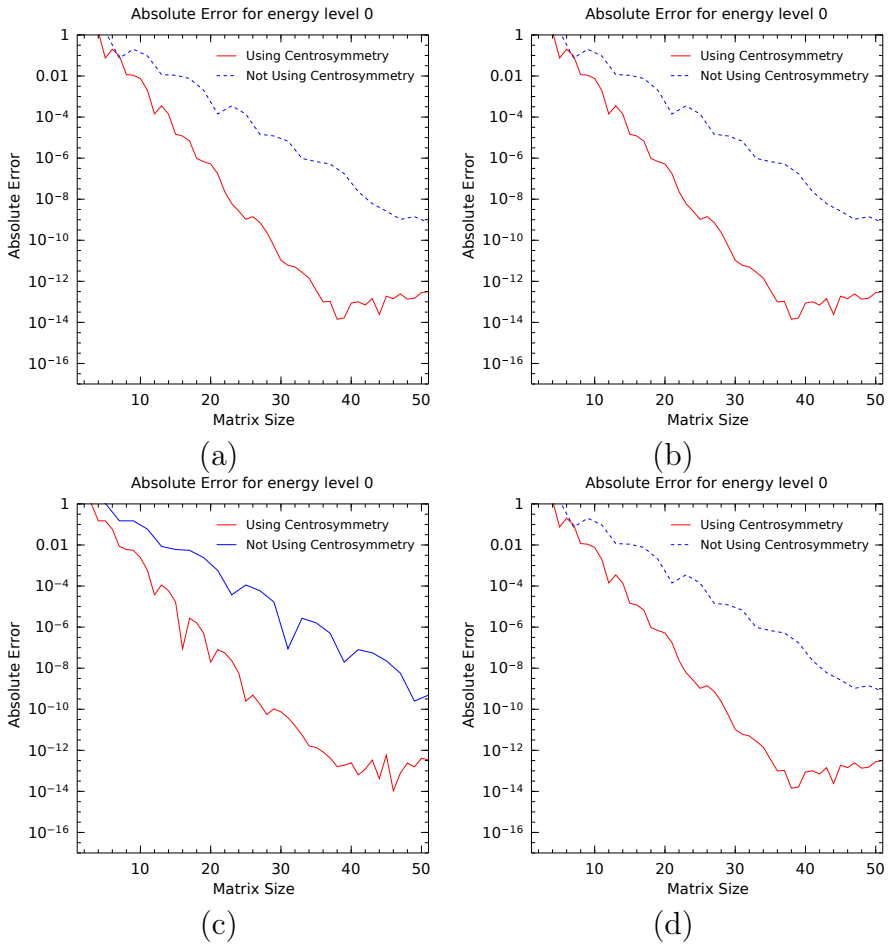

Figure 5.1: Absolute error for the potentials $V_i(x)$ for $i = 1, 2, 3, 4$ given by (5.40) with $\phi(x) = \sinh(x)$.
(a) $V_1(x) = x^2 - 4x^4 + x^6$ with exact eigenvalue $E_0 = -2$. (b) $V_2(x) = 4x^2 - 6x^4 + x^6$ with exact eigenvalue $E_1 = -9$. (c) $V_3(x) = (105/64)x^2 - (43/8)x^4 + x^6 - x^8 + x^{10}$ with exact eigenvalue $E_0 = 3/8$. (d) $V_4(x) = (169/64)x^2 - (59/8)x^4 + x^6 - x^8 + x^{10}$ with exact eigenvalue $E_1 = 9/8$.

only $\dfrac{1}{N+1}$ of all entries need to be computed and stored at every iteration in order to find all of their eigenvalues. Numerical results are presented for the time independent Schrödinger equation (5.34) with an anharmonic oscillator potential (5.35). Four exact potentials with known eigenvalues are tested and the results clearly demonstrated the reduction in complexity and increase in

convergence.

Chapter 6

A Numerical Treatment of Energy Eigenvalues of Harmonic Oscillators Perturbed by a Rational Function

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Abstract.

In the present contribution, we apply the algorithm for the double exponential Sinc-collocation method (DESCM) to the one-dimensional time independent Schrödinger equation for a class of rational potentials of the form $V(x) = p(x)/q(x)$. This algorithm is based on the discretization of the Hamil-

tonian of the Schrödinger equation using Sinc functions expansions. This discretization results in a generalized eigenvalue problem where the eigenvalues correspond to approximations of the energy values of the corresponding Hamiltonian. A systematic numerical study is conducted, beginning with test potentials with known eigenvalues and moving to rational potentials of increasing degree.

6.1 Introduction

Over the last three decades, the study of perturbed quantum harmonic oscillators has been on the edge of thrilling and exciting new research. Numerous methods have been developed to numerically evaluate the energy eigenvalues of the Schrödinger equation $\mathcal{H}\psi = E\psi$. More specifically, the Hamiltonian $\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$, where $V(x)$ is a rational function of the form $V(x) = x^2 + \frac{p(x)}{q(x)}$ has been the subject of much interest. Historically, the potential:

$$V(x) = x^2 + \frac{\lambda x^2}{1 + gx^2}, \tag{6.1}$$

with $\lambda \in \mathbb{R}$ and $g > 0$ was among the first rational potentials to manifest interest in the scientific community. The Schrödinger equation with such a potential is the analogue of a zero-dimensional field theory with a nonlinear Lagrangian, which is still of interest in particle physics today [112, 118, 137, 165]. Additionally, outside the realm of field theory, double-well potentials are among the most important potentials in quantum mechanics [85, 95]. Double well potentials occur abundantly in the study of quantum information theory

or quantum computing. Concisely, quantum information theory attempts to generalize the ideas of classical information theory to the quantum world. Recently, systems of two particles in double well potentials have been studied experimentally with ultracold atoms [11, 178]. In 2009, it was theoretically proposed that neutral atoms held in double well potentials could be used to create quantum logic gates to be used for quantum information processing [78]. Recently, Murmann et al. demonstrated that the quantum state of two ultracold fermionic atoms in an isolated double-well potential was completely controllable [122]. They were able to control the interaction strength between these two particles, the tilt of the potential as well as their tunneling rates between the two wells. These experiments provide a starting point for quantum computation with neutral atoms. Hence, further investigations into quantum systems with multiple wells could be an asset in constructing an efficient and reliable quantum computer.

There is a rich and diverse collection of techniques and algorithms available in literature to compute the energy eigenvalues of the Schrödinger equation with the rational potential (6.1). Among others, the use of variational methods, perturbation series, and perturbed ladder operators methods have been readily used to approximate the energy eigenvalues of this potential [26, 27, 29, 63, 118, 160]. To understand the innate structure of the potential (6.1), several exact representations for the energy eigenvalues of this potential were found for specific relations between the parameters λ and g [25, 32, 41, 73, 74, 76, 77, 80, 87, 113, 139–142, 181, 188]. Moreover, the Hill determinant method as well as the Hill determinant method with a variational parameter have been used extensively to numerically calculate the energy eigenvalues of

(6.1) [3, 60, 86]. Methods utilizing power series, Taylor series and Padé approximants have also been used frequently in literature [64, 65, 67, 90, 96, 99]. More general numerical techniques have also been studied and applied to the potential (6.1) such as finite differences, numerical integration, Runge-Kutta methods and transfer matrix methods [31, 62, 79, 92, 146, 147, 191].

Despite the amount of attention the potential (6.1) has received in literature, there have been some attempts to treat more general rational potentials. In [49], the potential:

$$V(x) = x^2 + \frac{2g^{m-1}x^{2m}}{1+\alpha g x^2} \quad \text{where} \quad m \in \mathbb{Z}^+,\ \alpha > 0 \ \text{ and } \ g \geq 0, \tag{6.2}$$

is examined. A perturbation series is used to investigate the spectrum of energy eigenvalues for this specific potential. A strong asymptotic condition of order $(m-1)$ is proved and this series is also shown to be summable in the sense of the Borel-Leroy method.

In [89], the potential:

$$V(x) = \omega^2 x^2 + \frac{f(x^2)}{g(x^2)}, \tag{6.3}$$

where $f(x^2)$ and $g(x^2)$ are polynomials in x^2 such that $\frac{f(x^2)}{g(x^2)} = o(x^2)$ as $x \to \infty$, is investigated. A method for obtaining quasi-exact solutions for the energy eigenvalues is outlined.

In [125], asymptotic expansions for the energy eigenvalues of the potential:

$$V(x) = x^{2N} + \frac{\lambda x^{m_1}}{1+gx^{m_2}} \tag{6.4}$$

with N, m_1, m_2 being arbitrary positive integers and real parameters λ and g are derived. These asymptotic expansions are subsequently shown to be related to the corresponding energy levels n. Numerical results are presented for a variety of potentials of the form in equation (6.4). The numerical accuracy of the proposed asymptotic estimates increase as their corresponding energy levels increases.

In [145], a matrix-continued-fraction algorithm is introduced to calculated the energy eigenvalues of rational potentials of the form:

$$V(x) = x^2 + \frac{\sum_{m=1}^{M} \lambda_{2m} x^{2m}}{1 + \sum_{m=1}^{M} g_{2m} x^{2m}} \qquad \text{and} \qquad V(x) = x^2 + \frac{\sum_{m=1}^{2M} \lambda_m x^m}{1 + \sum_{m=1}^{2M} g_m x^m}. \quad (6.5)$$

This method is based on an expansion of the eigenfunctions into complete sets. In addition to the proposed method, numerical results are given only for the nested potential in equation (6.1) as well as polynomial potentials (i.e. $g_m = 0 \quad \forall m$). The numerical results provided demonstrate a high accuracy in comparison to previous results available in literature.

In [190], the energy levels of the one dimensional potentials:

$$V(x) = x^2 + \frac{\lambda x^N}{1 + g x^2} \qquad \text{and} \qquad V(x) = \mu x^{2I} \pm \frac{g x^{2N}}{1 + g\alpha x^{2M}} \quad (6.6)$$

are evaluated using a finite difference approach. Numerical results are presented for a variety of parameters and they are in good agreement with other results obtained in literature.

As can be seen by the numerous approaches which have been made to solve

this problem, there is a lack of uniformity in its resolution. Moreover, the task of evaluating energy eigenvalues for any general rational potential has only been studied lightly. While several of these methods yield excellent results for specific cases of rational potentials namely the potential in equation (6.1), it would be favorable to have one algorithm capable of handling any rational potential of the form $V(x) = \omega x^{2m} + \frac{p(x)}{q(x)}$, which can deliver all eigenvalues at any desired level of accuracy in an acceptable computational time. It is the purpose of this research work to present such a general algorithm based on the double exponential Sinc-collocation method presented in [84]. In this work, we will begin by summarizing the algorithm based on the double exponential Sinc-collocation method (DESCM). The DESCM starts by approximating the wave function as a series of weighted Sinc functions. By substituting this approximation in the Schrödinger equation and evaluating this expression at several collocation points, we obtain a generalized eigensystem where the generalized eigenvalues are approximations to the energy eigenvalues. As will be shown in this contribution, the more terms we include in our series of weighted Sinc functions, the better the approximation to the energy eigenvalues becomes. This method has numerous advantages over previous methods as it is insensitive to large changes in the numerous parameters in addition to having a near-exponential convergence rate. Moreover, the matrices generated by the DESCM have very nice symmetric properties which make numerical calculations of their eigenvalues much easier than standard non-symmetric matrices.

6.2 General definitions, properties and preliminaries

The sinc function, analytic for all $z \in \mathbb{C}$ is defined by the following expression:

$$\operatorname{sinc}(z) = \begin{cases} \dfrac{\sin(\pi z)}{\pi z} & \text{for} \quad z \neq 0 \\ 1 & \text{for} \quad z = 0 \end{cases} . \tag{6.7}$$

The Sinc function $S(j,h)(x)$ for $h \in \mathbb{R}^+$ and $j \in \mathbb{Z}$ is defined by:

$$S(j,h)(x) = \operatorname{sinc}\left(\frac{x}{h} - j\right). \tag{6.8}$$

It is possible to expand well-defined functions as series of Sinc functions. Such expansions are known as Sinc expansions or Whittaker Cardinal expansions.

Definition 6.2.1. *[155] Given any function $v(x)$ defined everywhere on the real line and any $h > 0$, the Sinc expansion of $v(x)$ is defined by the following series:*

$$C(v,h)(x) = \sum_{j=-\infty}^{\infty} v_j S(j,h)(x), \tag{6.9}$$

where $v_j = v(jh)$. The symmetric truncated Sinc expansion of the function $v(x)$ is defined by the following series:

$$C_N(v,h)(x) = \sum_{j=-N}^{N} v_j \, S(j,h)(x) \qquad \textit{for} \qquad N \in \mathbb{N}. \tag{6.10}$$

The Sinc functions defined in (6.8) form an interpolatory set of functions

with the discrete orthogonality property:

$$S(j,h)(kh) = \delta_{j,k} \qquad \text{for} \qquad j,k \in \mathbb{Z}, \tag{6.11}$$

where $\delta_{j,k}$ is the Kronecker delta function. In other words, $C_N(v,h)(x) = v(x)$ at all the Sinc grid points given by $x_k = kh$.

A major motivation behind the use of Sinc expansions stems from numerical integration. As it happens, integration of Sinc expansions have a direct connection with the the composite trapezoidal rule. It is well known from the Euler-Maclaurin summation formula that the error in approximating the integral of a measurable function v defined on the interval (a,b) by the composite trapezoidal rule is given by:

$$h\sum_{k=1}^{N-1}\frac{v(x_{k-1})+v(x_k)}{2} - \int_a^b v(x)\mathrm{d}x \sim \sum_{l=1}^{\infty} h^{2l}\frac{B_{2l}}{(2l)!}\left(v^{2l-1}(b) - v^{2l-1}(a)\right), \tag{6.12}$$

where B_{2l} are the Bernoulli numbers and N is the number of points in the interval of integration, from $x_0 = a$ to $x_N = b$. Hence, for a periodic function or a function for which $v^{(n)}(x) \to 0$ at the endpoints, the convergence is faster than any power of h. This observation has lead to much research on the use of conformal maps that decay to zero at infinities. Indeed, given a conformal map $\phi^{-1}(x)$ of a simply connected domain in the complex plane with boundary points $a \neq b$ such as $\phi^{-1}(a) = -\infty$ and $\phi^{-1}(b) = \infty$ and a Lebesgue measurable function v defined on the interval (a,b) we can derive

the following elegant result using Sinc expansions:

$$\begin{aligned}\int_a^b v(x)\mathrm{d}x &= \int_{-\infty}^{\infty}(v\circ\phi)(y)\phi'(y)\mathrm{d}y \\ &\approx \int_{-\infty}^{\infty}\sum_{j=-N}^{N}\tilde{v}_j\, S(j,h)(y)\mathrm{d}y \\ &= \sum_{j=-N}^{N}\tilde{v}_j\int_{-\infty}^{\infty}S(j,h)(y)\mathrm{d}y \\ &= h\sum_{j=-N}^{N}\tilde{v}_j, \end{aligned} \tag{6.13}$$

where $\tilde{v}_j = (v\circ\phi)(jh)\phi'(jh)$. As we can see, equation (6.13) is exactly the trapezoidal rule.

In [155], Stenger introduced a class of functions which are successfully approximated by a Sinc expansion. We present the definition for this class of functions bellow.

Definition 6.2.2. *[155] Let $d > 0$ and let $\mathscr{D}_d$ denote the strip of width $2d$ about the real axis:*

$$\mathscr{D}_d = \{z \in \mathbb{C} : |\,\Im(z)| < d\}. \tag{6.14}$$

For $\epsilon \in (0,1)$, let $\mathscr{D}_d(\epsilon)$ denote the rectangle in the complex plane:

$$\mathscr{D}_d(\epsilon) = \{z \in \mathbb{C} : |\,\Re(z)| < 1/\epsilon,\ |\,\Im(z)| < d(1-\epsilon)\}. \tag{6.15}$$

Let $\mathbf{B}_2(\mathscr{D}_d)$ denote the family of all functions g that are analytic in $\mathscr{D}_d$, such

that:

$$\int_{-d}^{d} |\, g(x+iy)|dy \to 0 \; as \; x \to \pm\infty \quad and \quad \mathcal{N}_2(g, \mathscr{D}_d) = \lim_{\epsilon \to 0} \left(\int_{\partial \mathscr{D}_d(\epsilon)} |g(z)|^2 |dz| \right)^{1/2} < \infty. \tag{6.16}$$

The time independent Schrödinger equation is given by the following expression:

$$\mathcal{H}\,\psi(x) \;=\; E\,\psi(x), \tag{6.17}$$

where the Hamiltonian is given by the following linear operator:

$$\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \tag{6.18}$$

where $V(x)$ is the potential energy function. The time independent Schrödinger equation (6.17) can be written as the following boundary value problem:

$$-\psi''(x) + V(x)\psi(x) = E\psi(x) \qquad \text{with} \qquad \lim_{|x| \to \infty} \psi(x) = 0. \tag{6.19}$$

Equation (6.19) is similar to the Schrödinger equation with an anharmonic oscillator potential to which we applied successfully the DESCM [83].

Eggert et al. [56] demonstrate that applying an appropriate substitution to the boundary value problem (6.19), results in a symmetric discretized system when using Sinc expansion approximations. The change of variable they propose is given by:

$$v(x) = \left(\sqrt{(\phi^{-1})'}\, \psi \right) \circ \phi(x) \qquad \Longrightarrow \qquad \psi(x) = \frac{v \circ \phi^{-1}(x)}{\sqrt{(\phi^{-1}(x))'}}, \tag{6.20}$$

where $\phi^{-1}(x)$ a conformal map of a simply connected domain in the complex plane with boundary points $a \neq b$ such that $\phi^{-1}(a) = -\infty$ and $\phi^{-1}(b) = \infty$.

Applying the substitution (6.20) to (6.19), we obtain:

$$\hat{\mathcal{H}}\, v(x) = -v''(x) + \tilde{V}(x)v(x) \;=\; E(\phi'(x))^2 v(x) \quad \text{with} \quad \lim_{|x|\to\infty} v(x) = 0, \tag{6.21}$$

where:

$$\tilde{V}(x) = -\sqrt{\phi'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\phi'(x)}\frac{\mathrm{d}}{\mathrm{d}x}(\sqrt{\phi'(x)})\right) + (\phi'(x))^2 V(\phi(x)). \tag{6.22}$$

6.3 The development of the method

A function $\omega(x)$ is said to decay double exponentially at infinities if there exist positive constants A, B, γ such that:

$$|\,\omega(x)| \leq A\exp(-B\exp(\gamma|\,x|)) \qquad \text{for} \qquad x \in \mathbb{R}. \tag{6.23}$$

The double exponential transformation is a conformal mapping $\phi(x)$ which allows for the solution of (6.21) to have double exponential decay at both infinities.

In order to implement the DESCM, we start by approximating the solution of (6.21) by a truncated Sinc expansion (6.10). Inserting (6.10) into (6.21),

we obtain the following system of equations:

$$\begin{aligned}\hat{\mathcal{H}}\, C_N(v,h)(x_k) &= \sum_{j=-N}^{N}\left[-\frac{\mathrm{d}^2}{\mathrm{d}x_k^2}S(j,h)(x_k)+\tilde{V}(x_k)S(j,h)(x_k)\right]v_j \\ &= \mathcal{E}\sum_{j=-N}^{N} S(j,h)(x_k)(\phi'(x_k))^2 v_j \qquad \text{for} \qquad k=-N,\ldots,N,\end{aligned} \tag{6.24}$$

where the collocation points $x_k = kh$ and $\mathcal{E}$ is an approximation of the eigenvalue E in (6.21).

The above equation can be re-written as follows:

$$\begin{aligned}\hat{\mathcal{H}}\, C_N(v,h)(x_k) &= \sum_{j=-N}^{N}\left[-\frac{1}{h^2}\,\delta_{j,k}^{(2)}+\tilde{V}(kh)\,\delta_{j,k}^{(0)}\right]v_j \\ &= \mathcal{E}\sum_{j=-N}^{N}\delta_{j,k}^{(0)}(\phi'(kh))^2 v_j \qquad \text{for} \quad k=-N,\ldots,N,\end{aligned} \tag{6.25}$$

where $\delta_{j,k}^{(l)}$ are given by [154]:

$$\delta_{j,k}^{(l)} = h^l\left(\frac{d}{dx}\right)^l S(j,h)(x)\bigg|_{x=kh}. \tag{6.26}$$

Equation (6.25) can be represented in a matrix form as follows:

$$\hat{\mathcal{H}}\,\mathbf{C}_N(v,h) = \mathbf{H}\mathbf{v} \;=\; \mathcal{E}\mathbf{D}^2\mathbf{v} \quad\Longrightarrow\quad (\mathbf{H}-\mathcal{E}\mathbf{D}^2)\mathbf{v} \;=\; 0, \tag{6.27}$$

where:

$$\mathbf{v} = (v_{-N},\ldots,v_N)^T \qquad \text{and} \qquad \mathbf{C}_N(v,h) = (C_N(v,h)(-Nh),\ldots,C_N(v,h)(Nh))^T.$$

$\mathbf{H}$ is a $(2N+1)\times(2N+1)$ matrix with entries $H_{j,k}$ given by:

$$H_{j,k} = -\frac{1}{h^2}\,\delta^{(2)}_{j,k} + \tilde{V}(kh)\,\delta^{(0)}_{j,k} \qquad \text{with} \quad -N \le j,k \le N, \tag{6.28}$$

and $\mathbf{D}^2$ is a $(2N+1)\times(2N+1)$ diagonal matrix with entries $D^2_{j,k}$ given by :

$$D^2_{j,k} = (\phi'(kh))^2\,\delta^{(0)}_{j,k} \qquad \text{with} \quad -N \le j,k \le N. \tag{6.29}$$

To obtain non-trivial solutions for (6.27), we have to set:

$$\det(\mathbf{H} - \mathcal{E}\mathbf{D}^2) = 0. \tag{6.30}$$

In order to find an approximation of the eigenvalues of equation (6.21), we will solve the above generalized eigenvalue problem. The matrix $\mathbf{D}^2$ is diagonal and positive definite. The matrix $\mathbf{H}$ is the sum of a diagonal matrix and a symmetric Toeplitz matrix. If there exits a constant $\delta > 0$ such that $\tilde{V}(x) \ge \delta^{-1}$, then the matrix $\mathbf{H}$ is also positive definite.

In [84, Theorem 3.2], we present the convergence analysis of DESCM which we state here in the case of the transformed Schrödinger equation (6.21). The proof of the Theorem is given in [84].

Theorem 6.3.1. *[84, Theorem 3.2] Let E and $v(x)$ be an eigenpair of the transformed Schrödinger equation:*

$$-v''(x) + \tilde{V}(x)v(x) = E(\phi'(x))^2 v(x), \tag{6.31}$$

where:

$$\tilde{V}(x) = -\sqrt{\phi'(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\phi'(x)}\frac{\mathrm{d}}{\mathrm{d}x}(\sqrt{\phi'(x)})\right)+(\phi'(x))^2 V(\phi(x)) \quad \textit{and} \quad \lim_{|x|\to\infty} v(x) = 0. \tag{6.32}$$

Assume there exist positive constants A, B, γ *such that:*

$$|v(x)| \leq A\exp(-B\exp(\gamma|x|)) \qquad \textit{for all} \qquad x \in \mathbb{R}, \tag{6.33}$$

and that $v \in \mathbf{B}_2(\mathscr{D}_d)$ *with* $d \leq \dfrac{\pi}{2\gamma}$.

Moreover, if there is a constant $\delta > 0$ *such that* $\tilde{V}(x) \geq \delta^{-1}$ *and the selection of the optimal mesh size* h *is such that:*

$$h = \frac{W(\pi d\gamma N/B)}{\gamma N}, \tag{6.34}$$

where $W(x)$ *is the Lambert W function.*

Then, there is an eigenvalue $\mathcal{E}$ *of the generalized eigenvalue problem satisfying:*

$$|\mathcal{E} - E| \leq \vartheta_{v,d}\sqrt{\delta E}\left(\frac{N^{5/2}}{\log(N)^2}\right)\exp\left(-\frac{\pi d\gamma N}{\log(\pi d\gamma N/B)}\right) \quad \textit{as} \quad N \to \infty, \tag{6.35}$$

where $\vartheta_{v,d}$ *is a constant that depends on* v *and* d.

As we can see from the results obtained in Theorem 6.3.1, $|\mathcal{E} - E| \to 0$ as $N \to \infty$ for all energy eigenvalues E. Moreover, it is important to notice that the convergence rate of the DESCM is dependent on the strip width of analyticity d.

6.4 Application to Rational Potentials

In this section, we will apply the DESCM to the time independent Schrödinger equation with a rational potential. The time independent Schrödinger equation is defined by the following equation:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right] \psi(x) \quad = \quad E\,\psi(x), \tag{6.36}$$

where the potential $V(x)$ is given by:

$$V(x) = \omega x^{2m} + \frac{p(x)}{q(x)} \quad \text{with} \quad (\omega, m) \in \mathbb{R}_{>0} \times \mathbb{N}, \tag{6.37}$$

where the functions $p(x)$ and $q(x)$ are polynomials in x. More specifically, we will investigate a subset of rational functions $\dfrac{p}{q} \in \mathcal{Q} \subset \mathbb{R}(x)$, where $\mathcal{Q}$ is defined by the following function space:

$$\mathcal{Q} = \left\{ \frac{p}{q} \in \mathbb{R}(x) : \left| \begin{array}{l} q(x) \neq 0, \quad \forall\, x \in \mathbb{R}, \\ \\ q(0) = 1, \\ \\ \dfrac{p(x)}{q(x)} = o(x^{2m}) \quad \text{as} \quad |x| \to \infty \end{array} \right. \right\}. \tag{6.38}$$

In (6.38), $\mathbb{R}(x)$ denotes the set of rational functions of x with real coefficients. The first condition, $q(x) \neq 0$, $\forall\, x \in \mathbb{R}$ is set in order for $V(x)$ to be continuous for all $x \in \mathbb{R}$. However, this conditions automatically imposes that $\deg(q(x))$ be even since any odd degree polynomial has at least one real root. The second condition imposes a uniqueness on the potentials. For example, we can create

the rational function:

$$\frac{p_1(x)}{q_1(x)} = \frac{2 + 2x + 2x^4}{2 + 2x^2} = \frac{1 + x + x^4}{1 + x^2} = \frac{p_2(x)}{q_2(x)}. \tag{6.39}$$

Although $p_1(x) \neq p_2(x)$ and $q_1(x) \neq q_2(x)$, we have $p_1(x)/q_1(x) = p_2(x)/q_2(x)$. The condition $q(0) = 1$ removes this ambiguity when defining new potentials. The third condition specifies that for large x, the rational potential $V(x)$ exhibits behaviour similar to an anharmonic potential of the form ωx^{2m}. Consequently, the potential $V(x)$ we will be investigating has the following general form:

$$V(x) = \omega x^{2m} + \frac{\sum_{i=0}^{k} \lambda_i x^i}{1 + \sum_{i=1}^{2l} g_i x^i} \qquad \text{with} \quad k - 2l < 2m, \tag{6.40}$$

It is worth noting that this current form also encompasses even potentials depending on the values of the coefficients $\{\lambda_i\}_{i=0}^{k}$ and $\{g_i\}_{i=1}^{2l}$. To implement the DE transformation, we choose a function ϕ which would result in the solution of (6.21) to decay doubly exponentially. Given the nature of the potential (6.40), we know that the wave function will be analytic everywhere in the complex plane except for the points $z \in \mathbb{C}$ where $q(z) = 0$. Since the anharmonic potential in equation (6.40) is analytic in $\mathbb{R}$ and grows to infinity as $x \to \pm\infty$, the wave function is also analytic and normalizable over $\mathbb{R}$. To find the decay rate of the solution to equation (6.19) with the rational potential, we can use a similar WKB analysis as the one presented in [83].

In [83], we considered the anharmonic potential:

$$V(x) = \sum_{i=1}^{m} c_i x^{2i} = \mathcal{O}(x^{2m}) \quad \text{as} \quad |x| \to \infty. \tag{6.41}$$

As we can see, the anharmonic potential (6.41) has the same asymptotic growth as the rational potential (6.40). Consequently, the function $\psi(x)$ has the same decay rate at both infinities:

$$\psi(x) = \mathcal{O}\left(|x|^{-m/2} \exp\left(-\frac{\sqrt{\omega}\,|x|^{m+1}}{m+1}\right)\right) \qquad \text{as} \qquad |x| \to \infty. \tag{6.42}$$

Away from both infinities, the wave function $\psi(x)$ undergoes oscillatory behaviour. From equation (6.42), we can see that the wave function $\psi(x)$ decays only single exponentially at infinities.

A possible choice for the conformal mapping is $\phi(x) = \sinh(x)$ since:

$$\begin{aligned} |v(x)| &= \left|\frac{\psi \circ \phi(x)}{\sqrt{\phi'(x)}}\right| \\ &\leq A|\sinh(x)|^{-m/2}|\cosh(x)|^{-1/2} \exp\left(-\frac{\sqrt{\omega}|\sinh(x)|^{m+1}}{m+1}\right) \\ &\leq A \exp\left(-\frac{\sqrt{\omega}}{(m+1)2^{m+1}} \exp((m+1)|x|)\right), \end{aligned} \tag{6.43}$$

for some positive constant A. However, as previously mentioned, Theorem 6.3.1 demonstrates that the convergence of the DESCM is dependent on the strip of width $2d \leq \dfrac{\pi}{\gamma}$ for which the function $v(x)$ is analytic. Since, we know that our original wave function $\psi(x)$ is analytic everywhere in the complex plane except for the points $z \in \mathbb{C}$ where $q(z) = 0$; we wish to find a conformal mapping which will result in the solution of the transformed wave equation,

$v(x)$, in (6.21) to be analytic up to the maximal strip width $d = \dfrac{\pi}{2\gamma}$. To choose this optimal mapping ϕ, we will utilize a result presented in [152]. Slevinsky et al. investigate the use of conformal maps for the acceleration of convergence of the trapezoidal rule and Sinc numerical methods [152]. The conformal map they propose is constructed as a polynomial adjustment to a sinh map, and allows for the treatment of a finite number of singularities in the complex plane. The polynomial adjustments achieve this goal by locating singularity pre-images on the boundary of the widest allowable strip $\partial\mathscr{D}_{\frac{\pi}{2\gamma}}$. The map they propose has the form:

$$\phi(x) = u_0 \sinh(x) + \sum_{j=1}^{n} u_j x^{j-1} \qquad \text{with} \quad u_0 > 0, \tag{6.44}$$

for the $(n+1)$ coefficients $\{u_k\}_{k=0}^{n}$ to be determined given a finite set of singularities $\{\delta_k \pm \epsilon_k\}_{k=1}^{n}$. Equation (6.44) still grows single-exponentially. Hence, the transformed wave equation in (6.21) will still result in a double exponential variable transformation. Indeed, using this conformal mapping, we see that for all $x \in \mathbb{R}$:

$$|v(x)| \leq A \exp\left(-\frac{\sqrt{\omega}}{m+1}\left(\frac{u_0}{2}\right)^{m+1} \exp((m+1)|x|)\right), \tag{6.45}$$

for some positive constant A. From equation (6.45), we deduce that:

$$\gamma = m+1 \qquad \text{and} \qquad B = \frac{\sqrt{\omega}}{m+1}\left(\frac{u_0}{2}\right)^{m+1}. \tag{6.46}$$

Concisely, the algorithm presented in [152] is as follows: Given a finite set of singularities $\{\delta_k \pm \epsilon_k\}_{k=1}^{n}$, we wish to solve the following system of complex

equations:

$$\phi\left(x_k + i\frac{\pi}{2\gamma}\right) = \delta_k + i\epsilon_k \qquad \text{for} \quad k = 1, \ldots, n. \tag{6.47}$$

This is a system of n complex equations for the $2n+1$ unknowns $\{u_k\}_{k=0}^{n}$ and the real parts of the pre-images of the singularities $\{x_k\}_{k=1}^{n}$. Since there is one more unknown then equations, we can maximize the value of u_0 which is proportional to B in equation (6.46). By summing all n equations in (6.47) and solving for u_0, we obtain the following non-linear program:

$$\begin{aligned} \text{maximize } u_0 \quad & \left(= \frac{\displaystyle\sum_{k=1}^{n}\left\{\epsilon_k - \Im\sum_{j=1}^{n} u_j\left(x_k + i\frac{\pi}{2\gamma}\right)^{j-1}\right\}}{\displaystyle\sin\left(\frac{\pi}{2\gamma}\right)\sum_{k=1}^{n}\cosh(x_k)} \right), \\ \text{subject to} \quad & \phi\left(x_k + i\frac{\pi}{2\gamma}\right) = \delta_k + i\epsilon_k \qquad \text{for} \quad k = 1, \ldots, n. \end{aligned} \tag{6.48}$$

For more information of the implementation of this algorithm, we refer the readers to [152]. Implementing this algorithm guarantees that all complex singularities of the potential in (6.40) will lie on the lines: $\pm i\frac{\pi}{2\gamma}$ implying that our transformed solution $v(x) \in \mathbf{B}_2(\mathscr{D}_{\frac{\pi}{2\gamma}})$. Hence, the convergence rate of the DESCM will now be given by:

$$|\mathcal{E} - E| \leq \vartheta_v\sqrt{\delta E}\left(\frac{N^{5/2}}{\log(N)^2}\right)\exp\left(-\frac{\pi^2 N}{2\log(\pi^2 N/2B)}\right) \quad \text{as} \quad N \to \infty, \tag{6.49}$$

6.5 Numerical discussion

In this section, we present numerical results for the energy values for rational potentials discussed in the previous section. All calculations are performed

using the programming language Julia [30] in double precision. A double-precision floating-point format is a computer number format that occupies 8 bytes (64 bits) in computer memory. In general, this corresponds to about 15-17 significant decimal digits on average. In the figures bellow, the saturation effect observed in all figures is merely a consequence of this computer number format resulting from rounding errors. The eigenvalue solvers in Julia utilize the linear algebra package *LAPACK* [13]. In order to obtain the optimal conformal map in equation (6.44), the non-linear program in (6.48) is solved using the package *DEQuadrature* [151]. The matrices $\mathbf{H}$ and $\mathbf{D}^2$ are constructed using equations (6.28) and (6.29). To produce our figures, we use the Julia package *PyPlot*.

In [25, 32, 41, 73, 74, 76, 77, 80, 87, 113, 139–142, 181, 188], several authors presented exact solutions for potentials of the form:

$$V(x) = x^2 + \frac{\lambda(g)x^2}{1+gx^2}, \tag{6.50}$$

where λ was dependant on g. A few examples are presented bellow:

$$\begin{aligned}
\lambda_1(g) &= -2g(2+g) && \Rightarrow \quad E_0 = 5 + \lambda_1(g)/g, \\
\lambda_2(g) &= -2g(2+3g) && \Rightarrow \quad E_1 = 7 + \lambda_2(g)/g, \\
\lambda_3(g) &= -g\left(7g+6-\sqrt{25g^2-12g+4}\right) && \Rightarrow \quad E_2 = 9 + \lambda_3(g)/g, \\
\lambda_4(g) &= -g\left(13g+6-\sqrt{49g^2-4g+4}\right) && \Rightarrow \quad E_3 = 11 + \lambda_4(g)/g.
\end{aligned} \tag{6.51}$$

Using these exact values as comparison, we present the following figures showing the convergence of the DESCM. Figure 6.1, shows the absolute error between our approximation and the exact values shown in equation (6.51). In

this case, the optimal map can be derived analytically and is given by:

$$\phi(t) = \left(\frac{2}{g}\right)^{1/2} \sinh(t) \tag{6.52}$$

Explicitly, we define the absolute error as:

$$\text{Absolute error} = |\mathcal{E}_n(N) - E_n| \qquad \text{for} \quad n = 0, 1, 2, 3. \tag{6.53}$$

As we can see from Figure 6.1, the proposed algorithm converges quite well.

We will now define an approximation to the absolute error as follows:

$$\epsilon_n(N) = |\mathcal{E}_n(N) - \mathcal{E}_n(N-1)| \qquad \text{for} \quad \begin{cases} N &= 1, 2, 3, \ldots \\ n &= 0, 1, 2, \ldots. \end{cases} \tag{6.54}$$

We will now consider the general potentials of the form in equation (6.40).

$$V(x) = \omega x^{2m} + \frac{\displaystyle\sum_{i=0}^{k} \lambda_i x^i}{1 + \displaystyle\sum_{j=1}^{2l} g_j x^j} \qquad \text{with} \quad k - 2l < 2m, \tag{6.55}$$

These potentials contains many free parameters. Indeed, we have $5 + k + 2l$ free parameters. The free parameters include:

1. the exponent: m
2. the coefficient parameters: ω, λ_i and g_j, $\quad i = 0, \ldots, k$ and $j = 1, \ldots, 2l$
3. the degrees of the polynomials in the numerator and denominator: $k, 2l$.

It is important to mention that choosing the parameters $g_i, i = 1, \ldots, 2l$ at random such that $q(x) \neq 0, \forall x \in \mathbb{R}$ might at first seem problematic. However, by the fundamental theorem of algebra, we are assured that $q(x)$ may be written as:

$$q(z) = 1 + \sum_{i=1}^{2l} g_i z^i = \frac{\prod_{i=1}^{l}(z - z_i)(z - \bar{z_i})}{\prod_{i=1}^{l} z_i \bar{z_i}}, \tag{6.56}$$

where $\{z_i, \bar{z_i}\}_{i=1}^{l}$ are the complex zeros of the strictly positive polynomial $q(x)$. In this cases, $\bar{z_i}$ denotes the complex conjugate of z_i. Hence, the polynomials $q(z)$ can be easily constructed by choosing values for $\{\Re\{z_i\}, \Im\{z_i\}\}_{i=1}^{l}$ and substituting them into equation (6.56).

To remove as much bias as possible in choosing these parameters, we let these parameters represent random variables such that:

$$\begin{aligned} \omega &\sim U(0, 10) \\ k &\sim U\{0, 1, \ldots, 2m + 2l - 1\} \\ \lambda_i &\sim U(-10, 10) \qquad i = 0, \ldots, k \\ \Re\{z_i\} &\sim U(-5, 5) \qquad i = 1, \ldots, l \\ \Im\{z_i\} &\sim U(0, 10) \qquad i = 1, \ldots, l, \end{aligned} \tag{6.57}$$

for fixed parameters m and l. We acknowledge that we have already used the the symbol " $\sim$ " to denote the concept of asymptoticity. However, in equation (6.57), the symbol $X \sim f$ denotes the common statistics notation that the random variable X follows the distribution f. In (6.57), $U(a, b)$ denotes the

continuous uniform distribution on the interval (a, b) and $U\{c, c+1, \ldots, d\}$ denotes the discrete uniform distribution for the integer support $\{c, c+1, \ldots, d\}$, $c, d \in \mathbb{N}_0$.

In figure 6.2, we applied the DESCM to 100 randomly generated potentials of the form in (6.40) according to (6.57) with $m = 1, 2, 3, 4$ and $l = 1$. In this case, we can also find the optimal map analytically which is given by:

$$\phi(t) = \left[\Im\{z_1\} \csc\left(\frac{\pi}{4}\right)\right] \sinh(t) + \Re\{z_1\}. \tag{6.58}$$

As we can, the DESCM performs quite well for a wide variety of parameters values.

In figure 6.3, we applied the DESCM to 100 randomly generated potentials of the form in (6.40) according to (6.57) with $m = 1, 2, 3, 4$ and $l = 2$. Unlike the previous examples, the optimal map cannot be found analytically for these types of potentials. This would lead us to solve the non-linear program in 6.47 for every randomly generated potential. However, this is much harder than anticipated because this non-linear program must be calibrated for any potential. More explicitly, solving this non-linear program requires a user input of two parameters, "obj_scaling_factor" which controls the scaling of the objective function and "Hint" which controls the homotopy solution process for the nonlinear program. Given the sensitivity of non-linear programming, these parameters must be tuned for any arbitrary potential. As such, it is an infeasible task to finely tune these parameters for any given list of randomly generated potentials. However, to demonstrate the power of the DESCM, figure 6.3 display the its implementation using the basic non-optimal $\phi(t) =$

$\sinh(t)$ conformal mapping. As we see, the DESCM still converges quite well for a wide range of parameters.

6.6 Conclusion

Several methods have been used to evaluate the energy eigenvalues of perturbed harmonic oscillators. In this work, we present a method based on the DESCM where the wave function of a transformed Schrödinger equation (6.21) is approximated by as a Sinc expansion. By summing over $2N+1$ collocation points, the implementation of the DESCM leads to a generalized eigenvalue problem with symmetric and positive definite matrices. In addition, we also show that the convergence of the DESCM in this case can be improved to the rate $\mathcal{O}\left(\left(\frac{N^{5/2}}{\log(N)^2}\right)\exp\left(-\kappa'\frac{N}{\log(N)}\right)\right)$ as $N\to\infty$ where $2N+1$ is the dimension of the resulting generalized eigenvalue system and κ' is a constant that depends on the potential. The convergence of this method can improved by adding a polynomial adjustment to the typical sinh conformal mapping to displace the complex singularities away from the real axis.

6.7 Tables and Figures

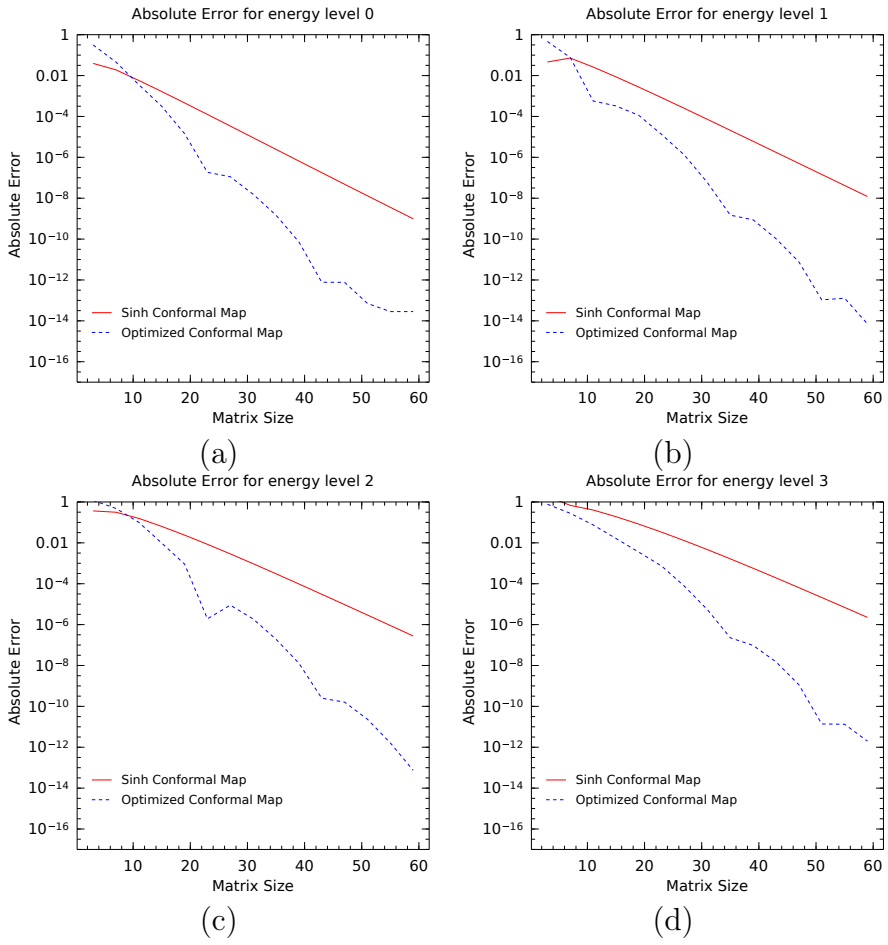
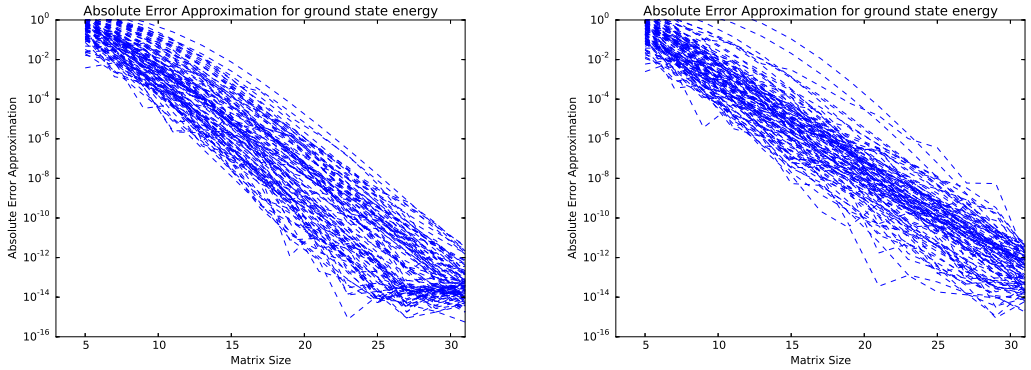
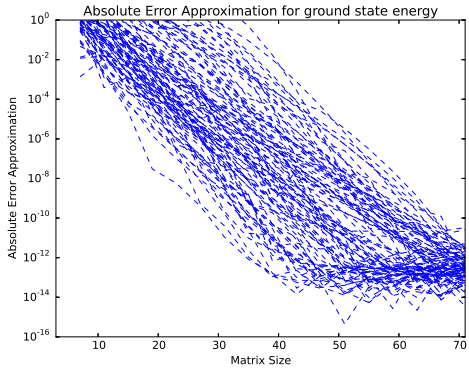


Figure 6.1: Numerical evaluation of the relative error for the potentials $V(x)$ in equation (6.50) with $\lambda_i(g)$ for $i = 1, 2, 3, 4$ as shown in equations (6.51) with $\phi(x) = \sinh(x)$. For all figures, we used the value $g = 1$. Figure (a) shows the relative error for the potential with $\lambda_1(1) = -6$ with exact eigenvalue $E_0 = -1$. Figure (b) shows the relative error for the potential with $\lambda_2(1) = -10$ with exact eigenvalue $E_1 = -3$. Figure (c) shows the relative error for the potential with $\lambda_3(1) = -13 + \sqrt{17}$ with exact eigenvalue $E_2 = -4 + \sqrt{17}$. Figure (d) shows the relative error for the potential with $\lambda_4(1) = -12$ with exact eigenvalue $E_3 = -1$.

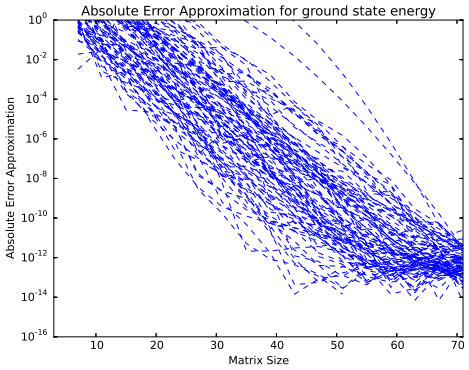


(a) $m = 1$

(b) $m = 2$

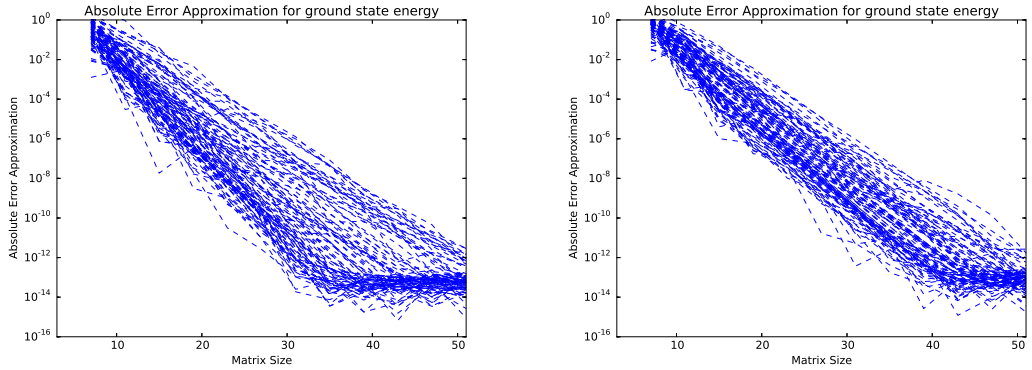


(c) $m = 3$



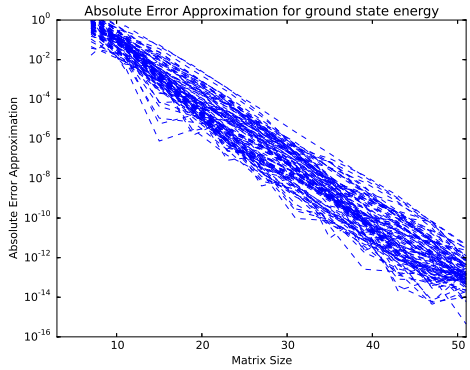
(d) $m = 4$

Figure 6.2: Application of the DESCM for 100 randomly generated potentials of the form $V(x) = \omega x^{2m} + \dfrac{\sum_{i=0}^{k} \lambda_i x^i}{1 + g_1 x + g_2 x^2}$. Figure (a) corresponds to $m = 1$. Figure (b) corresponds to $m = 2$. Figure (c) corresponds to $m = 3$. Figure (d) corresponds to $m = 4$.

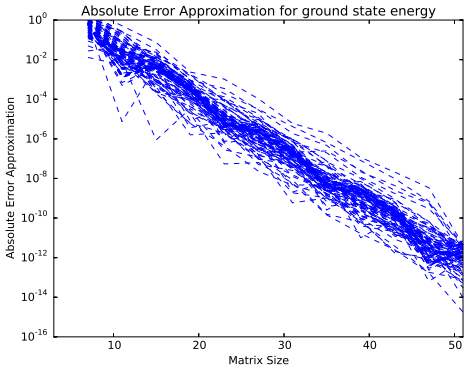


(a) $m = 1$

(b) $m = 2$



(c) $m = 3$



(d) $m = 4$

Figure 6.3: Application of the DESCM for 100 randomly generated potentials of the form $V(x) = \omega x^{2m} + \dfrac{\sum_{i=0}^{k} \lambda_i x^i}{1 + g_1 x + g_2 x^2 + g_3 x^3 + g_4 x^4}$. Figure (a) corresponds to $m = 1$. Figure (b) corresponds to $m = 2$. Figure (c) corresponds to $m = 3$. Figure (d) corresponds to $m = 4$.

Chapter 7

On the Computation of Eigenvalues of the Anharmonic Coulombic Potential

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Abstract.

In this work, we propose a method combining the Sinc collocation method with the double exponential transformation for computing the eigenvalues of the anharmonic Coulombic potential. We introduce a scaling factor that improves the convergence speed and the stability of the method. Further, we apply this method to Coulombic potentials leading to a highly efficient and accurate computation of its eigenvalues.

7.1 Introduction

The Coulombic anharmonic oscillator potential, which is given by $V(x) = \frac{a_{-2}}{x^2} + \frac{a_{-1}}{x} + \sum_{i=1}^{n} a_i x^i$, has been of considerable interest in the study of the Schrödinger equation. The potential describes the interaction between charged particles and consistently arises in physical applications. These applications include interactions in atomic, molecular and particle physics, and between nuclei in plasma [132, 143]. The study of the Schrödinger equation involves computation of the energy states, and many different methods have been proposed for accurate and efficient calculation of the energy eigenvalues [40,69,91, 109, 132]. In [40], the authors use the Hill determinant method to numerically evaluate the Coulomb potential in N dimensions. They initially transform the N dimension differential equation into a $(2N - 4)$ dimensional problem. This transformation produces the structure of a one dimensional Schrödinger equation with a spherically symmetric potential. The authors then reduce the dimension of the problem by transforming the Schrödinger equation into a radial differential equation, leading to numerical approximations of the energy eigenvalues. In [91], the authors use an appropriate ansatz to the wavefunction and the Hill determinant method to find energy eigenvalues for the Coulomb potential and the sextic oscillator problem. They also produce a relation between parameters leading to exactly solvable equations. However, the Hill determinant method presents several limitations, including a lack of convergence to higher order eigenvalues and the production of non physically realistic results [170]. In addition, the method does not account for an important aspect of the wavefunction, for instance, decay at the boundaries [170].

Conversely, the Riccati-Padé method has been used in the calculation of bound states and resonances in the Coulomb potential [69]. This method consists of transforming the Schrödinger equation into a Riccati type equation for the logarithmic derivative of the wavefunction. Analysis of the Riccati equation provides a deeper understanding of the overall nature of both the wavefunction and the energy eigenvalues. In [69], the method shows convergence towards eigenvalues of the Schrödinger equation for bounded and unbounded states. In a separate work [68], the Riccati-Padé method is combined with Hankel determinants to find resonance states of the Coulomb potential. While useful, the Riccati-Padé method can only produce bounds on the eigenvalues. These bounds can give quite good approximations of the energy eigenvalues, but can also be so large that they do not produce any meaningful information [72]. Achieving acceptable error bounds on the eigenvalues requires an increase in the dimension of the Hankel determinants. Further, the complexity of the method increases with the complexity of the potential. Finally, the method can also yield unwanted and unrealistic solutions [72].

The super symmetric quantum mechanic approach has also produced results with potentials of the form $V(x) = \frac{\alpha}{r} + \sum_{i=1} 4p_i r^i$. In [143], the authors solved the equation using supersymmetric quantum mechanics. Their results are mostly in agreement with exact values. Nevertheless, poor agreement seems to arise when the potential has multiple wells or roots. There has also been advancement in the combination of supersymmetric quantum mechanics and perturbation theory. In [132], a combination of these techniques to find exact solutions to the perturbed Coulomb potential is proposed. This method can be expanded to include many other potentials and their excited states.

However, the method requires constraints on the parameters of the potential and these constraints differ for different eigenvalues [132].

In [109], the Sinc collocation method (SCM) have been used in a combination with the single exponential (SE) transformation to compute the energy eigenvalues of the radial Schrödinger equation. The Sinc function and Sinc collocation method have been used extensively since their introduction to solve a variety of numerical problems [154, 155, 158]. The applications include numerical integration, linear and non-linear ordinary differential equations as well as partial differential equations [5, 6, 9, 37, 56–58, 83, 84, 153]. The single exponential Sinc collocation method (SESCM) have been shown to offer an exponential convergence rate and works well in the presence of singularities. The double exponential (DE) transform, introduced in 1974 [166], yields near optimal accuracy when using the trapezoidal rule in numerical integration [121,163]. Since the introduction of the DE transform, its effectiveness has been studied extensively [162,168]. While exponential convergence is produced using the SESCM, it has been shown that the double exponential transformation provides an improved numerical convergence [120, 129, 167]. It should be noted that the assumption for DE convergence is more severe than the one for SE. Given the fact that $\mathcal{F}_{DE} \subsetneq \mathcal{F}_{SE}$, where $\mathcal{F}_{SE}$ (respectively $\mathcal{F}_{DE}$) denotes the class of functions for which SE is suitable (respectively DE is suitable), there exist examples such that Sinc expansion with SE achieves its usual rate, whereas it does not with DE [129, 167]. However, in [129, 167], the authors present a theoretical convergence analysis for Sinc methods with DE for functions in $\mathcal{F}_{SE} \backslash \mathcal{F}_{DE}$ for which DE does not achieve its usual rate of $\mathcal{O}\left(e^{-\kappa_1 n/\log(\kappa_2 n)}\right)$, and they were able to prove that DE still works for these

functions with errors bounded by $\mathcal{O}\left(e^{-\kappa_3\sqrt{N}/\log(\kappa_4 N)}\right)$ which is slightly lower than the rate of SE; however, as stated in [129, 167] one can consider that there is almost no difference between the two transformations. This result also illustrates the great advantage of using DE over SE.

The combination of SCM with the DE transformation was used to compute eigenvalues of the anharmonic oscillator $V(x) = \sum_{i=1}^{n} a_i x^{2i}$ [83] and to Sturm-Liouville boundary value problems [84]. This method, referred to as the DESCM, is shown to be highly accurate, efficient and stable for computing the energy eigenvalues of the Schrödinger equation. In [83], an optimal mesh size for potentials with multiple wells was derived leading to a substantial improvement of the convergence of the method.

In this work, we provide a refinement for the DESCM and we apply the metod to the anharmonic Coulombic potential. The improved method is capable of dealing with a vast variety of potentials efficiently. The DESCM approximates the wavefunction with a series of weighted Sinc functions. By substituting the approximation into the Schrödinger equation, we obtain a generalized eigensystem where the generalized eigenvalues are approximations to the exact energy eigenvalues. We preform asymptotic analysis on the Schrödinger equation with the anharmonic Coulombic potential. We use the asymptotic solutions to produce optimized double exponential transformations. We also present a numerical scaling that improves both the numerical convergence and stability of the method. Finally, we compare the results of the refined DESCM with the SESCM to illustrate the superiority of the proposed method.

7.2 Definitions and properties

The sinc function is defined by the following expression:

$$\operatorname{sinc}(z) = \begin{cases} \dfrac{\sin(\pi z)}{\pi z} & \text{for} \quad z \in \mathbb{C}/\{0\} \\ 1 & \text{for} \quad z = 0. \end{cases} \tag{7.1}$$

For $k \in \mathbb{Z}$ and h a positive number, we define the Sinc function $S(k,h)(x)$ by:

$$S(j,h)(x) = \operatorname{sinc}\left(\frac{x - jh}{h}\right). \tag{7.2}$$

We also note the discrete orthogonality of the Sinc functions [158]. For every $k \in \mathbb{Z}$, we have:

$$S(j,h)(k\,h) = \begin{cases} 1 & \text{if} \quad k = j \\ 0 & \text{if} \quad k \neq j. \end{cases} \tag{7.3}$$

Definition 7.2.1. *[155, Chapter 1] Given a function v: $\mathbb{R} \to \mathbb{R}$ and any h positive, the Sinc expansion also known as the Whittaker Cardinal expansion of v is defined as:*

$$C(v,h)(x) = \sum_{j=-\infty}^{\infty} v(kh) S(j,h)(x). \tag{7.4}$$

The symmetric truncated Sinc expansion given by:

$$C_N(v,h)(x) = \sum_{j=-N}^{N} v(jh)\, S(j,h)(x) \quad \textit{with} \quad N \in \mathbb{N}. \tag{7.5}$$

In [155], Stenger proposed the following space of functions which are well suited to Sinc approximations.

Definition 7.2.2. *[155, Definition 3.1] Let* $0 < d < \frac{\pi}{2}$ *and consider the set* $\mathcal{D}_d$ *to be a strip of width* $2d$ *about the real axis defined as follows:*

$$\mathcal{D}_d = \left\{ z \in \mathbb{C} : |\Im(z)| < d < \frac{\pi}{2} \right\}. \tag{7.6}$$

We also define a rectangle in $\mathbb{C}$ *such that, for* $\varepsilon \in (0, 1)$*:*

$$\mathcal{D}_d(\varepsilon) = \{ z \in \mathbb{C} : |\Re(z)| < 1/\varepsilon,\ |\Im(z)| < d(1-\varepsilon) \}. \tag{7.7}$$

Let $\mathbf{B}_2(\mathcal{D}_d)$ *be the family of functions* g *that are analytic in* $\mathcal{D}_d$ *such that:*

$$\lim_{|x|\to\infty} \left(\int_{-d}^{d} |g(x+iy)|\,dy \right) = 0 \quad \textit{and} \quad \mathcal{N}_2(g, \mathcal{D}_d) := \lim_{\varepsilon \to 0} \left(\int_{\partial \mathcal{D}_d(\varepsilon)} |g(z)|^2 |dz| \right)^{\frac{1}{2}} < \infty. \tag{7.8}$$

An analysis of the error induced when approximating a function in the function space $\mathbf{B}_2(\mathcal{D}_d)$ using a Sinc expansion can be found in [155].

7.3 The double exponential Sinc-Collocation method

The Schrödinger equation with semi-infinite zero boundary conditions is given by:

$$\begin{aligned} \mathcal{H}\,\psi(x) &= E\,\psi(x) \quad \text{for} \quad 0 < x < \infty \\ \psi(0) &= \psi(\infty) = 0, \end{aligned} \tag{7.9}$$

where the Hamiltonian operator is given by:

$$\mathcal{H} = -\frac{d^2}{dx^2} + V(x), \tag{7.10}$$

and where $V(x)$ stands for the potential.

In [56], the authors proposed the following change of variable:

$$v(x) = \left(\sqrt{(\phi^{-1})'}\,\psi\right) \circ \phi(x), \tag{7.11}$$

where the conformal map $\phi(x)$ is defined according to the following definition.

Definition 7.3.1. *[56] Let Ω_d be a simply connected domain in the complex plane with boundary points a and b. Define a conformal map, ϕ^{-1}, from Ω_d onto the infinite strip $\mathcal{D}_d$ with $\phi^{-1}(a) = -\infty$ and $\phi^{-1}(b) = \infty$. Denote the inverse of ϕ^{-1} by ϕ.*

The proposed transformation (7.11) produces a symmetric discretized system when employing the Sinc collocation method on Sturm-Liouville problems.

Applying the transformation (7.11) to the Schrödinger equation (7.9) pro-

duces the following equation:

$$-v''(x) + \tilde{V}(x)v(x) = E\,(\phi'(x))^2 v(x) \quad \text{with} \quad \lim_{|x|\to\infty} v(x) = 0, \tag{7.12}$$

where:

$$\tilde{V}(x) = -\sqrt{\phi'(x)}\frac{d}{dx}\left(\frac{1}{\phi'(x)}\frac{d}{dx}\sqrt{\phi'(x)}\right) + (\phi'(x))^2\, V(\phi(x)). \tag{7.13}$$

We note that for analytic $V(x)$ the transformed differential equation has analytic coefficients. Therefore, basic ordinary differential equation theory assures us of the existence of an analytic solution.

To utilize the optimality of the double exponential transformation [163], we search for a conformal mapping $\phi(x)$ that will result in the eigenfunction $v(x)$ involved in (7.11) to decay double exponentially. The function $v(x)$ decays double exponentially if there exists positive constants A, β, γ such that for all $x \in \mathbb{R}$, we have:

$$|v(x)| \leq A \exp(\beta \exp(\gamma|x|)). \tag{7.14}$$

To approximate the solution using the Sinc collocation method, we use the truncated Sinc expansion (7.5) given by:

$$C_N(v,h)(x) = \sum_{j=-N}^{N} v_j\, S(j,h)(x) \quad \text{with} \quad v_j = v(jh), \tag{7.15}$$

and h is the mesh size and $N \in \mathbb{N}$. In this case, the $2N+1$ function values $v_j = v(jh)$ are unknown. Consequently, we will proceed to find $2N+1$ equations to solve for these unknown values.

Inserting the truncated Sinc expansion (7.5) into the differential equation (7.12) and evaluating at the collocation points $x_k = kh$, $k = -N, \ldots, N$ leads to the following $2N+1$ equations:

$$\sum_{j=-N}^{N} \left[-\frac{1}{h^2}\delta_{j,k}^{(2)} + \tilde{V}(kh)\delta_{j,k}^{(0)} \right] v_j = \mathcal{E} \sum_{j=-N}^{N} \left[(\phi'(jh))^2 \delta_{j,k}^{(0)} \right] v_j \quad \text{for} \quad k = -N, \ldots, N, \tag{7.16}$$

where:

$$\delta_{j,k}^{(2)} = \begin{cases} -\dfrac{\pi^2}{3} & \text{if} \quad j = k \\ \dfrac{(-2)(-1)^{k-j}}{(k-j)^2} & \text{if} \quad j \neq k \end{cases} \qquad \text{and} \qquad \delta_{j,k}^{(0)} = \begin{cases} 1 & \text{if} \quad j = k \\ 0 & \text{if} \quad j \neq k. \end{cases} \tag{7.17}$$

In (7.16), the value $\mathcal{E}$ is an approximation of the exact energy eigenvalue E of the system (7.12).

Equation (7.16) can be re-writen in a matrix form as follows:

$$\mathbf{A}\mathbf{v} = \mathcal{E}\,\mathbf{D^2}\,\mathbf{v} \quad \Rightarrow \quad (\mathbf{A} - \mathcal{E}\,\mathbf{D^2})\,\mathbf{v} = \mathbf{0}, \tag{7.18}$$

where $\mathbf{v} = [v_{-N}, ..., v_N]^T$ and the matrix $\mathbf{A}$ and the diagonal matrix $\mathbf{D^2}$ are given by:

$$\mathbf{A} = \left[-\frac{1}{h^2}\delta_{j,k}^{(2)} + \tilde{V}(jh)\delta_{j,k}^{(0)} \right]_{j,k=-N,\ldots,N} \qquad \text{and} \qquad \mathbf{D^2} = \left[(\phi'(jh))^2 \delta_{j,k}^{(0)} \right]_{j,k=-N,\ldots,N}. \tag{7.19}$$

As can be seen from (7.18), the eigenfunctions and eigenvalues of the differential equation (7.12) can be approximated by the generalized eigenvalue problem (7.18).

Now, let us denote by $W(x)$ the Lambert W function which is defined as follows:

Definition 7.3.2. *[46, Equation (1.5)]*

The Lambert W function denoted by $W(x)$ is defined implicitly by the solution of the following equation:

$$z = W(x)e^{W(x)}. \tag{7.20}$$

In our case, we restrict the Lambert W function to be real valued with the additional constraint $W(x) \geq -1$. This additional constraint forces the Lambert W function to be single-valued. This branch is commonly denoted by $W_0(x)$. For the numerical evaluation of the Lambert W function, we refer the readers to [46].

Theorem 7.3.3. *[83] Let $(v(x), E)$ be an eigenpair of the transformed Schrödinger equation given by:*

$$-v''(x) + \tilde{V}(x)v(x) = E(\phi'(x))^2 v(x) \quad \textit{with} \quad \lim_{|x|\to\infty} v(x) = 0, \tag{7.21}$$

where $\tilde{V}(x) = -\sqrt{\phi'(x)}\frac{d}{dx}\left(\frac{1}{\phi'(x)}\frac{d}{dx}\sqrt{\phi'(x)}\right) + (\phi'(x))^2\, V(\phi(x))$. If

1. *$\exists\, A, \beta, \gamma > 0$ such that: $|v(x)| \leq A\exp\left(-\beta\exp(\gamma|x|)\right)$,*
2. *$v(x) \in \mathbf{B}_2(\mathcal{D}_d)$ with $d \leq \dfrac{\pi}{2\gamma}$,*
3. *$\exists\, q > 0$ such that $\tilde{V}(x) \geq q^{-1}$,*
4. *The mesh size h is chosen such that $h = \dfrac{W(\pi d\gamma N/\beta)}{\gamma N}$,*

where $W(z)$ is the Lambert-W function, then the eigenvalue $\mathcal{E}$ obtained by solving the system (7.18) *satisfies the following asympotic bound with respect to E:*

$$|\mathcal{E} - E| = O\left[\sqrt{qE}\left(\frac{N^{\frac{5}{2}}}{\log(N)}\right)\exp\left(-\frac{\pi d\gamma N}{\log(\pi d\gamma N/\beta)}\right)\right] \quad as \quad N \to \infty. \tag{7.22}$$

Since this process can be done for any arbitrary eigenpair $\{(v_n(x), E_n)\}_n$, it is clear from Theorem 7.3.3 that every eigenvalue E will satisfy the error bound for the appropriate sequence of generalized eigenvalues $\mathcal{E}$.

7.4 The Coulombic anharmonic potential

The Coulombic anharmonic potential $V(x)$ is given by:

$$\begin{aligned} V(x) &= \frac{a_{-2}}{x^2} + \frac{a_{-1}}{x} + \sum_{i=1}^{n} a_i x^i \\ &= \sum_{i=-2}^{n} a_i x^i \qquad \text{with} \quad a_{-2} > 0,\ a_0 = 0 \ \text{ and } \ a_n > 0. \end{aligned} \tag{7.23}$$

The negative powers of x and the singularity at $x = 0$ are some of the defining features of the anharmonic Coulombic potential. To utilize the Sinc collocation method to compute eigenvalues of Coulombic potential, we search for an appropriate double exponential transform as defined in Definition 7.3.1. To find such a transformation, we must first perform an asymptotic analysis of the differential equation (7.9).

As $x \to \infty$, the potential is dominated by the term x^n term and our

differential equation becomes:

$$-\psi''(x) + a_n x^n \psi(x) \sim 0 \quad \text{as} \quad x \to \infty. \tag{7.24}$$

Making the substitution $\psi(x) = e^{S(x)}$ where $S(x)$ is such that $S''(x) = o(S'(x)^2)$ as $x \to \infty$ leads to:

$$-S'(x)^2 + a_n x^n \sim 0 \quad \text{as} \quad x \to \infty. \tag{7.25}$$

Solving this equation and taking the negative root to satisfy the boundary conditions, we obtain:

$$S(x) \sim -\frac{2\sqrt{a_n}}{n+2} x^{\frac{n+2}{2}} \quad \text{as} \quad x \to \infty. \tag{7.26}$$

Hence, we deduce the following bound for our wavefunction:

$$\psi(x) = O\left(\exp\left[-\frac{2\sqrt{a_n}}{n+2}\, x^{\frac{n+2}{2}}\right]\right) \quad \text{as} \quad x \to \infty. \tag{7.27}$$

Conversely, as $x \to 0^+$ the Coulomb potential is dominated by x^{-2} term. We see that $x = 0$ is a regular singular point and the equation requires the use of a Frobenius series type solutions. The solution is of the form $\psi(x) = O(x^r)$, where r is a solution of the indicial equation:

$$-r(r-1) + a_{-2} = 0 \quad \Longrightarrow \quad r = \frac{1 \pm \sqrt{1 + 4a_{-2}}}{2}. \tag{7.28}$$

The boundary condition $\psi(0) = 0$ leads us to reject the negative root,

leading us to the following asymptotic bound as $x \to 0^+$:

$$\psi(x) = O\left(x^r\right) \quad \text{with} \quad r = \frac{1 + \sqrt{1 + 4a_{-2}}}{2}. \tag{7.29}$$

Finally, we notice that the wavefunction exhibits exponential decay at infinity and algebraic decay at zero. Now, we search for a transformation $\phi(x)$ that satisfies Definition 7.3.1 and produces double exponential decay at infinities. We begin by using the transformation proposed in [168]:

$$\phi(x) = \log\left[e^{\sinh(x)} + 1\right] \sim \begin{cases} \dfrac{e^x}{2} & \text{as} \quad x \to \infty \\ \exp\left[-\dfrac{e^{-x}}{2}\right] & \text{as} \quad x \to -\infty. \end{cases} \tag{7.30}$$

From the definition of $v(x)$ given by (7.11), our asymptotic bounds in (7.27) and (7.29), as well as the asymptotic behavior of the conformal map in (7.30), we can deduce the following asymptotic bounds for $v(x)$:

$$v(x) = \begin{cases} O\left(\exp\left[-\dfrac{\sqrt{a_n}}{(n+2)2^{n/2}} \exp\left(\frac{n+2}{2}x\right)\right]\right) & \text{as} \quad x \to \infty \\ O\left(\exp\left[-\dfrac{1 + \sqrt{1 + 4a_{-2}}}{4} \exp\left(-x\right)\right]\right) & \text{as} \quad x \to -\infty. \end{cases} \tag{7.31}$$

From (7.31), we notice that the conformal map (7.30) indeed leads to a double exponential decaying function $v(x)$. In order for $v(x)$ to belong to the function space $\mathbf{B}_2(\mathcal{D}_d)$ as defined in Definition 7.2.2, given its asymptotic behavior (7.31), proper attention must be given to the quantity $\mathcal{N}_2(g, \mathcal{D}_d)$. For $\mathcal{N}_2(g, \mathcal{D}_d)$ to remain bounded, we require $\gamma = \max\left\{\dfrac{n+2}{2}, 1\right\} = \dfrac{n+2}{2}$.

7.5 Numerical discussion

We use the DESCM to find energy eigenvalues of the anharmonic Coulomb potential. The codes are written in double precision using the programming language MATLAB [114] and are available upon request. A double-precision floating-point format is a computer number format that occupies 8 bytes (64 bits) in computer memory. In general, this corresponds to about 15-17 significant decimal digits on average. In the Figures bellow, the saturation effect observed in all Figures is merely a consequence of this computer number format resulting from rounding errors in addition to numerical instabilities rcaused by the increasing condition numbers of the matrices involved in the DESCM. The matrices $\mathbf{A}$ and $\mathbf{D}^2$ are constructed using (7.19).

To evaluate the effectiveness of the DESCM, we define the relative error between known eigenvalues E and numerical eigenvalues $\mathcal{E}$ as:

$$\text{Relative Error} = \frac{|E - \mathcal{E}|}{|E|}. \tag{7.32}$$

When moving to higher order energy eigenvalues or potentials without known analytic solutions, we use the following aproximation to the relative error:

$$\text{Relative Error Approximation} = \frac{|\mathcal{E}_i(N+1) - \mathcal{E}_i(N)|}{|\mathcal{E}_i(N+1)|}, \tag{7.33}$$

where $\mathcal{E}_i(N+1)$ denotes the $(N+1)$th approximation of the ith energy eigenvalue.

To illustrate the convergence of our method, we compute the eigenvalues of

potentials that have known analytic solutions [40, 109]. These potentials are:

$$\begin{array}{lcll} V_1(x) & = & \frac{2}{x^2} - \frac{16}{x} + 2x + \frac{x^2}{16} & \Longrightarrow \quad E_0 = -\frac{59}{4} \\ V_2(x) & = & \frac{6}{x^2} - \frac{24}{x} + 2x + \frac{x^2}{16} & \Longrightarrow \quad E_0 = -\frac{57}{4} \\ V_3(x) & = & \frac{15}{4x^2} - \frac{20}{x} + 2x + \frac{x^2}{16} & \Longrightarrow \quad E_0 = -\frac{58}{4} \\ V_4(x) & = & \frac{35}{4x^2} - \frac{28}{x} + 2x + \frac{x^2}{16} & \Longrightarrow \quad E_0 = -14 \\ V_5(x) & = & \frac{2}{x^2} + x^2 & \Longrightarrow \quad E_0 = 5 \\ V_6(x) & = & \frac{3}{4x^2} + x^2 & \Longrightarrow \quad E_0 = 4 \end{array} \tag{7.34}$$

7.5.1 Refinement of the DESCM

We notice that we have a singularity at the left end point of the potential at $x = 0$. Following the approach detailed in [119], we search for a general transformation of the form:

$$\phi(x) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right] \quad \text{with} \quad \alpha_i > 0 \quad \text{for} \quad i = 1, 2, 3, 4. \tag{7.35}$$

We find that this transformation is ideal as it produces double exponential decay at both boundaries and is suitable to Sinc expansion. In fact, we have the following asymptotic behavior at both infinities:

$$\log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right] \sim \begin{cases} \alpha_1 e^{\alpha_2 x} & \text{as} \quad x \to \infty \\ \exp\left[-\alpha_3 e^{-\alpha_4 x}\right] & \text{as} \quad x \to -\infty. \end{cases} \tag{7.36}$$

From the definition of $v(x)$ given by (7.11), our asymptotic bounds in

(7.27) and (7.29) in addition to the asymptotic behavior of the conformal map in (7.36), we can deduce the following asymptotic bounds for $v(x)$:

$$v(x) = \begin{cases} O\left(\exp\left[-\dfrac{2\sqrt{a_n}\alpha_1^{n+2}}{n+2}\,\exp\left(\dfrac{\alpha_2(n+2)}{2}x\right)\right]\right) & \text{as} \quad x \to \infty \\ O\left(\exp\left[-\dfrac{(1+\sqrt{1+4a_{-2}})\alpha_3}{2}\exp\left(-\alpha_4 x\right)\right]\right) & \text{as} \quad x \to -\infty. \end{cases} \tag{7.37}$$

Similarly to what was mentioned before, by taking $\gamma = \max\left\{\dfrac{\alpha_2(n+2)}{2}, \alpha_4\right\}$ and $d = \dfrac{\pi}{2\gamma}$, we ensure that $v(x) \in \mathbf{B}_2(\mathcal{D}_d)$ and is well suited to a Sinc approximation.

The matrices involved in the calculation become ill-conditioned. This is to be expected as the Schrödinger equation produces eigenvalues that grow unboundedly. We notice that the numerical blow ups correspond to the increasing condition number.

As our transformation $\phi(x) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right]$ includes four arbitrary positive parameters α_1, α_2, α_3 and α_4, we have more freedom in tailoring the transformation to our potential. We define our optimal parameters to be those that increase our numerical stability. Our potential has an algebraic singularity at $x = 0$ resulting in a significant numerical instability.

We considered the potential $V_1(x)$ and define the optimal parameter set $\{\alpha_i\}$ as the parameter set that maximized the number of convergent eigenvalues found for $N = 50$ collocation points. Where two or more parameter sets gave the same number of convergent eigenvalues, we chose the parameter set requiring the least number of collocation points to converge to the ground

state eigenvalue. We performed a systematic search of parameter space. We began the search with $\alpha_1 = \alpha_3 = 0.5$ and $\alpha_2 = \alpha_4 = 1$. We began our search of parameter space by incrementing parameter values by 0.1. This led to a first optimal parameter set of $\alpha_1 = 1, \alpha_2 = 1.3, \alpha_3 = 1.2$ and $\alpha_4 = 0.9$.

We then iterated this process, taking the first optimal parameter set as an initial guess and taking steps of 0.01 in parameter space.

We anticipate that further optimization of the transformation parameters will produce further numerical stability. However, finding the optimal combination is quite costly, as we are optimizing a non-linear function with 4 input values. Finding an efficient way to calculate the optimal parameters remains an open question. In our calculations, we used $\alpha_1 = 1.05, \alpha_2 = 1.30, \alpha_3 = 1.20$ and $\alpha_4 = 0.94$. As can be seen from Figure 7.2, implementing the generalized transformation improves considerably the numerical stability of the method.

To improve the stability of the method, we introduce a scaling factor leading to a considerable increase in convergence.

Corollary 7.5.1. *Scaling the transformed energy eigenvalue problem using $x = \tau y$ with $\tau \neq 0$ will transform the computed eigenvalues by $E = \dfrac{\widetilde{E}}{\tau^2}$ where E is the original eigenvalue and $\widetilde{E}$ is the energy eigenvalue of the scaled problem.*

Proof. Consider the potential $V(x) = \sum_{j=-i}^{n} a_j x^j$ and the vector $\mathbf{a} := [a_{-i}, a_{-i+1}, ..., a_n]$ consisting of the coefficients of the potential. Consider also the vector $\mathbf{x} = [x^{-i}, x^{-i+1}, ..., x^n]$. Recognize that the energy eigenvalues are functions of the coefficients of the potential. We can thus write $E(\mathbf{a})$.

We write the problem in the following form:

$$-\psi''(x) + (\mathbf{a}\cdot\mathbf{x})\psi(x) = E(\mathbf{a})\psi(x). \tag{7.38}$$

Implementing the change of variable $x = \tau y$ with $\tau \in \mathbb{R}$ and $\tau \neq 0$, and using:

$$\frac{d^2}{dx^2}\psi(\tau y) = \frac{1}{\tau^2}\frac{d^2}{dy^2}\psi(y), \tag{7.39}$$

leads to:

$$\frac{\psi''(\tau y)}{\tau^2} + (\mathbf{b}\cdot\mathbf{y})\psi(\tau y) = E(\mathbf{b})\psi(\tau y), \tag{7.40}$$

where $\mathbf{b} = [\tau^{-i}a_i, \tau^{-i+1}a_{-i+1}..., \tau^n a_n]$ and $\mathbf{y} = [y^{-i}, y^{-i+1}, ..., y^n]$.

If we let $\mathbf{c} = [\tau^{-i+2}a_i, \tau^{-i+2}a_{-i+1}...\tau^{n+2}a_n]$, then (7.40) becomes:

$$-\psi''(\tau y) + \mathbf{c}\cdot\mathbf{y} = E(\mathbf{c})\psi(\tau y) = \tau^2 E(\mathbf{a})\psi(x). \tag{7.41}$$

We can recover the energy eigenvalues corresponding to a_j by noticing that:

$$E(\mathbf{a}) = \frac{E(\mathbf{c})}{\tau^2}, \tag{7.42}$$

as desired. □

The scaling vastly improves the number of convergent eigenvalues found by the method. We fixed the matrix size at 201×201, and computed the number of convergent eigenvalues with and without the scaling factor for each transformation and we report the substantial increase in the number of convergent eigenvalues found as can be seen from Table 7.1. In Figure 7.2, we used 1001×1001 matrix illustrating the increased stability of the method when the

scaling factor is used.

In Table 7.1, we calculate the number of convergent eigenvalues in 100 iterations for the potentials V_1, V_2, V_3 and V_4. For higher order eigenvalues, where the analytic solution is not known, we use the relative error threshold of $5 \cdot 10^{-12}$. We consider a higher order eigenvalue to be found if the relative error approximation is within the relative error threshold. Our choice of relative error threshold is influenced by the accuracy of the eigensolvers in Matlab as well as the presence of round off error. In this Table, the improvement resulting from utilizing the generalized transformation and the introduction of the scaling factor is obvious.

In Table 7.2, we plot the evolution of the convergence for increasing matrix size for the potential V_1. We see convergence towards the known ground state eigenvalue as well as the convergence towards the first and second excited states.

However, we would like to be able to compute arbitrarily many energy eigenvalues. This will require dealing with matrices of increasingly large size. Further, these matrices become more and more ill-conditioned as they grow. In fact, for the potential V_1, when using the transformation $\phi(x) = \log\left[e^{\sinh(x)} + 1\right]$, numerical blow ups occur for a 141×141 matrix and higher. We plot the condition number of the generalized eigenvalue problem, and notice that the numerical blow ups occur as the condition number of the eigenvalue problem passes 10^{16}. This increase in the condition number is to be expected as the energy eigenvalues of the system grow without bound. The scaling factor presents a simple way to improve stability of the method and is evidenced in Figure 7.2. The Figure shows the improved convergence of the

transformation $\phi_2(x) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right]$ when compared with $\phi_1(x) = \log\left[e^{\sinh(x)} + 1\right]$. We also see the vastly improved stability of the scaled transformation.

The refined DESCM provides increased convergence speed when compared with the SESCM presented in [109]. To compare the two methods, we implement the SESCM following the procedure in [109]. The improved convergence speed offered by the refined DESCM is predicted in theoretical work done by Sugihara and others [121, 163, 168]. As we have shown that the solution of the Schrödinger equation is well suited to the DESCM, our results are remarkable. The convergence of both methods is plotted in Figure 7.1. For the potentials V_5 and V_6, we utilize the same single exponential transformation and step size as proposed in [109]. Moreover, we show that the refinements presented in this work also improve the convergence of the SESCM.

7.6 Conclusion

In this paper, we apply the DESCM method to the Schrödinger equation with an anharmonic Coulombic potential. This potential presents several numerical difficulties, including a singularity at $x = 0$. The DESCM proves to be a powerful choice for computing the energy eigenvalues and produces convergence towards known eigenvalues quickly. Further, we show that for the Coulombic potential, the double exponential transformation is the optimal transformation for an accurate computation of the eigenvalues. Further, we introduced an improvement of the numerical stability as well as the convergence of the DESCM. The scaling factor that utilizes the symmetry of the eigenvalues is,

to our knowledge, a novel suggestion that vastly improves stability and increases convergence. Our numerical results imply that the instability is due to the problem becoming ill-conditioned for large matrix sizes. Future work will include implementing preconditioning methods in the generalized eigenvalue problem as well as exploring other methods of increasing stability.

7.7 Numerical tables and figures

Table 7.1: The numberof convergent eigenvalues computed in 100 iterations for different transformations. $\phi_1(t) = \log(\exp(\sinh(t)) + 1)$, $\phi_2(t) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right]$. The τ value denotes the scaling factor used in the calculations.

Potential	$\phi_1(t)$ $\tau = 1$	$\phi_1(t)$ $\tau = 1.75$	$\phi_2(t)$ $\tau = 1$	$\phi_2(t)$ $\tau = 1.75$
$V_1(x)$	8	22	22	36
$V_2(x)$	9	23	20	35
$V_3(x)$	8	20	19	37
$V_4(x)$	9	22	20	34

Table 7.2: Numerical calculations for the ground states and first two excited states of the potential $V_1(x)$ Here we used the potential ϕ_2 with the scaling factor $\tau = 1.00$.

N	$\tilde{E}_0(N)$	$\tilde{E}_1(N)$	$\tilde{E}_2(N)$
10	-14.7499998222764	-4.09661939808125	1.13533983977096
15	-14.7499999935935	-4.09661597228020	1.13571953379622
20	-14.7499999989570	-4.09661597504977	1.13571957570939
25	-14.7499999997938	-4.09661597544138	1.13571957544272
30	-14.7499999999506	-4.09661597551624	1.13571957539198
35	-14.7499999999867	-4.09661597553405	1.13571957537878
40	-14.7499999999960	-4.09661597553543	1.13571957537729
45	-14.7500000000008	-4.09661597553923	1.13571957537739
50	-14.7499999999961	-4.09661597554020	1.13571957537189

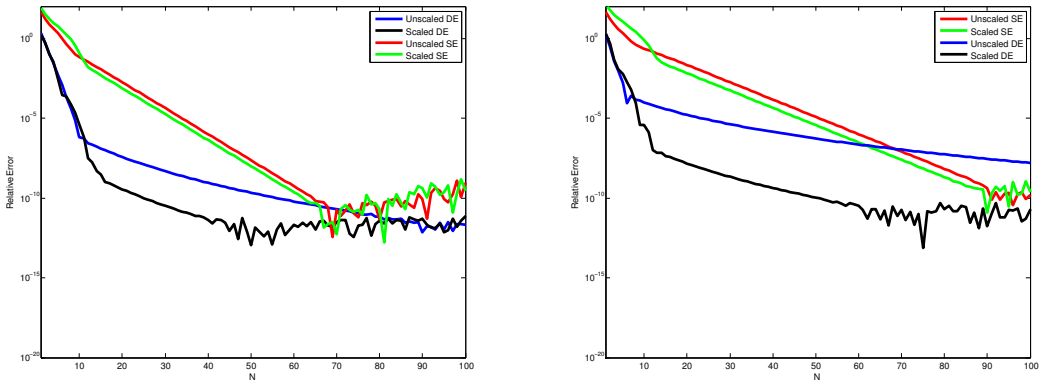

Figure 7.1: Comparison of the DESCM and the SESCM. (a) represents the convergence of the DESCM and the SESCM towards known eigenvalues of the potential V_5. (b) represents the convergence of the DESCM and the SESCM towards the eigenvalues of the potential V_6. The scaled plots correspond to the convergence diagrams using the scaling factor τ. (a) uses a scaling factor of $\tau = 0.75$. (b) uses a scaling factor of $\tau = 0.55$.

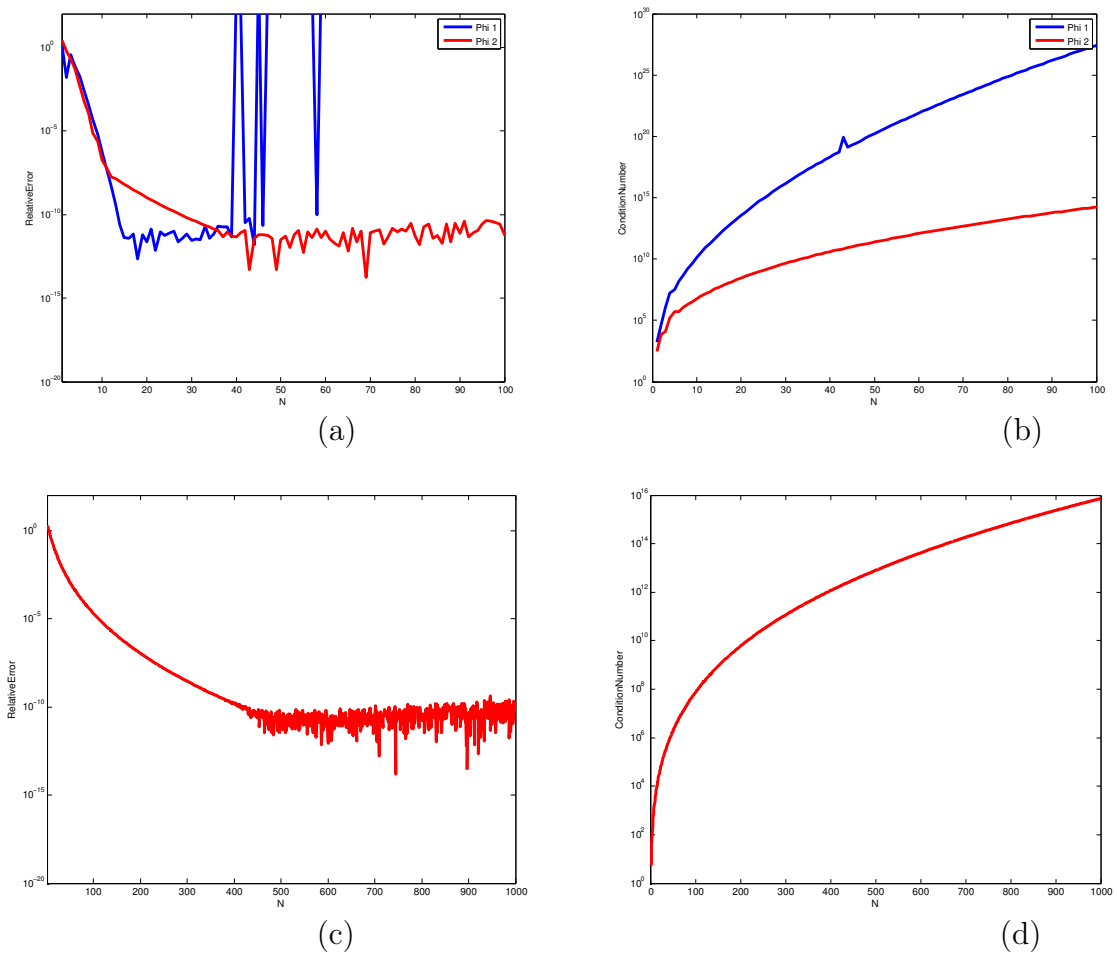

Figure 7.2: The improved numerical stability of the DESCM for the potential V_1. (a) shows the convergence of the method with $\phi_1(x) = \log\left[e^{\sinh(x)} + 1\right]$ and $\phi_2(x) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right]$ over 100 iterations. (b) compares the condition numbers of the different transformation for the generalized eigenvalue problem. (c) shows the convergence and stability of the generalized transformation following the introduction of a scaling factor $\tau = 3.00$ over 1000 iterations. (d) shows the condition number of the scaled generalized transformation.

Chapter 8

Concluding Remarks

In this thesis work, we investigated the solutions of the Schrödinger equation in one dimension. Starting with asymptotic and WKB methods, we proposed an algorithm for the evaluation of the energy eigenvalues of simple anharmonic potentials. We derived an asymptotic expansion for the energy eigenvalues of anharmonic oscillators for potentials of the form $V(x) = \kappa\, x^{2q} + \omega\, x^2$ for $q = 2, 3, \ldots$ using the WKB approach. This leads to an asymptotic series relating the energy levels to their corresponding energy values. Using series reversion theory, we reverted this series to obtain an analytic expression for the energy values in terms of their corresponding energy levels. This was significantly more efficient as it only required the summation of a series for different values of n eliminating the need for a root-finding method. Despite the success of this method, more complicated potentials could not be tackled efficiently using WKB methods.

Moving on the Sinc-collocation method, we were able to achieve much higher accuracy for the resolution of a much broader class of anharmonic po-

tentials. However, to establish the convergence of the Sinc-collocation method with a double exponential transformation for the Schrödinger equation, we tackled a more general differential eigenvalue problem: the Sturm-Liouville eigenvalue problems. Studying the convergence properties of this equation, we found that the DESCM achieved an accuracy of $O\left(\exp\left(-\kappa N/\log(N)\right)\right)$ for some $\kappa > 0$ and where N is proportional to the number of collocation points involved in the DESCM.

After establishing the convergence of the DESCM, we retackled the classical anharmonic potentials of the form:

$$V(x) = \sum_{i=1}^{m} c_i x^{2i}, \qquad m > 2, \tag{8.1}$$

achieving unprecedented accuracy for a wide variety of coefficients c_i. Moreover, we proposed an alternate method for computing an optimal mesh size h in the DESCM when these types of potentials were highly oscillatory.

Upon studying the matrices involved in the DESCM when working with potentials of the form in (8.1), we realized that an added symmetry was present when the potentials where even. In fact, the matrices of the DESCM are centrosymmetric when the potentials were even. This realization lead us to discover that this symmetry was intrisincly linked to the commutativity of the Sturm-Liouville differential operator with the parity operator. Additionally, this discovery lead us to an improved algorithm which reduces the computational complexity of the DESCM by half.

The potentials in (8.1) are relatively well behaved since they do not have any singularities on the real line or the complex plane. As such, we decided to

tackle a more general type of rational potential of the form:

$$V(x) = \omega x^{2m} + \frac{\sum_{i=0}^{k} \lambda_i x^i}{1 + \sum_{i=1}^{2l} g_i x^i} \qquad \text{with} \quad k - 2l < 2m. \tag{8.2}$$

The position of the complex singularties present in (8.2) with respect to the real line influence the convergence of the DESCM. To accelerate the convergence for these types of potentials, we use tailored double exponential transformation which move these singluarites away from the real line. As such, an optimal convergence of the DESCM is achieved. We tested these tailored transformations on a large variety of randomly generated potentials and achieved an unprecendeted accuracy for all of them.

Lastly, we applied the DESCM to Coulombic potentials of the form:

$$V(x) = \sum_{i=-2}^{n} a_i x^i. \tag{8.3}$$

The singularity at the origin, presented some numerical difficulties in computing the eigenvalues of such a potential. By using a scaling factor, we wer able to reduce the condition number of the resulting matrices, leading to a better convergence.

For future work, it would be interesting to apply the DESCM to the 2-dimensional Schrödinger equation:

$$[-\nabla^2 + V(x,y)]\psi(x,y) = E\psi(x,y), \quad (x,y) \in \Omega \subseteq \mathbb{R}^2 \quad \text{with} \quad \psi(x,y)|_{\partial\Omega} = 0 \tag{8.4}$$

Complications might arise when trying to identify the asympotic behaviour of the wave function $\psi(x, y)$ at the border of its domain Ω in two dimensions. This information would be important when trying to identify the optimal conformal mappings given any potential $V(x, y)$.

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