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ORIGINAL PAPER

On the Computation of Eigenvalues of the Anharmonic Coulombic Potential

Tyler Cassidy[1] · **Philippe Gaudreau**[1] · **Hassan Safouhi**[1]

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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 the eigenvalues.

Keywords Coulombic anharmonic potentials · Schrödinger equation · Sinc collocation method · Double exponential transformation

Mathematics Subject Classification 65L10 · 65L20

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 [1,2]. The study

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✉ Hassan Safouhi
hassan.safouhi@ualberta.ca

[1] Mathematical Section, Campus Saint-Jean, University of Alberta, 8406, 91 Street, Edmonton, AB T6C 4G9, Canada

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 [2–6]. In [3], 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 [4], the authors use an appropriate wavefunction ansatz 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 [7]. In addition, the method does not account for an important aspect of the wavefunction, for instance, decay at the boundaries [7].

Conversely, the Riccati-Padé method has been used in the calculation of bound states and resonances in the Coulomb potential [5]. 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 [5], the method shows convergence towards eigenvalues of the Schrödinger equation for bounded and unbounded states. In a separate work [8], 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 [9]. 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 [9].

The super symmetric quantum mechanic approach has also produced results with potentials of the form $V(x) = \frac{\alpha}{r} + \sum_{i=1} 4 p_i r^i$. In [1], 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 [2], 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 [2].

In [6], the Sinc collocation method (SCM) has 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 [10–12]. The applications include numerical integration, linear and non-linear ordinary dif-

ferential equations as well as partial differential equations [13,14,16–23]. The single exponential Sinc collocation method (SESCM) has been shown to offer an exponential convergence rate and works well in the presence of singularities. The double exponential (DE) transform, introduced in 1974 [24], yields near optimal accuracy when using the trapezoidal rule in numerical integration [25,26]. Since the introduction of the DE transform, its effectiveness has been studied extensively [27,28]. While exponential convergence is produced using the SESCM, it has been shown that the double exponential transformation provides an improved numerical convergence [29–31]. It should be noted that the assumption for DE convergence is stronger 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 [30,31]. However, in [30,31], 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 [30,31] 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 $V(x) = \sum_{i=1}^{n} a_i x^{2i}$ [13] and to Sturm–Liouville boundary value problems [14]. 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 [13], 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 method 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.

2 Definitions and properties

The sinc function is defined by the following expression:

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

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

$$S(k, h)(x) = \operatorname{sinc}\left(\frac{x - kh}{h}\right). \tag{2}$$

We also note the discrete orthogonality of the Sinc functions [12]. For every $j \in \mathbb{Z}$, we have:

$$S(k, h)(j\,h) = \begin{cases} 1 & \text{if } \ k = j \\ 0 & \text{if } \ k \neq j. \end{cases} \tag{3}$$

Definition 2.1 [11, Chapter 1] Given a function $v\colon \mathbb{R} \to \mathbb{R}$ and any h positive, the Sinc expansion, also known as the Whittaker Cardinal expansion, of v is defined as:

$$C(v, h)(x) = \sum_{k=-\infty}^{\infty} v(kh) S(j, h)(x). \tag{4}$$

The symmetric truncated Sinc expansion given by:

$$C_N(v, h)(x) = \sum_{k=-N}^{N} v(kh)\, S(k, h)(x) \quad \text{with} \quad N \in \mathbb{N}. \tag{5}$$

In [11], Stenger proposed the following space of functions which are well suited to Sinc approximations.

Definition 2.2 [11, 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:

$$\mathcal{D}_d = \left\{ z \in \mathbb{C} : |\Im(z)| < d < \frac{\pi}{2} \right\}. \tag{6}$$

We also define a rectangle in $\mathbb{C}$ such that, for $\varepsilon \in (0, 1)$:

$$\mathcal{D}_d(\varepsilon) = \{ z \in \mathbb{C} : |\Re(z)| < 1/\varepsilon, \ \ |\Im(z)| < d(1 - \varepsilon) \}. \tag{7}$$

Let $\mathbf{B}_2(\mathcal{D}_d)$ be the family of functions g that are analytic in $\mathcal{D}_d$ such that:

$$\lim_{|x| \to \infty} \left(\int_{-d}^{d} |g(x + iy)| \mathrm{d}y \right) = 0 \quad \text{and} \quad \mathcal{N}_2(g, \mathcal{D}_d) := \lim_{\varepsilon \to 0} \left(\int_{\partial \mathcal{D}_d(\varepsilon)} |g(z)|^2 |dz| \right)^{\frac{1}{2}} < \infty. \tag{8}$$

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 [11].

3 The double exponential Sinc-collocation method

The Schrödinger equation with semi-infinite zero boundary conditions is given by:

$$\begin{aligned} \mathcal{H}\,\psi(x) &= E\,\psi(x) \quad \text{for} \quad 0 < x < \infty \\ \psi(0) &= \psi(\infty) = 0, \end{aligned} \tag{9}$$

where the Hamiltonian operator is given by:

$$\mathcal{H} = -\frac{d^2}{dx^2} + V(x), \tag{10}$$

and where $V(x)$ stands for the potential.

In [23], the authors proposed the following change of variable:

$$v(x) = \left(\sqrt{(\phi^{-1})'}\,\psi\right) \circ \phi(x), \tag{11}$$

where the conformal map $\phi(x)$ is defined according to the following definition.

Definition 3.1 [23] 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 (11) produces a symmetric discretized system when employing the Sinc collocation method on Sturm–Liouville problems.

Applying the transformation (11) to the Schrödinger equation (9) produces the following equation:

$$-v''(x) + \tilde{V}(x)v(x) = E\,(\phi'(x))^2 v(x) \quad \text{with} \quad \lim_{|x|\to\infty} v(x) = 0, \tag{12}$$

where:

$$\tilde{V}(x) = -\sqrt{\phi'(x)}\,\frac{d}{dx}\left(\frac{1}{\phi'(x)}\,\frac{d}{dx}\sqrt{\phi'(x)}\right) + (\phi'(x))^2\,V(\phi(x)). \tag{13}$$

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 [26], we search for a conformal mapping $\phi(x)$ that will result in the eigenfunction $v(x)$ involved in (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:

$$|v(x)| \le A \exp(-\beta \exp(\gamma|x|)). \tag{14}$$

To approximate the solution using the Sinc collocation method, we use the truncated Sinc expansion (5) given by:

$$C_N(v,h)(x) = \sum_{k=-N}^{N} v_k\, S(k,h)(x) \quad \text{with} \quad v_k = v(kh), \tag{15}$$

and h is the mesh size and $N \in \mathbb{N}$. In this case, the $2N+1$ function values $v_k = v(kh)$ are unknown. Consequently, we will proceed to find $2N+1$ equations to solve for these unknown values.

Inserting the truncated Sinc expansion (5) into the differential equation (12) and evaluating at the collocation points $x_j = jh$, $j = -N, \ldots, N$ leads to the following $2N+1$ equations:

$$\sum_{k=-N}^{N} \left[-\frac{1}{h^2}\delta_{j,k}^{(2)} + \tilde{V}(jh)\delta_{j,k}^{(0)} \right] v_k = \mathcal{E} \sum_{k=-N}^{N} \left[(\phi'(jh))^2 \delta_{j,k}^{(0)} \right] v_k \quad \text{for} \quad j = -N, \ldots, N, \tag{16}$$

where:

$$\delta_{j,k}^{(2)} = \begin{cases} -\dfrac{\pi^2}{3} & \text{if} \quad j = k \\ \dfrac{(-2)(-1)^{k-j}}{(k-j)^2} & \text{if} \quad j \neq k \end{cases} \quad \text{and} \quad \delta_{j,k}^{(0)} = \begin{cases} 1 & \text{if} \quad j = k \\ 0 & \text{if} \quad j \neq k. \end{cases} \tag{17}$$

In (16), the value $\mathcal{E}$ is an approximation of the exact energy eigenvalue E of the system (12).

Equation (16) can be re-written in a matrix form as follows:

$$\mathbf{A}\mathbf{v} = \mathcal{E}\,\mathbf{D^2}\,\mathbf{v} \quad \Rightarrow \quad \left(\mathbf{A} - \mathcal{E}\,\mathbf{D^2}\right)\mathbf{v} = \mathbf{0}, \tag{18}$$

where $\mathbf{v} = [v_{-N}, \ldots, v_N]^T$ and the matrix $\mathbf{A}$ and the diagonal matrix $\mathbf{D^2}$ are given by:

$$\mathbf{A} = \left[-\frac{1}{h^2}\delta_{j,k}^{(2)} + \tilde{V}(jh)\delta_{j,k}^{(0)} \right]_{j,k=-N,\ldots,N} \quad \text{and}$$
$$\mathbf{D^2} = \left[(\phi'(jh))^2 \delta_{j,k}^{(0)} \right]_{j,k=-N,\ldots,N}. \tag{19}$$

As can be seen from (18), the eigenfunctions and eigenvalues of the differential equation (12) can be approximated by the generalized eigenvalue problem (18).

Now, we denote the Lambert W function by $W(x)$ which is defined as follows:

Definition 3.2 [15, Equation (1.5)] The Lambert W function denoted by $W(x)$ is defined implicitly by the solution of the following equation:

$$z = W(x)e^{W(x)}. \tag{20}$$

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 [15].

Theorem 3.3 [13] *Let $(v(x), E)$ be an eigenpair of the transformed Schrödinger equation given by:*

$$-v''(x) + \tilde{V}(x)v(x) = E(\phi'(x))^2 v(x) \quad \textit{with} \quad \lim_{|x|\to\infty} v(x) = 0, \tag{21}$$

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:* $|v(x)| \leq A\exp(-\beta\exp(\gamma|x|))$,
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 (18) satisfies the following asymptotic bound with respect to E:

$$|\mathcal{E} - E| = O\left[\sqrt{qE}\left(\frac{N^{\frac{5}{2}}}{\log(N)}\right)\exp\left(-\frac{\pi d\gamma N}{\log(\pi d\gamma N/\beta)}\right)\right] \quad as \quad N \to \infty. \tag{22}$$

Since this process can be done for any arbitrary eigenpair $\{(v_n(x), E_n)\}_n$, it is clear from Theorem 3.3 that every eigenvalue E will satisfy the error bound for the appropriate sequence of generalized eigenvalues $\mathcal{E}$.

4 The Coulombic anharmonic potential

The Coulombic anharmonic potential $V(x)$ is given by:

$$\begin{aligned} V(x) &= \frac{a_{-2}}{x^2} + \frac{a_{-1}}{x} + \sum_{i=1}^{n} a_i x^i \\ &= \sum_{i=-2}^{n} a_i x^i \quad \text{with} \quad a_{-2} > 0,\ a_0 = 0 \ \text{and} \ a_n > 0. \end{aligned} \tag{23}$$

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 3.1. To find such a transformation, we must first perform an asymptotic analysis of the differential equation (9).

As $x \to \infty$, the potential is dominated by the term x^n term and our differential equation becomes:

$$-\psi''(x) + a_n x^n \psi(x) \sim 0 \quad \text{as} \quad x \to \infty. \tag{24}$$

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:

$$-S'(x)^2 + a_n x^n \sim 0 \quad \text{as} \quad x \to \infty. \tag{25}$$

Solving this equation and taking the negative root to satisfy the boundary conditions, we obtain:

$$S(x) \sim -\frac{2\sqrt{a_n}}{n+2} x^{\frac{n+2}{2}} \quad \text{as} \quad x \to \infty. \tag{26}$$

Hence, we deduce the following bound for our wavefunction:

$$\psi(x) = O\left(\exp\left[-\frac{2\sqrt{a_n}}{n+2} x^{\frac{n+2}{2}}\right]\right) \quad \text{as} \quad x \to \infty. \tag{27}$$

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:

$$-r(r-1) + a_{-2} = 0 \quad \Longrightarrow \quad r = \frac{1 \pm \sqrt{1 + 4a_{-2}}}{2}. \tag{28}$$

The boundary condition $\psi(0) = 0$ leads us to reject the negative root, leading us to the following asymptotic bound as $x \to 0^+$:

$$\psi(x) = O\left(x^r\right) \quad \text{with} \quad r = \frac{1 + \sqrt{1 + 4a_{-2}}}{2}. \tag{29}$$

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 3.1 and produces double exponential decay at infinities. We begin by using the transformation proposed in [27]:

$$\phi(x) = \log\left[e^{\sinh(x)} + 1\right] \sim \begin{cases} \dfrac{e^x}{2} & \text{as } x \to \infty \\ \exp\left[-\dfrac{e^{-x}}{2}\right] & \text{as } x \to -\infty. \end{cases} \tag{30}$$

From the definition of $v(x)$ given by (11), our asymptotic bounds in (27) and (29), as well as the asymptotic behavior of the conformal map in (30), we can deduce the following asymptotic bounds for $v(x)$:

$$v(x) = \begin{cases} O\left(\exp\left[-\dfrac{\sqrt{a_n}}{(n+2)2^{n/2}} \exp\left(\frac{n+2}{2}x\right)\right]\right) & \text{as} \quad x \to \infty \\ O\left(\exp\left[-\dfrac{1 + \sqrt{1 + 4a_{-2}}}{4} \exp(-x)\right]\right) & \text{as} \quad x \to -\infty. \end{cases} \tag{31}$$

From (31), we notice that the conformal map (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 8, given its asymptotic behavior (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 $\gamma = \max\left\{\frac{n+2}{2}, 1\right\} = \frac{n+2}{2}$.

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 [33] 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 below, 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 caused by the increasing condition numbers of the matrices involved in the DESCM. The matrices $\mathbf{A}$ and $\mathbf{D}^2$ are constructed using (19).

To evaluate the effectiveness of the DESCM, we define the relative error between known eigenvalues E and numerical eigenvalues $\mathcal{E}$ as:

$$\text{Relative Error} = \frac{|E - \mathcal{E}|}{|E|}. \tag{32}$$

When moving to higher order energy eigenvalues or potentials without known analytic solutions, we use the following approximation to the relative error:

$$\text{Relative Error Approximation} = \frac{|\mathcal{E}_i(N+1) - \mathcal{E}_i(N)|}{|\mathcal{E}_i(N+1)|}, \tag{33}$$

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 [3,6]. These potentials are:

$$\begin{array}{lcl}
V_1(x) = \frac{2}{x^2} - \frac{16}{x} + 2x + \frac{x^2}{16} & \Longrightarrow & E_0 = -\frac{59}{4} \\
V_2(x) = \frac{6}{x^2} - \frac{24}{x} + 2x + \frac{x^2}{16} & \Longrightarrow & E_0 = -\frac{57}{4} \\
V_3(x) = \frac{15}{4x^2} - \frac{20}{x} + 2x + \frac{x^2}{16} & \Longrightarrow & E_0 = -\frac{58}{4} \\
V_4(x) = \frac{35}{4x^2} - \frac{28}{x} + 2x + \frac{x^2}{16} & \Longrightarrow & E_0 = -14 \\
V_5(x) = \frac{2}{x^2} + x^2 & \Longrightarrow & E_0 = 5 \\
V_6(x) = \frac{3}{4x^2} + x^2 & \Longrightarrow & E_0 = 4
\end{array} \tag{34}$$

5.1 Refinement of the DESCM

We note the singularity at the left end point of the potential at $x = 0$. Following the approach detailed in [32], we search for a general transformation of the form:

$$\phi(x) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right] \quad \text{with} \quad \alpha_i > 0 \quad \text{for} \quad i = 1, 2, 3, 4. \tag{35}$$

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:

$$\log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right] \sim \begin{cases} \alpha_1 e^{\alpha_2 x} & \text{as} \quad x \to \infty \\ \exp\left[-\alpha_3 e^{-\alpha_4 x}\right] & \text{as} \quad x \to -\infty. \end{cases} \tag{36}$$

From the definition of $v(x)$ given by (11), our asymptotic bounds in (27) and (29) in addition to the asymptotic behavior of the conformal map in (36), we can deduce the following asymptotic bounds for $v(x)$:

$$v(x) = \begin{cases} O\left(\exp\left[-\dfrac{2\sqrt{a_n \alpha_1^{n+2}}}{n+2} \exp\left(\dfrac{\alpha_2(n+2)}{2} x\right)\right]\right) & \text{as} \quad x \to \infty \\ O\left(\exp\left[-\dfrac{(1+\sqrt{1+4a_{-2}})\alpha_3}{2} \exp\left(-\alpha_4 x\right)\right]\right) & \text{as} \quad x \to -\infty. \end{cases} \tag{37}$$

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 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 $\alpha_1 = 1, \alpha_2 = 1.3, \alpha_3 = 1.2$

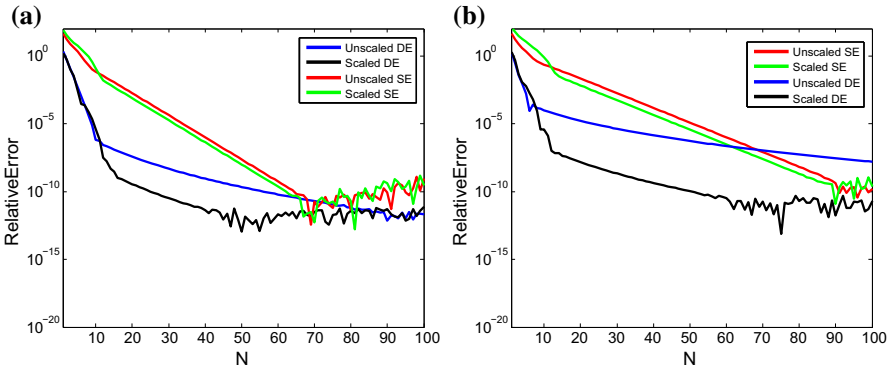

Fig. 1 Comparison of the DESCM and the SESCM. **a** Represents the convergence of the DESCM and the SESCM towards known eigenvalues of the potential V_5. **b** Represents the convergence of the DESCM and the SESCM towards the eigenvalues of the potential V_6. The *scaled plots* correspond to the convergence diagrams using the scaling factor τ. **a** Uses a scaling factor of $\tau = 0.75$. **b** Uses a scaling factor of $\tau = 0.55$

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 (Fig. 1).

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 Fig. 2, implementing the generalized transformation improves considerably the numerical stability of the method. We performed the same procedure to find the optimal parameter sets for other potentials V_2, V_3, V_4, V_5, and V_6. Optimizing the generalized transformation (35) for each potential gives six different parameter sets. In each case, using the optimized parameter sets yields improved performance of the DESCM that is similar to the V_1 case.

To improve the stability of the method, we introduce a scaling factor leading to a considerable increase in convergence.

Corollary 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 $\mathbf{a} := [a_{-i}, a_{-i+1}, \ldots, a_n]$ consisting of the coefficients of the potential. Consider also the vector $\mathbf{x} = [x^{-i}, x^{-i+1}, \ldots, x^n]$. Recognizing 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:

$$-\psi''(x) + (\mathbf{a} \cdot \mathbf{x})\psi(x) = E(\mathbf{a})\psi(x). \tag{38}$$

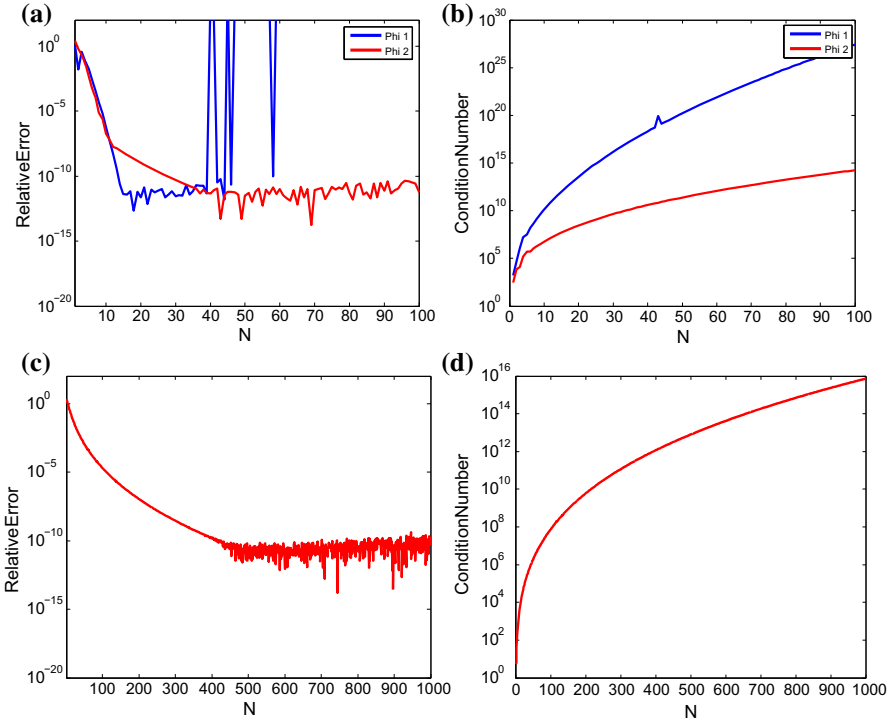

Fig. 2 The improved numerical stability of the DESCM for the potential V_1. **a** Shows the convergence of the method with $\phi_1(x) = \log\left[e^{\sinh(x)} + 1\right]$ and $\phi_2(x) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right]$ over 100 iterations. **b** 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

Implementing the change of variable $x = \tau y$ with $\tau \in \mathbb{R}$ and $\tau \neq 0$, and using:

$$\frac{d^2}{dx^2}\psi(\tau y) = \frac{1}{\tau^2}\frac{d^2}{dy^2}\psi(y), \tag{39}$$

leads to:

$$\frac{\psi''(\tau y)}{\tau^2} + (\mathbf{b}\cdot\mathbf{y})\psi(\tau y) = E(\mathbf{b})\psi(\tau y), \tag{40}$$

where $\mathbf{b} = [\tau^{-i}a_i, \tau^{-i+1}a_{-i+1}, \ldots, \tau^n a_n]$ and $\mathbf{y} = [y^{-i}, y^{-i+1}, \ldots, y^n]$.

If we let $\mathbf{c} = [\tau^{-i+2}a_i, \tau^{-i+2}a_{-i+1}\cdots\tau^{n+2}a_n]$, then (40) becomes:

$$-\psi''(\tau y) + \mathbf{c}\cdot\mathbf{y} = E(\mathbf{c})\psi(\tau y) = \tau^2 E(\mathbf{a})\psi(x). \tag{41}$$

Table 1 The number of convergent eigenvalues computed in 100 iterations for different transformations: $\phi_1(t) = \log(\exp(\sinh(t)) + 1)$, and $\phi_2(t) = \log\left[\exp\left(\alpha_1 e^{\alpha_2 x} - \alpha_3 e^{-\alpha_4 x}\right) + 1\right]$

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

The τ value denotes the scaling factor used in the calculations

We can recover the energy eigenvalues corresponding to a_j by noticing that:

$$E(\mathbf{a}) = \frac{E(\mathbf{c})}{\tau^2}, \tag{42}$$

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 using 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 1. In Fig. 2, we used 1001×1001 matrix illustrating the increased stability of the method when the scaling factor is used.

In Table 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 5×10^{-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 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 $\phi_1(x) = \log\left[e^{\sinh(x)} + 1\right]$, 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 Fig. 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.

Table 2 Numerical calculations for the ground states and first two excited states of the potential $V_1(x)$

N	$\mathcal{E}_0(N)$	$\mathcal{E}_1(N)$	$\mathcal{E}_2(N)$
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

Here we used the potential ϕ_2 with the scaling factor $\tau = 1.00$. ($E_0 = -14.75$)

The refined DESCM provides increased convergence speed when compared with the SESCM presented in [6]. To compare the two methods, we implement the SESCM following the procedure in [6]. The improved convergence speed offered by the refined DESCM is predicted in theoretical work done by Sugihara and others [25–27]. 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 Fig. 1. For the potentials V_5 and V_6, we utilize the same single exponential transformation and step size as proposed in [6]. Moreover, we show that the refinements presented in this work also improve the convergence of the SESCM.

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.

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