

Matrix methods for radial Schrödinger eigenproblems defined on a semi-infinite domain

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Abstract

In this paper, we discuss numerical approximation of the eigenvalues of the one-dimensional radial Schrödinger equation posed on a semi-infinite interval. The original problem is first transformed to one defined on a finite domain by applying suitable change of the independent variable. The eigenvalue problem for the resulting differential operator is then approximated by a generalized algebraic eigenvalue problem arising after discretization of the analytical problem by the matrix method based on high order finite difference schemes. Numerical experiments illustrate the performance of the approach.

Keyword: Radial Schrödinger equation, Infinite domain, Eigenvalues, Finite difference schemes

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1 Introduction

The aim of this paper is to investigate certain aspects arising in the numerical treatment of the following eigenvalue problem (EVP):

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

subject to boundary conditions

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

where $\ell \in \mathbb{N}$, the function $V(r)$ satisfies $\lim_{r \rightarrow \infty} V(r) = 0$, λ is an eigenvalue, and $u(r)$ is the associated eigenfunction.

Equation (1) is known in the literature as *radial* Schrödinger equation with *underlying potential* $V(r)$. An important example of this type of problems is the hydrogen atom equation corresponding to $V(r) = -Z/r$ with $Z > 0$.

Many currently available numerical techniques to handle this problem are based on the so-called *regularization* which, in our context, may mean replacing (2) by

$$u(\varepsilon) = u(R) = 0, \quad (3)$$

where ε is strictly positive and small and R is large. Clearly, equation (1) subject to (3) is a regular Sturm-Liouville problem on $[\varepsilon, R]$ and classical methods can be used to approximate its eigenvalues. The accuracy of these approximations, however, strongly depends on the choice of the cutoff points ε and R as discussed, for example, in [16]. Concerning the choice of R , a generalization of the so-called WKB-approximation introduced in [12] for nonharmonic oscillators, was proposed in [14]. In case of a problem whose potential has a Coulomb-like tail, the authors proposed to impose suitably adapted boundary conditions at the right endpoint R which allowed a noticeable reduction of the size of R . On the other hand, an ad-hoc procedure, treating $V(r)$ as a perturbation of the reference potential $\ell(\ell + 1)/r^2$ in a neighborhood of the origin, was investigated in [13, 14]. The aim of this procedure was to find an approximation for $u(\varepsilon)$ and $u'(\varepsilon)$. All these estimates were then used in a two-sided shooting procedure.

The approach proposed here is different. We first apply suitable change of variable, $t(r)$, in order to transform the problem posed on $r \in (0, \infty)$ to a problem posed on a finite domain $t \in (0, 1)$. After the transformation the EVP assumes the following general form:

$$-A_2(t) \mathbf{v}''(t) + A_1(t) \mathbf{v}'(t) + A_0(t) \mathbf{v}(t) = \lambda \mathbf{v}(t), \quad t \in (0, 1), \quad (4)$$

where $A_i(t)$, $i = 0, 1, 2$, are singular at $t = 0$ and/or $t = 1$. The EVP (4) is then augmented by suitable boundary conditions. We use results provided in [9, 10, 18] to show that the above singular EVP is well-posed and to describe the smoothness of its solution.

Numerical approximations of the eigenvalues are obtained by applying the so-called matrix methods which transform the EVP for the differential operator into a generalized algebraic EVP. More precisely, the equation (4) is discretized in its original second order formulation by using the finite difference schemes introduced in [4]. We stress that the application of these methods is possible in spite of the singularities at $t = 0, 1$, since the corresponding discrete problem does not involve the values of the coefficients functions in (4) at the interval endpoints.

It is worth mentioning that the idea of reducing the continuous problem to a finite domain was already used in the development of the codes SLEIGN2 [6] and SLF02F [15]. Nevertheless, the numerical schemes used in the implementation of the shooting procedure make use of the coefficient functions at the endpoints.

This means that, in our case, where such functions become unbounded, cutting off the interval ends becomes inevitable.

We have organized the paper as follows. In Section 2, we propose two ways of changing the independent variable for the transformation of the original problem to a finite domain and discuss the properties of the resulting singular BVPs and EVPs. In Section 3, we describe in some detail the numerical procedure based on the matrix method. Finally, Section 4 contains the results of the numerical simulation for the hydrogen atom equation and models studied in [17]. Here, we also show numerical results related to a third change of independent variable, which is analyzed in detail in [2].

2 Reformulation of the problem on a finite domain

The first question we would like to address is how to transform problem (1)-(2) posed on the semi-infinite interval to a finite domain. In general, if $t(r)$ is given and $u(r) =: z(t(r))$, then we can rewrite (1) as

$$-\frac{d^2}{dt^2}z(t) \left(\frac{d}{dr}t(r) \right)^2 - \frac{d}{dt}z(t) \frac{d^2}{dr^2}t(r) + \left(\frac{\ell(\ell+1)}{r^2} + V(r) \right) z(t) = \lambda z(t). \quad (5)$$

2.1 Transformation doubling the size of the ODE system: TDS

The transformation TDS is based on the following change of the independent variable:

$$t(r) = \frac{1}{r}, \quad r \in [1, \infty). \quad (6)$$

We use (6) to reformulate (5) as follows:

$$-z''(t) - \frac{2}{t}z'(t) + \left(\frac{\ell(\ell+1)}{t^2} + \frac{1}{t^4}V\left(\frac{1}{t}\right) \right) z(t) = \lambda \frac{z(t)}{t^4}, \quad t \in (0, 1],$$

and therefore (1) posed on the interval $(0, \infty)$ can be transformed to the finite interval,

$$\begin{aligned} -u''(t) + \left(\frac{\ell(\ell+1)}{t^2} + V(t) \right) u(t) &= \lambda u(t), \quad t \in (0, 1], \\ -z''(t) - \frac{2}{t}z'(t) + \left(\frac{\ell(\ell+1)}{t^2} + \frac{1}{t^4}V\left(\frac{1}{t}\right) \right) z(t) &= \lambda \frac{z(t)}{t^4}, \quad t \in (0, 1]. \end{aligned}$$

In matrix notation, this system of equations can be written as

$$-\mathbf{v}''(t) + \tilde{A}_1(t) \mathbf{v}'(t) + \tilde{A}_0(t) \mathbf{v}(t) = \lambda B(t) \mathbf{v}(t), \quad t \in (0, 1], \quad (7)$$

with $\mathbf{v}(t) = (u(t), z(t))^T$ and

$$\begin{aligned}\tilde{A}_1(t) &= \begin{pmatrix} 0 & 0 \\ 0 & -2t^{-1} \end{pmatrix}, \\ \tilde{A}_0(t) &= \begin{pmatrix} \ell(\ell+1)t^{-2} + V(t) & 0 \\ 0 & \ell(\ell+1)t^{-2} + t^{-4}V(t^{-1}) \end{pmatrix}, \\ B(t) &= \begin{pmatrix} 1 & 0 \\ 0 & t^{-4} \end{pmatrix}.\end{aligned}$$

Note that $B(t)$ is nonsingular for $t \in (0, 1)$, and hence, (7) can be written in the general form (4).

In the sequel, we investigate if the above singular EVP is well-posed. This is done by first examining the boundary conditions. To this aim, we follow the arguments from [8, 10]. Although, we will numerically simulate the EVPs in form (4), for the analysis, we have to rewrite the problem into its first order form. It turns out that here $t = 0$ is a singular point and therefore, we have to investigate the local behavior of the ODE in the vicinity of this point.

If we transform (7) to a first order system of ODEs for the new vector

$$\mathbf{y}(t) = (y_1(t), y_2(t), y_3(t), y_4(t))^T := (\mathbf{v}(t), t\mathbf{v}'(t))^T \in \mathbb{R}^4, \quad (8)$$

then we obtain

$$t^4 \mathbf{y}'(t) - M(t) \mathbf{y}(t) = \lambda G(t) \mathbf{y}(t), \quad t \in (0, 1], \quad (9)$$

where the matrices $M(t)$ and $G(t)$ include the data from (7), namely

$$\begin{aligned}M(t) &= \begin{pmatrix} 0 & 0 & t^3 & 0 \\ 0 & 0 & 0 & t^3 \\ t^3 \ell(\ell+1) + t^5 V(t) & 0 & t^3 & 0 \\ 0 & t^3 \ell(\ell+1) + tV(t^{-1}) & 0 & -t^3 \end{pmatrix}, \\ G(t) &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -t^5 & 0 & 0 & 0 \\ 0 & -t & 0 & 0 \end{pmatrix}.\end{aligned}$$

For the investigation of the local behavior of (9) around $t = 0$, note that $\lim_{t \rightarrow 0^+} V(t^{-1}) = \lim_{r \rightarrow \infty} V(r) = 0$. Moreover, we assume that $\lim_{t \rightarrow 0^+} t^5 V(t) = 0$, and the higher derivatives of $t^5 V(t)$ exist and are continuous on $[0, 1]$. This means that in (9), $M(t) = M + A(t)$ and $G(t) = N + C(t)$, where $M = M(0)$ and $N = G(0)$ are zero matrices. Consequently, (9) has the form

$$t^4 \mathbf{y}'(t) - A(t) \mathbf{y}(t) = \lambda C(t) \mathbf{y}(t), \quad t \in (0, 1]. \quad (10)$$

The associated boundary conditions read:

$$y_1(0) = y_2(0) = 0, \quad y_1(1) = y_2(1), \quad y_3(1) = -y_4(1), \quad (11)$$

which is equivalent to

$$B_0\mathbf{y}(0) + B_1\mathbf{y}(1) = \mathbf{0}, B_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, B_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \quad (12)$$

First note that the form of the EVP (10)-(11) corresponds exactly to the one of the EVP (1.2) studied in [10]. To discuss the boundary conditions, we have to look at the associated BVP

$$t^4\mathbf{y}'(t) - M(t)\mathbf{y}(t) = t^4\mathbf{y}'(t) - (M + A(t))\mathbf{y}(t) = \mathbf{g}(t), \quad t \in (0, 1], \quad (13)$$

subject to (12), cf. [10, problem (3.9)]. Since the matrix $M = M(0)$ is a zero matrix, its eigenvalues are $\mu_1 = \mu_2 = \mu_3 = \mu_4 := \mu = 0$ and the corresponding eigenspace is \mathbb{R}^4 . Consequently, the orthogonal projection R onto the eigenspace of M associated with $\mu = 0$ is $R = I$ and the condition $(I - R)A(0) = O$ is satisfied, see [10, requirement (3.10)]. Moreover, due to [10, Theorem 3.2], for any $\mathbf{g}, A \in C[0, 1]$ there exists a unique solution $\mathbf{y} \in C^1[0, 1]$ of the BVP (12)-(13) since $\text{rank}[B_0, B_1] := k = 4$, and the linear differential operator $t^4\mathbf{y}'(t) - A(t)\mathbf{y}(t)$ is Fredholm with index equal to $\text{rank}[R] - k = 0$. This result immediately carries over to the EVP problem (10)-(11). Here, $(I - R)C(0) = O$ holds, cf. [10, (7.1)] and A, C are smooth functions. Therefore, according to [10, Theorem 7.2] the EVP is well-posed and has a solution in $C^\infty[0, 1]$.

For the numerical treatment, we use system (7), where the second equation is premultiplied by t^4 , together with boundary conditions, see (8) and (11),

$$\mathbf{v}(0) = \mathbf{0}, \quad (1, -1)\mathbf{v}(1) = 0, \quad (1, 1)\mathbf{v}'(1) = 0. \quad (14)$$

2.2 Transformation compressing the infinite interval: TCII

We now consider an alternative change of independent variable described by

$$t(r) = \frac{r}{r + \xi}, \quad \xi > 0, \quad r \in [0, \infty). \quad (15)$$

Using (15) in (5) yields the following new form of (1):

$$-z''(t) + \frac{2}{1-t}z'(t) + \left(\frac{\ell(\ell+1)}{t^2(1-t)^2} + \frac{\xi^2}{(1-t)^4}V\left(\frac{\xi t}{1-t}\right) \right) z(t) = \frac{\lambda\xi^2}{(1-t)^4}z(t), \quad (16)$$

subject to boundary conditions

$$z(0) = z(1) = 0. \quad (17)$$

First of all we note that there are two critical points $t = 0$ and $t = 1$ in the differential operator in (16). Our aim is to show that boundary conditions (17)

are posed in such a way that the associated BVP is well-posed. To this aim, we have to investigate the ODE in the vicinity of $t = 0$ and $t = 1$. Let us first consider $t = 0$. Setting

$$a_1(t) = \frac{2t}{1-t}, \quad a_0(t) = \frac{\ell(\ell+1)}{(1-t)^2} + \frac{t^2\xi^2}{(1-t)^4}V\left(\frac{\xi t}{1-t}\right), \quad b(t) = -\frac{\xi^2}{(1-t)^4},$$

we rewrite (16) to obtain the form

$$z''(t) - \frac{a_1(t)}{t}z'(t) - \frac{a_0(t)}{t^2}z(t) = \lambda b(t)z(t),$$

and transform it to the following first order system for the vector $\mathbf{y}(t) = (y_1(t), y_2(t))^T := (z(t), tz'(t))^T$

$$t\mathbf{y}'(t) - M(t)\mathbf{y}(t) = \lambda G(t)\mathbf{y}(t), \quad (18)$$

subject to

$$B_0\mathbf{y}(0) + B_1\mathbf{y}(1) = \mathbf{0}, \quad B_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad B_1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (19)$$

where

$$M(t) = \begin{pmatrix} 0 & 1 \\ a_0(t) & 1 + a_1(t) \end{pmatrix}, \quad G(t) = \begin{pmatrix} 0 & 0 \\ t^2b(t) & 0 \end{pmatrix}. \quad (20)$$

Also here, if we assume that $\lim_{r \rightarrow 0^+} rV(r)$ is finite we have $M(t) = M + A(t)$ and $G(t) = N + C(t)$, where N is a zero matrix and

$$M = M(0) = \begin{pmatrix} 0 & 1 \\ a_0(0) & 1 + a_1(0) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \ell(\ell+1) & 1 \end{pmatrix}.$$

In contrast to (9), where due to t^4 in the leading term the ODE admits a singularity of the second kind, in (18) a singularity of the first kind arises. Therefore, we can apply results from [8] to analyze the boundary conditions of the problem. We first calculate the eigenvalues of the matrix $M(0)$ and obtain $\mu_1 = -\ell \leq 0$ and $\mu_2 = 1 + \ell > 0$. Let us focus on two cases used in the numerical simulations.

Case 1: $\ell = 0$ For $\ell = 0$, the eigenvalues of the matrix M are $\mu_1 = 0$ and $\mu_2 = 1$. First, we have to calculate the related eigenvectors \mathbf{w}_1 and \mathbf{w}_2 and construct two projection matrices R and S , $R + S = I_2$, projecting onto eigenspaces of M associated with μ_1 and μ_2 , respectively. This yields

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{w}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad R = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}.$$

According to [8, Theorem 3.2], the linear operator $t\mathbf{y}'(t) - M(t)\mathbf{y}(t)$ is Fredholm with index equal to $\text{rank}(R + S) - \text{rank}[B_0R, B_1] = 2 - 2 = 0$ since

$$\text{rank}[B_0R, B_1] = \text{rank} \left[\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \right] = 2.$$

Again, this means that for any $\mathbf{g}, A \in C[0, 1]$ the BVP,

$$t\mathbf{y}'(t) - M(t)\mathbf{y}(t) = \mathbf{g}(t), \quad t \in (0, 1), \quad B_0\mathbf{y}(0) + B_1\mathbf{y}(1) = \mathbf{0}, \quad (21)$$

where the problem data has been specified in (19)-(20), is well-posed and has as solution $\mathbf{y} \in C[0, 1] \cap C^1(0, 1]$. We have an analogous result for the EVP (18)-(19) with $A, G \in C[0, 1]$. Since the positive eigenvalue of M is relatively small, we would need further investigations to show that also higher derivatives of \mathbf{y} are smooth, cf. [8, Theorem 10.2].

Case 2: $\ell = 3$ Here, the eigenvalues of the matrix M are $\mu_1 = -3$ and $\mu_2 = 4$. Again, we first calculate the related eigenvectors \mathbf{w}_1 and \mathbf{w}_2 and construct two projection matrices Q and S , $Q + S = I_2$, projecting onto eigenspaces of M associated with μ_1 and μ_2 , respectively. This yields

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ -3 \end{pmatrix}, \quad \mathbf{w}_2 = \begin{pmatrix} 1 \\ 4 \end{pmatrix}, \quad Q = \frac{1}{7} \begin{pmatrix} 4 & -1 \\ -12 & 3 \end{pmatrix}, \quad S = \frac{1}{7} \begin{pmatrix} 3 & 1 \\ 12 & 4 \end{pmatrix}.$$

First of all, $S\mathbf{y} \in C^1[0, 1]$ and $S\mathbf{y}(0) = S\mathbf{y}'(0) = \mathbf{0}$, see [8, Lemma 3.5]. Moreover, condition $Q\mathbf{y}(0) = \mathbf{0}$ is necessary and sufficient for \mathbf{y} to be in $C[0, 1]$. To see that this condition is satisfied, we have to take into account that the ODE in (21) arises from

$$z''(t) - \frac{a_1(t)}{t}z'(t) - \frac{a_0(t)}{t^2}z(t) = g(t), \quad t \in (0, 1],$$

and thus $\mathbf{g}(t) = t^2(0, g(t))^T$. Using the special structure of \mathbf{g} and [18, Lemma 3.1], we see that from $z(0) = y_1(0) = 0$, $y_1 \in C^1[0, 1]$ follows and therefore

$$(1, 0)Q\mathbf{y}(0) = \frac{4}{7}y_1(0) - \frac{1}{7}y_2(0) = -\frac{1}{7} \lim_{t \rightarrow 0^+} ty_1'(t) = 0$$

holds.

Now, according to [8, Theorem 3.2], the linear operator $t\mathbf{y}'(t) - M(t)\mathbf{y}(t)$ is Fredholm with index equal to $\text{rank}(S) - \text{rank}[B_0R, B_1] = 1 - 1 = 0$ since the orthogonal projection R onto the eigenspace of M associated with $\mu = 0$ is zero and

$$\text{rank}[B_0R, B_1] = \text{rank}[B_1] = \text{rank} \left[\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right] = 1.$$

Thus, for any $\mathbf{g}, A \in C^3[0, 1]$ the BVP (21) with the problem data given in (19)-(20) is well-posed and has as solution $\mathbf{y} \in C^3[0, 1] \cap C^4(0, 1]$. We have an analogous result for the EVP (18)-(19) for $A, G \in C^3[0, 1]$. Since the positive eigenvalue of M is slightly larger than in Case 1, we can show more smoothness in \mathbf{y} , cf. [8, Theorem 10.2].

Similar investigations for $t = 1$ show that this point is not a critical point and the solution is analytic at $t = 1$, see [2, 5].

For the numerical experiments, we use (16) premultiplied by $(1 - t)^4/\xi^2$ together with boundary conditions (17).

3 Finite difference schemes

The numerical methods that we have used discretize equation (4) in its original second order formulation. In particular, given the uniform mesh

$$t_i = i h, \quad i = 0, 1, \dots, N + 1, \quad h = 1/(N + 1),$$

for the interval $[0, 1]$, the first and second order derivatives of the solution at the inner grid points are approximated by applying suitable $(2k)$ -step finite difference schemes introduced in [4]. More precisely, for each $i = k, k + 1, \dots, N + 1 - k$,

$$\mathbf{v}'(t_i) \approx \frac{1}{h} \sum_{j=-k}^k \beta_{j+k} \mathbf{v}_{i+j}, \quad \mathbf{v}''(t_i) \approx \frac{1}{h^2} \sum_{j=-k}^k \gamma_{j+k} \mathbf{v}_{i+j}, \quad (22)$$

where $\mathbf{v}_i \approx \mathbf{v}(t_i)$, for each i . The coefficients $\{\beta_j\}_{j=0}^{2k}$ and $\{\gamma_j\}_{j=0}^{2k}$ are uniquely determined by imposing the formulas to be of consistency order $2k$. The resulting methods turn out to be symmetric, i.e., $\beta_j = -\beta_{2k-j}$ and $\gamma_j = \gamma_{2k-j}$, for each $j = 0, 1, \dots, k$. In particular, the 2-step schemes coincide with the ones used in [11, Section 5.3]. Using the terminology of Boundary Value Methods the formulas in (22) are called *main methods* [7]. When $k > 1$, these formulas are augmented by suitable *initial* and *final additional methods* which provide approximations of the first and second order derivatives at the meshpoints close to the interval ends. In particular, for each $i = 1, 2, \dots, k - 1$,

$$\mathbf{v}'(t_i) \approx \frac{1}{h} \sum_{j=0}^{2k} \beta_j^{(i)} \mathbf{v}_j, \quad \mathbf{v}''(t_i) \approx \frac{1}{h^2} \sum_{j=0}^{2k+1} \gamma_j^{(i)} \mathbf{v}_j,$$

while, for each $i = N + 2 - k, \dots, N$ and $r = N + 1 - 2k$,

$$\mathbf{v}'(t_i) \approx \frac{1}{h} \sum_{j=0}^{2k} \beta_j^{(i-r)} \mathbf{v}_{r+j}, \quad \mathbf{v}''(t_i) \approx \frac{1}{h^2} \sum_{j=0}^{2k+1} \gamma_j^{(i-r)} \mathbf{v}_{r+j-1}.$$

The involved coefficients are determined by requiring that the additional schemes are of the same order as the main formulas, i.e. $2k$, [4]. It is worth mentioning that such schemes have been already used for solving singular Sturm-Liouville problems in [1, 3].

Since for both transformations, TDS and TCII, $\mathbf{v}(0) = \mathbf{0}$ holds, the following system of equations arises after the discretization of (4):

$$\mathcal{R}\hat{\mathbf{v}} := \left(-D_2 \left(\hat{\Gamma} \otimes I_m\right) + D_1 \left(\hat{B} \otimes I_m\right) + \hat{D}_0\right) \hat{\mathbf{v}} = \lambda \mathbf{v}. \quad (23)$$

Here I_m is the identity matrix of dimension m , with $m = 2, 1$ for TDS and TCII, respectively,

$$\begin{aligned} D_i &= \text{blockdiag}(A_i(t_1), A_i(t_2), \dots, A_i(t_N)), \quad i = 0, 1, 2, \\ \hat{D}_0 &= (D_0 \mid \mathbf{0}_N \otimes I_m), \quad \mathbf{0}_N = (0, \dots, 0)^T \in \mathbb{R}^N, \\ \hat{\mathbf{v}}^T &= (\mathbf{v}^T \ \mathbf{v}_{N+1}^T) = (\mathbf{v}_1^T \ \dots \ \mathbf{v}_N^T \ \mathbf{v}_{N+1}^T) \approx (\mathbf{v}^T(t_1) \ \dots \ \mathbf{v}^T(t_N) \ \mathbf{v}^T(t_{N+1})) \end{aligned} \quad (24)$$

Finally, $\hat{\Gamma}, \hat{B} \in \mathbb{R}^{N \times (N+1)}$ contain the coefficients of the difference schemes. For example, for the method of order 4,

$$\begin{aligned} \hat{\Gamma} &= \frac{1}{12h^2} \begin{pmatrix} -15 & -4 & 14 & -6 & 1 & & & & & & \\ 16 & -30 & 16 & -1 & & & & & & & \\ -1 & 16 & -30 & 16 & -1 & & & & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\ & & & -1 & 16 & -30 & 16 & -1 & & & \\ & & & 1 & -6 & 14 & -4 & -15 & 10 & & \end{pmatrix}, \\ \hat{B} &= \frac{1}{12h} \begin{pmatrix} -10 & 18 & -6 & 1 & & & & & & & \\ -8 & 0 & 8 & -1 & & & & & & & \\ 1 & -8 & 0 & 8 & -1 & & & & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\ & & & 1 & -8 & 0 & 8 & -1 & & & \\ & & & -1 & 6 & -18 & 10 & 3 & & & \end{pmatrix}. \end{aligned}$$

Let us now describe the discretization of the boundary conditions at $t = 1$. We have to distinguish between TDS and TCII. For TDS, the last two conditions in (14) are approximated as follows:

$$(1, -1) \mathbf{v}_{N+1} = 0, \quad (1, 1) \mathbf{v}'(1) \approx (1, 1) \sum_{j=0}^{2k} \beta_j^{(2k)} \mathbf{v}_{N-2k+j} = 0, \quad (25)$$

where $\beta_j^{(2k)}$ are the coefficients of the classical $(2k)$ -step BDF method. Equation (23) augmented with (25) form the following generalized algebraic EVP,

$$\mathcal{R}_1 \hat{\mathbf{v}} = \lambda \mathcal{S} \hat{\mathbf{v}}, \quad \mathcal{S} = \begin{pmatrix} I_{2N} & \\ & O_2 \end{pmatrix},$$

where \mathcal{R}_1 is obtained by adding to \mathcal{R} two rows whose entries are all zeros except for

$$\begin{aligned} (\mathcal{R}_1)_{2N+1, 2N+1} &= -(\mathcal{R}_1)_{2N+1, 2N+2} = 1, \\ (\mathcal{R}_1)_{2N+2, 2(N-s)+1} &= (\mathcal{R}_1)_{2N+2, 2(N-s)+2} = \beta_{2k-s}^{(2k)}, \quad s = 0, 1, \dots, 2k. \end{aligned}$$

Concerning TCII, the treatment of the boundary condition in (17) is simpler: it is sufficient to remove the last entry of the vector $\hat{\mathbf{v}}$ thus obtaining the vector

\mathbf{v} (see (24)) and the last column of the matrices $\hat{\Gamma}$, \hat{B} , \hat{D}_0 . More precisely, by setting

$$\hat{\Gamma} = [\Gamma | \gamma_{N+1}], \quad \hat{B} = [B | \beta_{N+1}], \quad \mathcal{R}_2 = -D_2\Gamma + D_1B + D_0,$$

the algebraic EVP reads:

$$\mathcal{R}_2 \mathbf{v} = \lambda \mathbf{v}.$$

4 Numerical experiments

For the numerical simulations we considered the following potentials:

$$V_1(r) = -\frac{2}{r}, \quad V_2(r) = -\frac{2\alpha e^{-\alpha r}}{1 - e^{-\alpha r}}, \quad \alpha > 0, \quad V_3(r) = -\frac{2e^{-\alpha r}}{r}, \quad \alpha > 0,$$

hydrogen atom, Hulthén potential, and Yukawa potential, respectively. When r is close to zero, these three potentials behave similarly, i.e. $V_j(r) \sim V_1(r)$ for $j = 2, 3$. On the other hand, $|V_2(r)|$ and $|V_3(r)|$ decrease faster than $|V_1(r)|$ when $r \rightarrow \infty$.

For the hydrogen atom problem, the exact eigenvalues are known to be $\lambda_n = -n^{-2}$, $n \geq \ell + 1$, where n and ℓ represent the radial and the angular momentum quantum numbers, respectively, and the corresponding eigenfunction $u_n(r)$ has exactly $\nu = n - \ell - 1$ zeros in $(0, \infty)$. In the terminology of Sturm-Liouville problems, λ_n has therefore index ν . We solved this problem with various values of ℓ by applying the $(2k)$ -step scheme of order $p = 2k$ described in the previous section with different values of k and different numbers of interior meshpoints N . The resulting generalized eigenvalue problems have been solved by using the `eig` routine of MATLAB. When dealing with TCII, numerical experiments indicate that a good heuristic law for the choice of the parameter ξ is given by

$$\xi = (1.35)^p (\ell + 1). \quad (26)$$

There are various alternative possibilities to compress the semi-infinite interval to a finite domain. Any transformation of the type (ATCII),

$$t(r) = 1 - (1 + r)^{-\beta}, \quad \beta > 0, \quad r \in [0, \infty),$$

reduces $[0, \infty)$ to $[0, 1)$. To see how this transformation performs in the context of EVPs, we used ATCII with $\beta = \frac{1}{2}$. For the respective analysis, we refer the reader to [2].

In Figure 1, we plotted the relative errors in the eigenvalues λ_6 and λ_{10} of the hydrogen atom problem with $\ell = 3$ versus N . In particular, the plots at the top of the picture refer to TDS, those in the center to TCII and (26), and the bottom ones to ATCII. We can see that when the radial quantum number n increases, the results obtained with TDS are not satisfactory, even for higher order methods. For TCII, we obtain good results using already a second order method. They can be further improved when we increase the order of the

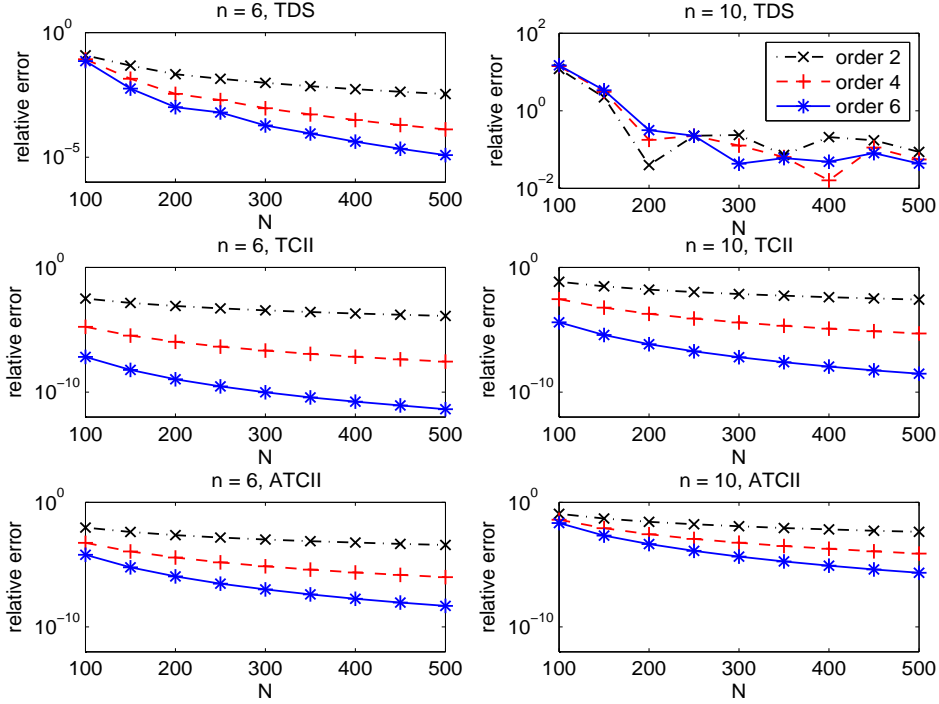


Figure 1: Hydrogen atom equation, $\ell = 3$: relative errors in the eigenvalues calculated using TDS, TCII with (26), and ATCII.

scheme. By virtue of these results and taking into account that for a fixed N the size of the generalized eigenvalue problem corresponding to TDS is approximately twice as large as the one corresponding to TCII, we do not include TDS in the sequel. Also, the accuracy obtained using TCII is considerably better than the accuracy of ATCII.

Let us now consider the Hulthén and the Yukawa potentials. The parameter α occurring in their definition is called *screening parameter* and it is known that the number of eigenvalues in the point spectrum of the corresponding problems varies with α [17]. Concerning the exact eigenvalues, these are known in closed form only for the Hulthén problem with $\ell = 0$. In all other cases, in order to evaluate the performance of our schemes, we calculated the reference eigenvalues using the method of order 8 with $N = 1500$. As an example, in Figure 2, the relative errors in the Hulthén eigenvalue approximations for $\ell = 0, 3$ and $\alpha = 0.02$ are shown. Observe that both plots on the left refer to the eigenvalues of index $\nu = n - \ell - 1 = 2$ while the plots on the right to those of index $\nu = 4$. The related data for ATCII can be found in Figure 3.

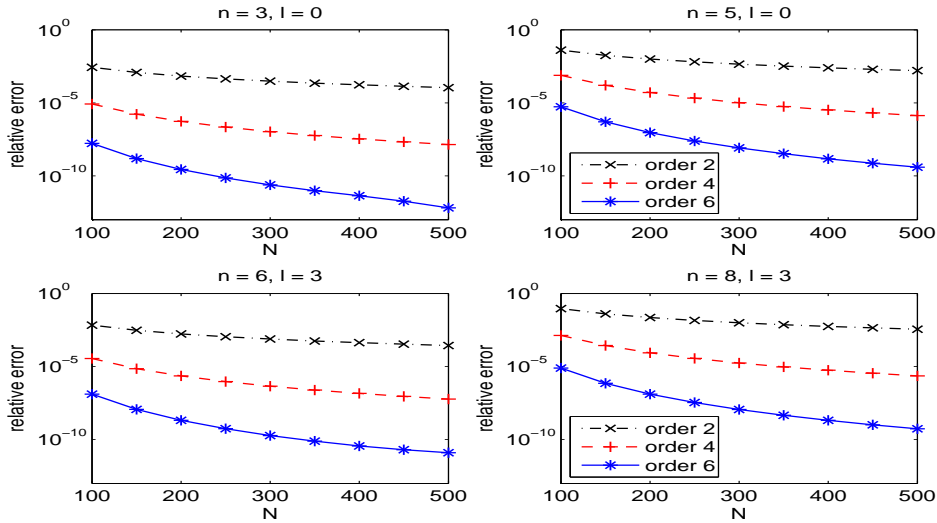


Figure 2: Hulthén potential, $\ell = 0, 3$, $\alpha = 0.02$: relative errors in the eigenvalues calculated using TCII with (26).

In Table 1, the eigenvalue approximations computed with TCII and (26) using the method of order $p = 8$ for the Yukawa potential have been listed and compared to those provided by [17].

5 Conclusions

In this paper we studied the numerical solution of the eigenvalue problems for singular Schrödinger equation posed on a semi-infinite interval

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

Our aim was to propose a transformation reducing the infinite domain to the finite interval $(0, 1]$ and then discretize the resulting ODE using finite difference schemes. Finally, the generalized algebraic eigenvalue problem was solved using the eigenvalue MATLAB routine. Three transformations have been used:

TDS: Here, the interval $(0, \infty)$ is split into two parts, $(0, \infty) = (0, 1] \cup [1, \infty)$, and the second interval is transformed to $(0, 1]$ using $t(r) := 1/r$. This transformation has two disadvantages: the number of equations is doubled which is not so critical since the original problem is scalar, but also a singularity of the first kind in the original problem changes to an essential singularity

Table 1: Yukawa potential: eigenvalues calculated using the method of order $p = 8$ as compared the those listed in Table 5 in [17].

$n = 9$				
ℓ	α	$\lambda/2, N = 200$	$\lambda/2, N = 1500$	[17]
0	0.010	-0.0005858266584	-0.0005858247613	-0.0005858247612
1	0.010	-0.0005665076452	-0.0005665076262	-0.0005665076261
2	0.010	-0.0005276644219	-0.0005276644203	-0.0005276644203
3	0.010	-0.0004688490639	-0.0004688490636	-0.0004688490636
4	0.010	-0.0003893108560	-0.0003893108559	-0.0003893108558
5	0.010	-0.0002878564558	-0.0002878564558	-0.0002878564558
6	0.005	-0.0022606077423	-0.0022606077423	-0.0022606077422
7	0.005	-0.0021997976659	-0.0021997976659	-0.0021997976659
8	0.005	-0.0021291265596	-0.0021291265596	-0.0021291265596
$n = 10$				
ℓ	α	$\lambda/2, N = 200$	$\lambda/2, N = 1500$	[17]
0	0.005	-0.0015083751962	-0.0015083559308	-0.0015083559307
1	0.005	-0.0015009237055	-0.0015009235029	-0.0015009235029
2	0.005	-0.0014860116411	-0.0014860116241	-0.0014860116240
3	0.005	-0.0014635239308	-0.0014635239276	-0.0014635239275
4	0.005	-0.0014333097815	-0.0014333097805	-0.0014333097805
5	0.005	-0.0013951561297	-0.0013951561294	-0.0013951561294
6	0.005	-0.0013487749861	-0.0013487749860	-0.0013487719860
7	0.005	-0.0012937846260	-0.0012937846260	-0.0012937846259
8	0.005	-0.0012296811836	-0.0012296811836	-0.0012296811835

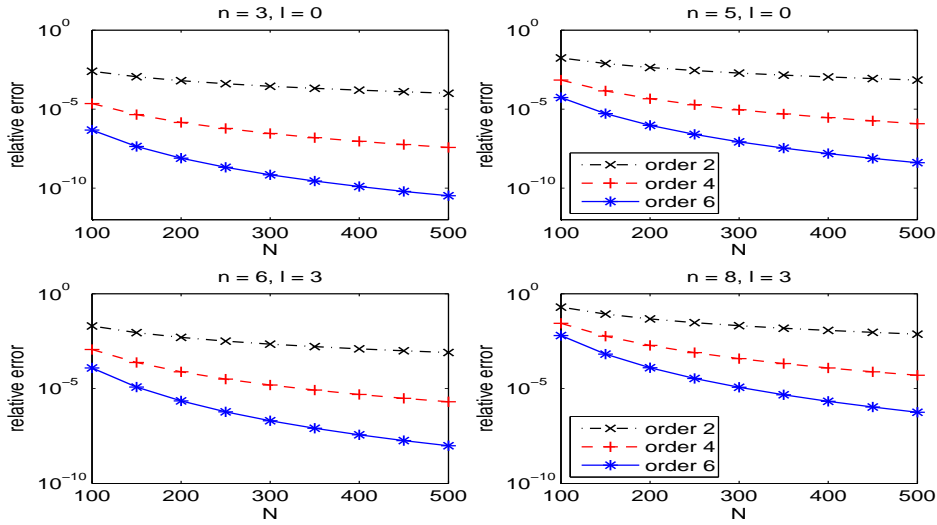


Figure 3: Hulthén potential, $\ell = 0, 3$, $\alpha = 0.02$: relative errors in the eigenvalues calculated using ATCII.

in the transformed equations. The latter singularity is considerably more difficult to handle numerically.

TCII: With the transformation $t(r) := r/(r + \xi)$ and a suitably chosen ξ , the semi-infinite interval is compressed to $(0, 1)$; the dimension of the problem and the type of the singularity do not change.

ATCII: Analogous compression is also done using $t(r) := 1 - 1/\sqrt{1+r}$.

We could show that the transformed problems are well-posed and discussed the smoothness of their solutions. Moreover, it turns out that the approach based on TCII outperforms the other two, and therefore, it could be recommended to be used in similar situations.

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