


Article

Accurate Spectral Collocation Computation of High Order Eigenvalues for Singular Schrödinger Equations.

Călin-Ioan Gheorghiu ^{1,†}  0000-0002-8512-2466¹ Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy; ghcalin@ictp.acad.ro

† Current address: Str. Fantanele 57, 400320 Cluj-Napoca, Romania

Abstract: We are concerned with the study of some classical spectral collocation methods as well as with the new software system Chebfun in computing high order eigenpairs of singular and regular Schrödinger eigenproblems. We want to highlight both the qualities as well as the shortcomings of these methods and evaluate them in conjunction with the usual ones. In order to resolve a boundary singularity we use Chebfun with domain truncation. Although it is applicable with spectral collocation, a special technique to introduce boundary conditions as well as a coordinate transform, which maps an unbounded domain to a finite one, are the special ingredients. A challenging set of “hard” benchmark problems, for which usual numerical methods (f. d., f. e. m., shooting etc.) fail, are analyzed. In order to separate “good” and “bad” eigenvalues we estimate the drift of the set of eigenvalues of interest with respect to the order of approximation and/or scaling of domain parameter. It automatically provides us with a measure of the error within which the eigenvalues are computed and a hint on numerical stability. We pay a particular attention to problems with almost multiple eigenvalues as well as to problems with a mixed spectrum.

Keywords: spectral collocation; Chebfun; singular Schrödinger; high index eigenpairs; multiple eigenpairs; accuracy; numerical stability

MSC: 34L40; 34L16; 65L15; 65L20; 65L60

1. Introduction

There is clearly an increasing interest to develop accurate and efficient methods of solution to singular Schrödinger eigenproblems. Our main interest here is to compare the capabilities of the new Chebfun package with those of classical spectral methods in solving such problems, showing their capabilities and weaknesses. The latter employ basis functions and/or grid points based on Chebyshev, Laguerre or Hermite polynomials as well as on sinc or Fourier functions. The effort expended by both classes of methods is also of real interest. It can be assessed in terms of the ease of implementation of the methods as well as in terms of computer resources required to achieve a specified accuracy.

Spectral methods have been shown to provide exponential convergence for a large variety of problems, generally with smooth solutions, and are often preferred. For details on Chebfun we refer to [1], [2], [3], [4], [5] and [6]. For Chebyshev collocation (ChC), Laguerre-Gauss-Radau collocation (LGRC), Hermite (HC) and sinc collocation (SiC) we refer among other sources to our contributions [7], [8] as well as to the seminal paper [9].

For problems on the entire real axis SiC proved to be particularly well suited. Moreover, this method has given excellent results recorded in our contribution [8] and in the works cited there. The so-called generalized pseudospectral (GPS) method, actually the Legendre collocation, is employed in [10] to calculate the bound states of the Hulthén and the Yukawa potentials in quantum mechanics, with special emphasis on higher excited states and stronger couplings. The author uses a two parameter dependent nonlinear transformation in order to map the half-line into the canonical interval $[-1, 1]$. In contrast, we will use an analogous transformation but which depends on only one parameter. Also,

very recently spectral methods based on non-classical orthogonal polynomials have been used in [11] in order to solve some Schrödinger problems connected with Fokker-Planck operator. A particular attention will be paid in this paper to the challenging issue of *continuous spectra vs. discrete (numerical) eigenvalues*. It is well known that some eigenvalue problems (see for instance the well known text [12]) for differential operators which are naturally posed on the whole real line or the half-line, often lead to some discrete eigenvalues plus a continuous spectrum. Actually, the usual numerical approximation typically involves three processes:

1. reduction to a finite interval;
2. discretization;
3. application of a numerical eigenvalue solver.

Reduction to a finite interval and discretization typically eliminate the continuous spectrum. Even if we do not truncate a priori the domain on which the problem is formulated such an inherent reduction can not be avoided.

It can be argued that, generally speaking, in solving various differential problems, the Chebfun software provides a greater flexibility than the classical spectral methods. This fact is fully true for regular problems.

Unfortunately, in the presence of various singularities, the maximum order of approximation N , of the unknowns can be reached ($N \geq 4000$) and then Chebfun issues a message that warns about the possible inaccuracy of the results provided.

We came out of this tangle using modified classical spectral methods. In this way, when we had serious doubts about the accuracy of the solutions given by Chebfun, we managed to establish the correctness of the numerical results.

As a matter of fact, in order to resolve a singularity on the ends of an unbounded integration interval, Chebfun uses only the arbitrary truncation of the domain. Classical spectral methods can also use this method, but it is not recommended. For singular points at finite distances (mainly origin) we will use the so-called *removing technique of independent boundary conditions*. The boundary conditions at infinity can be enforced using basis functions that satisfy these conditions (Laguerre, Hermite, sinc). An alternative method, which proved to be very accurate, is the Chebyshev collocation (ChC) method in combination with a change of variables (coordinates) which transform the half line into the canonical Chebyshev interval $[-1, 1]$. Then the removing technique of independent boundary conditions is essential in order to remove the singularities at the end points of integration interval.

A Chebfun code and two MATLAB codes, one for ChC and another for SiC method, are provided in order to exemplify. With minor modifications they could be fairly useful for various numerical experiments.

The structure of this work is as follows. In Section 2 we recall some specific issues for the regular as well as singular Schrödinger eigenproblems. The main comment refers to the notion of *mixed spectrum*. In Section 3 we review on the Chebfun structure and the classical spectral methods (differentiation matrices, enforcing boundary conditions, etc.). The Section 4 is the central part of the paper. Here we analyze some benchmark problems. In order to separate the “good” from the “bad” eigenvalues we estimate their relative drift with respect to some parameters. The accuracy in computing eigenfunctions is estimated by their departure from orthogonality. We end up with Section 5 where we underline some conclusions and suggest some open problems.

2. Regular and singular Schrödinger eigenproblems

The Schrödinger equation reads

$$u'' + [\lambda - q(x)]u = 0, \quad -\infty \leq a < x < b \leq +\infty. \quad (1)$$

It is a Liouville normal form of a general Sturm-Liouville (SL) equation where λ is proportional with the *energy levels* of the physical system, $q(x)$ is directly proportional with the *potential energy* and the

“wave function” u may be real or complex such that $u^* u dx = |u|^2 dx$ is the probability that the particle under consideration will be “observed” in the interval $(x, x + dx)$. In problems involving Schrödinger equations, it is customary among chemists and physicists to define the *spectrum* of this Sturm-Liouville problem as the all eigenvalues λ for which eigenfunctions u exist. The set of isolated points (if any) in this spectrum is called the *discrete spectrum*; the part (if any) that consists of entire interval is called *continuous spectrum*. We shall adopt this suggestive terminology here.

The equation (1) can be given on a finite, semi-infinite, or infinite interval. Only on a closed and finite interval $a \leq x \leq b$ can Schrödinger equation be associated with a *regular* Sturm-Liouville problem. If the interval of definition is semi-infinite or infinite, or is finite and $q(x)$ vanishes at one or both endpoints, or if q is discontinuous, we can not obtain from (1) a regular Sturm-Liouville problem. In any such case, the Schrödinger equation (1) is called *singular*. We obtain a *singular eigenproblem* from a singular Schrödinger equation by imposing suitable homogeneous boundary conditions. They can not always be described by formulae like $\alpha u(e) + \beta u'(e) = 0$, where e can be the end point a or b . For instance, the condition that u be bounded near a singular end point, which can be finite or $\pm\infty$, is a common boundary condition defining a singular eigenproblem. For regular SL problems, it is proved (see for instance [12]) that the spectrum is always discrete, and the eigenfunctions are (trivially) square-integrable. For singular problems the situation is completely different. For instance in their textbook [12] Birkhoff and Rota consider the eigenproblem attached to the *free particle* equation and show that the spectrum of the free particle is continuous. Some software packages have been designed over time to solve various singular SL problems. The most important would be SLEIGN and SLEIGN2, SLEDGE, SL02F and MATSLISE. The SLDRIVER interactive package supports exploration of a set of SL problems with the four previously mentioned packages. In [13] (see also [14]) the authors designed the software package SLEDGE. They observed that for a class of singular problems their method either fails or converges very slowly. Essentially, the numerical method used in this software package replaces the coefficient function $q(x)$ by step function approximation. Similar behavior has been observed on the NAG code SL02F introduced in [15] and [16] as well as on the packages SLEIGN and SLEIGN2 introduced in [17] and [18]. The MATSLISE code introduced in [19] can solve some Schrödinger eigenvalue problem by a constant perturbation method of a higher order.

The main purpose of this paper is to argue that Chebfun, along with the spectral collocation methods, can be a very feasible alternative to these software packages regarding accuracy, robustness as well as simplicity of implementation. In addition, these methods can compute the “whole” set of eigenvectors and provide some details on the accuracy and numerical stability of the results provided.

3. Chebfun vs. spectral collocation (ChC, LGRC, SiC)

3.1. Chebfun

The Chebfun system, in object-oriented MATLAB, contains algorithms which amount to spectral collocation methods on Chebyshev grids of automatically determined resolution. Its properties are briefly summarized in [2]. In [1] the authors explain that *chebops* are the fundamental Chebfun tools for solving ordinary differential (or integral) equations. One may then use them as tools for more complicated computations that may be nonlinear and may involve partial differential equations. This is analogous to the situation in MATLAB itself. The implementation of chebops combines the numerical analysis idea of spectral collocation with the computer science idea of *lazy or delayed evaluation of the associated spectral discretization matrices*. The grammar of chebops along with a lot of illustrative examples is displayed in the above quoted paper as well as in the text [5]. Thus one can get a suggestive image of what they can do.

In [1] p.12 the authors explain clearly how the Chebfun works, i.e., it solves the eigenproblem for two different orders of approximation, automatically chooses a reference eigenvalue and checks the convergence of the process. At the same time, it warns about the possible failures due to the high non-normality of the analyzed operator (matrix).

Actually, we want to show in this paper that Chebfun along with chebops can do much more, i.e., can accurately solve highly (double) singular Schrödinger eigenproblems.

3.2. ChC, LGRC and SiC

In the spectral collocation method the unknown solution to a differential equation is expanded as a global interpolant, such as a trigonometric or polynomial interpolant. In other methods, such as f. e. and f. d., the underlying expansion involves local interpolants such as piecewise polynomials. This means that the accuracy of spectral collocation is superior. For problems with smooth solutions convergence rates are typically of order e^{-cN} or $e^{-c\sqrt{N}}$ where N is the order of approximation or resolution, i.e., the number of degree of freedom in expansion. In contrast, f. e. or f. d. yield convergence rates that are only algebraic in N , typically of orders N^{-2} or N^{-4} . The net superiority of global spectral methods on local methods is discussed in detail in [20]. In all spectral collocation methods designed so far we have used the collocation differentiation matrices from the seminal paper [9]. We preferred this MATLAB differentiation suite for the accuracy, efficiency as well as for the ingenious way of introducing various boundary conditions.

In order to impose (enforce) the boundary conditions we have used two methods that are conceptually different, namely the *boundary bordering* as well as the *basis recombination*. A very efficient way to accomplish the boundary bordering is available in [21] and is called *removing technique of independent boundary conditions*. We have used this technique in the large majority of our papers except [22] where the latter technique has been employed. In the last quoted paper a modified Chebyshev tau method based on basis recombination has been used in order to solve an Orr-Sommerfeld problem with an eigenparameter dependent boundary condition. Even in eigenproblems that contain the spectral parameter in the definition of the boundary conditions we have used the boundary bordering technique (see [23]).

In [24] (see also [25]) we have solved some multiparameter eigenproblems (MEP) which come from separation of variables, in several orthogonal coordinate systems, applied to the Helmholtz, Laplace, or Schrödinger equation. Important cases include Mathieu's system, Lamé's system, and a system of spheroidal wave functions. We show that by combining spectral collocation methods, ChC and LGRC, and new efficient numerical methods for solving algebraic MEPs, it is possible to solve such problems both very efficiently and accurately. We improve on several previous results available in the literature, and also present a MATLAB toolbox for solving a wide range of problems.

3.3. The drift of eigenvalues

Two techniques are used in order to eliminate the “bad” eigenvalues as well as to estimate the stability (accuracy) of computations. The first one is the *drift*, with respect to the order of approximation or the scaling factor, of a set of eigenvalues of interest. In a simplified form this concept has been introduced by J. P. Boyd in [26]. The second one is based on the check of the *eigenvectors' orthogonality*.

In other words, we want to separate the “good” eigenvalues from the “bad” ones, i.e., inaccurate eigenvalues. An obvious way to achieve this goal is to compare the eigenvalues computed for different orders of some parameters such as the approximation order (cut-off parameter) N or the scaling factor. Only those whose difference or “resolution-dependent drift” is “small” can be believed. Actually, in [26] the so called *absolute (ordinal) drift* with respect to the order of approximation has been introduced.

We extend this definition to the following one. The *absolute (ordinal) drift* of the j th eigenvalue with respect to the parameter α is defined as

$$\delta_{j,absolute,\alpha} := \left| \lambda_j^{(\alpha_1)} - \lambda_j^{(\alpha_2)} \right|, \quad \alpha_1 \neq \alpha_2, \quad (2)$$

where $\lambda_j^{(\alpha)}$ is the j th eigenvalue, after the eigenvalues have been sorted, as computed using a specific value of the parameter. In the most common cases this parameter can be N or c .

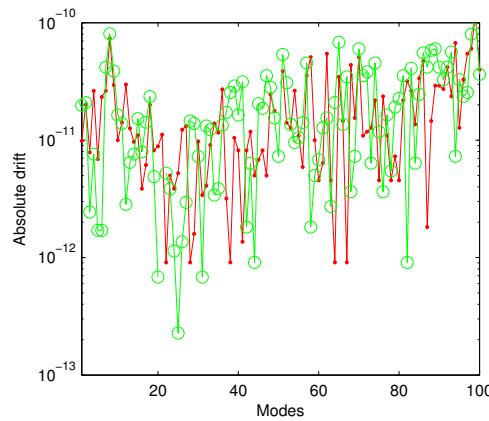


Figure 1. The drift of the first 100 eigenvalues of Coffey-Evans problem. ChC used the orders of approximations $N_1 := 256$ and $N_2 := 512$ -red dotted line and respectively $N_1 := 400$ and $N_2 := 512$ -green circled line.

The dependence of $\delta_{j,absolute,\alpha}$, $j = 1, 2, \dots, Ne$, where Ne is the number of analyzed eigenvalues, on the index (mode) j will be displayed in a log-linear plot. If we divide the right hand side of (2) by $|\lambda_j^{(a_1)}|$ we get the so called *relative drift* denote by $\delta_{j,relative,\alpha}$.

4. Numerical benchmark problems and discussions

4.1. A regular Schrödinger eigenproblem

The bounded Coffey-Evans potential reads

$$q(x) := -2\beta \cos(2x) + \beta^2 \sin^2(2x), \quad \beta \in \mathbb{R}. \quad (3)$$

We attach to equation (1) the homogeneous Dirichlet boundary conditions $u(\pm\pi/2) = 0$ and use $\beta := 30$. In spite of being regular, the Coffey-Evans problem is one of the most difficult test problems in the literature because there are very close eigenvalue triplets as β increases.

We have used a short Chebfun code in order to solve this regular eigenproblem. It is available in the next lines. With appropriate changes, this code can be used to analyze any other Schrödinger eigenproblem.

```
dom=[-pi/2,pi/2];
x=chebfun('x',dom);beta=30; sigma=-1;
L=chebop(dom);
L.op=@(x,y) -diff(y,2)+(-2*beta*cos(2*x)+(beta*sin(2*x))^2)*y;
L.rbc=0; L.lbc=0; N=201;
[V,D]=eigs(L,N,sigma); D=diag(D)
```

The eigenvalues obtained by ChC and Chebfun are extremely close, practically indistinguishable. They also compare very well with those computed in [27] by some coefficient approximation methods of orders 2, 4 and 8 and reported in Table 3 of this paper.

The absolute drift reported in Fig. 1 means that we can compute the first hundred eigenvalues with better accuracy than 10^{-10} . Unfortunately no accuracy analysis is reported in [27] (see also [19] and [28]). The eigenvectors are either symmetric (the even ones) or anti-symmetric (the odd ones). The first four of them are depicted in Fig. 2. They look fairly smooth and satisfy the boundary conditions. The Chebyshev coefficients of the first four eigenvectors of Coffey-Evans problem computed by Chebfun are displayed in Fig. 3. These coefficients decrease sharply and smoothly to a rounding-off plateau below 10^{-15} . Roughly speaking this means they are computed with the machine precision.

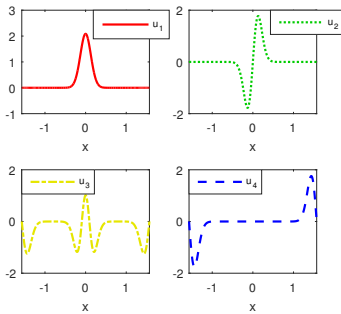


Figure 2. The first four eigenvectors of Coffey-Evans problem computed by Chebfun.

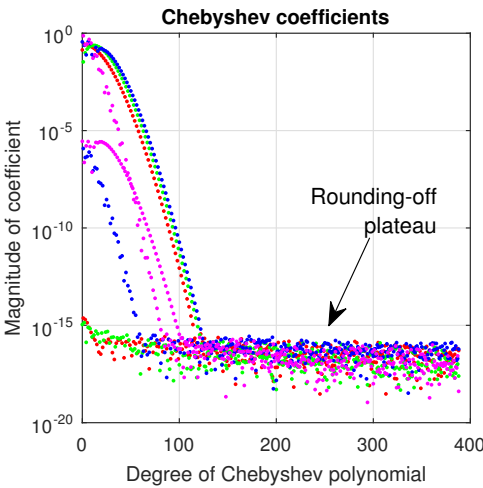


Figure 3. The Chebyshev coefficients of the first four eigenvectors of Coffey-Evans problem computed by Chebfun.

Table 1. High index eigenvalues of Schrödinger eigenproblem equipped with Coffey-Evans potential (3) computed by three different methods.

j	λ_j by Chebfun	λ_j computed in [27]	λ_j by ChC
20	951.878 806 795 878 3	951.878806796591	951.8788067965993
30	1438.295244640637	1438.295244640802	1438.295244640797
40	2146.405360539156	2146.405360539854	2146.405360539845
50	3060.923491511540	3060.923491511421	3060.923491511401
100	10653.52543568510	10653.525435875921	10653.52543587600
200	40851.63764596094	40851.637646050455	40851.63764605047

For this potential the first eigenvalue λ_0 is close to zero (actually we have got $\lambda_0 = -6.254\,959\,429\,708\,980 \cdot 10^{-12}$) and there are very close eigenvalue triplets $(\lambda_2, \lambda_3, \lambda_4)$, $(\lambda_6, \lambda_7, \lambda_8)$, \dots as β increases. The common numeric part of the eigenvalues in the first triplet is 2.31664929 and that of the eigenvalues in the second is a little shorter, i.e. 4.45283.

4.2. Two singular Schrödinger eigenproblem on the half line

In this section we study the *mixed spectrum* of some Schrödinger eigenproblems having a “potential well” dying out at infinity.

4.2.1. Hydrogen atom equation

The first example consists in the equation (1) equipped with the potential

$$q(x) := -\frac{1}{x} + \frac{l(l+1)}{x^2}, \quad l \in \mathbb{R}, \quad (4)$$

along with the boundary conditions

$$u(0) = 0, \quad u \rightarrow 0 \text{ as } x \rightarrow \infty. \quad (5)$$

The problem (1)-(4)-(5) is clearly singular. We must mention from the beginning that our numerical experiments performed with LGRC and Chebfun together with the truncation of the domain did not produce satisfactory results. In these conditions we have resorted to the *mapped ChC method*.

In order to implement this method we use the *algebraic map*

$$x := c \frac{1+s}{1-s}, \quad s \in [-1, 1], \quad x \in [0, +\infty), \quad c \in \mathbb{R}, \quad c > 0, \quad (6)$$

which, for each c , transforms the interval $[-1, 1]$ into the half line, and its inverse. The parameter c is free to be tuned for optimum accuracy.

The mapping (6) has been introduced in [29] where its practical effects have been discussed. The author observed that the convergence of the Chebyshev expansion is governed by the closeness of the singularities of the function being expanded to the expansion region. The major effect of such mapping is to allow us to move the singularities further away from the expansion region. The mapping may also weaken the effect of the singularities by modifying the strength of the singularity as well as moving it. The value of the scaling parameter c used in our computation was chosen essentially by trial and error along with the drift with respect to this parameter.

In order to write down any second order differential equation in independent variable s , we need the following derivatives:

$$\begin{aligned} u'(x) &= u'(s) \frac{1}{x'_s}, \quad x'_s = \frac{2c}{(1-s)^2}, \\ u''(x) &= u''(s) \frac{1}{(x'_s)^2} - u'(s) \frac{x''_s}{(x'_s)^3}. \end{aligned} \quad (7)$$

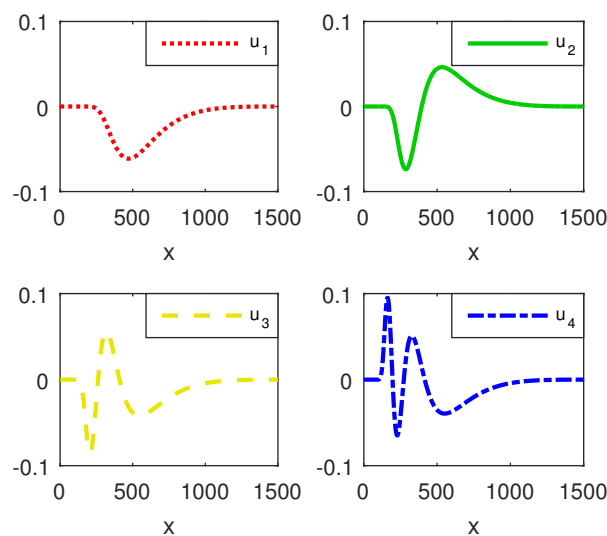


Figure 4. The first four eigenvectors for hydrogen atom eigenproblem (1)-(4)-(5) with $l := 1$ computed by mapped ChC with scaling factor $c := 2$ and $N := 512$.

Now it is easy to write the differential equation for $u(s)$ and to attach to this new equation the homogeneous Dirichlet boundary conditions $u(\pm 1) = 0$. As usual we implement these conditions by deleting the first and the last rows and columns of the collocation matrix attached to the left hand side of the equation (1)-(4). This is the most simplified version of removing technique of the independent boundary conditions introduced in [21]. With (7) the following MATLAB code solve this problem.

```
% approximation order and parameter l
N=1600; l=1;
% number of displayed eigenvalues
Ne=50;
c=2;          % scaling factor
% Chebyshev differentiation matrices (Weideman & Reddy)
[st,D]=chebdif(N,2);
% N-2 kept nodes; 1 and N are removed nodes
k=2:N-1; s=st(k);
% enforced boundary conditions in differentiation matrices
D2=D(k,k,2); D1=D(k,k,1);
% collocation matrix of the system
A=-diag((1-x).^4)*D2/(4*(c^2))+diag((1-x).^3)*D1/(2*(c^2))+...
    diag(l*(l+1)*((1-x).^2)./(((1+x).^2)*(c^2))-(1-x)./(c*(1+x))));
% computed and sorted eigenpairs
[U,S]=eig(A); S=diag(S); [t,o]=sort(S); S=S(o); U=U(:,o);
disp(S(1:Ne))
% Chebyshev coefficients of the first four eigenvectors by FCT
Ucoeff=fcgltran(U(:,1:4),1);
```

The first four vectors of the problem are displayed in Fig. 4. It is clear that they satisfy both boundary conditions but in the right neighborhood of origin they have a totally different behavior from the eigenvectors of regular problems, i.e., they vanish out on continuous portions and not in discrete points. However, they clearly approximate square-integrable eigenfunctions and thus confirm some theoretical results proved in [12]. Their Chebyshev coefficients obtained using FCT (fast Chebyshev transform-see [30] for details) are displayed in Fig.5. They decrease sharply and smoothly to some

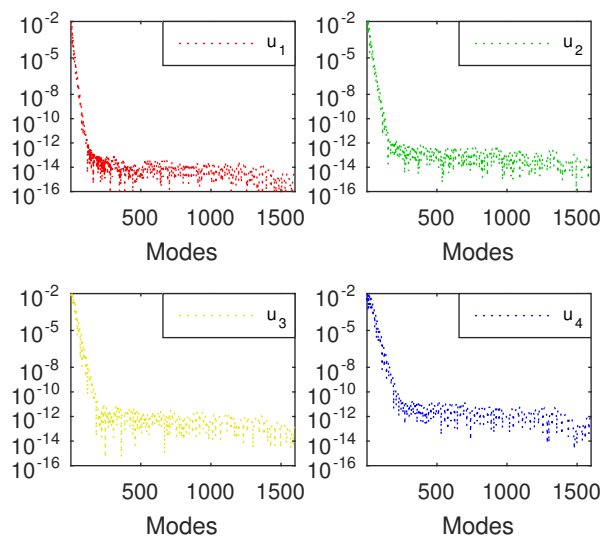


Figure 5. The coefficients of the first four eigenvectors for hydrogen atom eigenproblem (1)-(4)-(5) with $l := 1$ computed by mapped ChC with scaling factor $c := 2$ and $N := 1600$.

limits, followed by a wide rounding-off plateau. For the first vector (the rightmost one) this limit is around 10^{-13} . It increases with the index of the vector. Roughly this means that we cannot hope for a better approximation than something of the order 10^{-13} when computing the first eigenvector.

When $N := 2048$ mapped ChC has found $\lambda_0 = -6.250\,000\,000\,166\,379 \cdot 10^{-02}$ which is a very good approximation of $-1/16$. The largest negative eigenvalue has been $\lambda_{66} = -7.865\,782\,521\,027\,431 \cdot 10^{-07}$ and the next eigenvalue, the smallest positive has been computed as $\lambda_{67} = 6.517\,056\,834\,998\,433 \cdot 10^{-05}$. To see how the mapped ChC method simulates the notion of continuous spectrum we will provide in Table 2 some significant eigenvalues.

Table 2. High index eigenvalues of hydrogen atom eigenproblem (1)-(4)-(5).

j	λ_j by mapped ChC
70	$3.346\,710\,010\,488\,799 \cdot 10^{-4}$
80	$2.246853675452558e - 3$
90	$6.551029735506819e - 3$
100	$1.474442763764248e - 2$
110	$2.890880952550005e - 2$
120	$5.183912194697291e - 2$

In the monograph [12] Sect. 18 it is proved that if the potential $q(x)$ is continuous and has the asymptotic behaviour $q(x) = \frac{A}{x} + O\left(\frac{1}{x^2}\right)$ as $x \rightarrow \infty$, for $\lambda > 0$ the spectrum is continuous and the eigenfunctions are not square-integrable and for $\lambda < 0$ the spectrum is discrete and the eigenfunctions are square-integrable. The numerical results gathered around this problem plainly confirm this analytical result.

Actually the eigenvector corresponding to the first positive eigenvalue (the sixty-seventh one) is depicted in the left panel of Fig. 7. It is hard to believe that this could approximate a square-integrable eigenfunction. In the right panel of the same figure we displayed the Chebyshev coefficients of the corresponding eigenvector. The oscillations of these coefficients mimic the steep oscillations of the eigenvector.

For the real *scaling factor* c we have to mention that in case of eigenvalue problems it can be adjusted only on the mathematical basis. Thus, it can be tuned in order to:

- improve the decaying rate of the coefficients of spectral expansions.

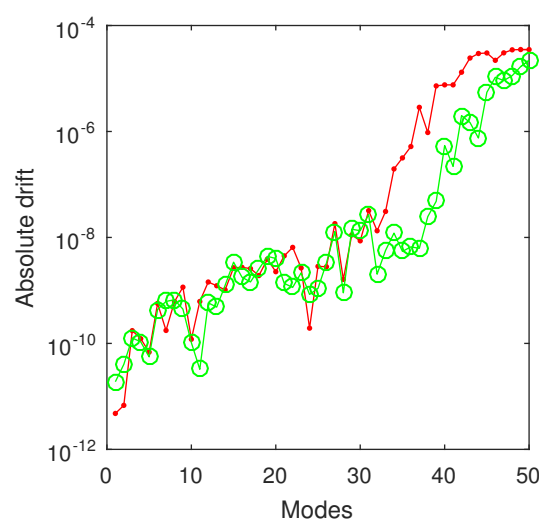


Figure 6. The absolute drift with respect to N of the first 50 negative eigenvalues of hydrogen atom eigenproblem (1)-(4)-(5) computed by mapped ChC with scaling factor $c := 2$ and $N_1 := 1600$ and $N_1 := 2048$ (red line). The green circled line signifies the drift of eigenvalues computed by mapped ChC using $N := 2048$ with respect to the exact eigenvalues $\lambda_n = -1/(2n+4)^2$, $n = 0, 1, 2, \dots, 50$ corresponding to $l := 1$.

- find as orthogonal as possible eigenvectors to an eigenproblem;

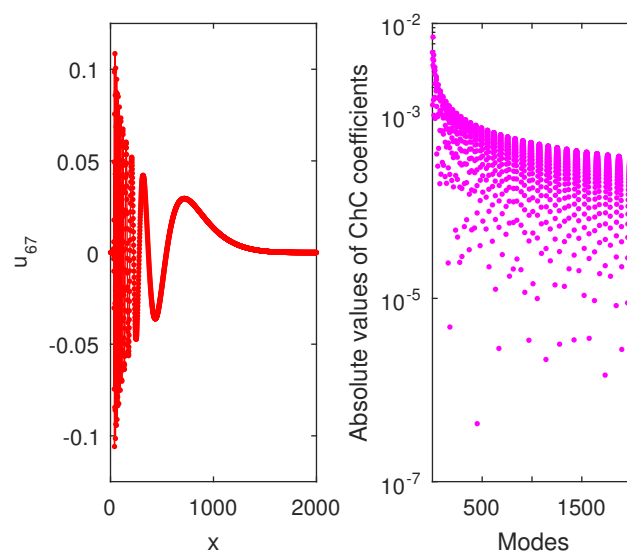


Figure 7. (a) The eigenvector corresponding to the first positive eigenvalue of hydrogen atom eigenproblem (1)-(4)-(5) computed by mapped ChC with scaling factor $c := 2$ and $N := 2024$, $l := 1$. (left panel). (b) In the right panel, in a log-linear plot we display the Chebyshev coefficients of this eigenvector.

4.2.2. Potential with a Coulomb type decay

Let's consider now the Schrödinger equation (1) equipped with the potential (8)

$$q(x) := -\frac{1 - 5 \exp(-2x)}{x} + \frac{l(l+1)}{x^2}, \quad l \in \mathbb{R}. \quad (8)$$

and supplied with boundary conditions (5). Some eigenvalues computed by ChC method when $c := 2$ and $N := 512$ are compared in Table 3 with their counterparts computed by LGRC and perturbation methods. If for the first eigenvalues the coincidence is excellent, the same does not happen for higher indices. That is why in Fig. 8 in a log-linear plot we illustrate the absolute drift in the case of the ChC method. It is observed that, for instance for the tenth mode, the difference between the values of this eigenvalue calculated with two very different orders of approximation N is of the order 10^{-10} . This leads us to believe that the eigenvalues computed with ChC are the most accurate. It is also clear from this figure that in the second case, i.e., $N_1 := 760$ and $N_2 := 1024$ the drift oscillates less than in the first case reported in this figure.

Table 3. The first five eigenvalues and the tenth one of the Schrödinger problem (1)-(5) when the potential has a Coulomb-type decay (8), computed by three different methods.

j	λ_j computed by LGRC in [8]	λ_j computed in [28]	λ_j by mapped ChC
1	-0.061 681 846 633 3	-0.061681846633	-0.06168184663316705
2	-0.0274980999429	-0.027498099943	-0.02749809994382280
3	-0.0155015616910	-0.015501561691	-0.01550156169420540
4	-0.0099354968508	-0.009935496851	-0.009935496853885005
5	-0.0069067013822	-0.006906701382	-0.006906701375461869
10	-0.001963685230	-0.001736111111	-0.002059879612641054

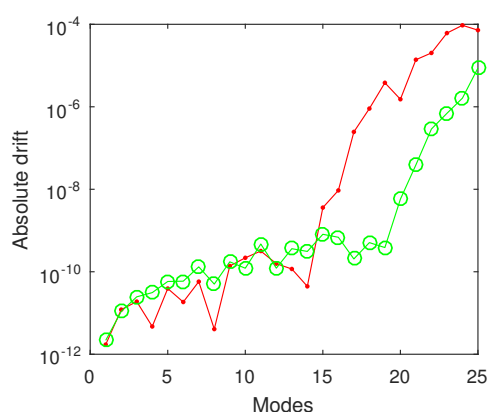


Figure 8. The absolute drift with respect to N of the first 25 eigenvalues for the Schrödinger problem (1)-(5) with Coulomb-type decay potential (8), computed by mapped ChC with scaling factor $c := 2$; red dotted line for the case $N_1 := 512$ and $N_2 := 1024$ and green circled line for the case $N_1 := 760$ and $N_2 := 1024$.

4.3. A singular Schrödinger eigenproblem on the real line

Let's consider now the equation (1) on the real line with the potential

$$q(x) := x^2 + \frac{vx^2}{1 + \mu x^2}, \quad (9)$$

where μ and v are real parameters. This is a more general (anharmonic) oscillator than the simpler harmonic one.

Two *behavioral* boundary conditions requiring the boundedness of the solutions at large distance, i.e., $x \rightarrow \pm\infty$ are attached to this equation. Actually we impose the conditions

$$u(x) \rightarrow 0 \text{ as } x \rightarrow \pm\infty. \quad (10)$$

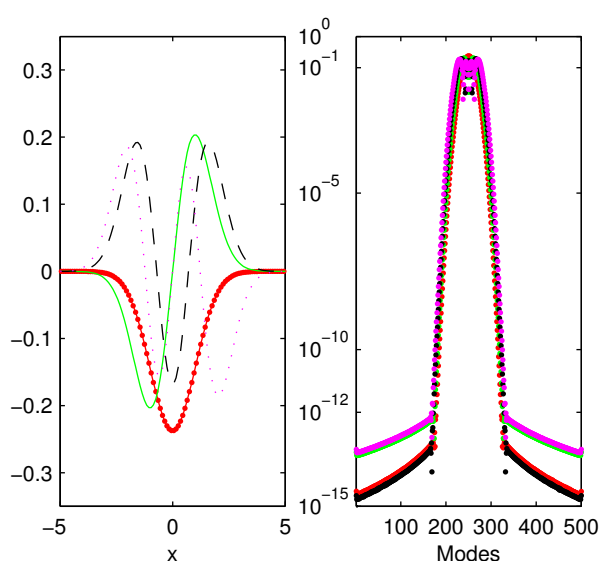


Figure 9. (a) Zoom in the first four eigenvectors computed by SiC for the Schrödinger eigenproblem (1)-(10) with potential (9) (left panel). (b) In the right panel we display the sinc coefficients for these vectors; red for the first, green for the second, black for the third and magenta for the fourth.

We have to observe that these conditions are automatically satisfied in spectral collocation based on Laguerre, Hermite and sinc functions.

SiC with $N := 500$ and scaling factor $h := 0.1$ has been used in order to produce the following results. The first four eigenvectors of Schrödinger eigenproblem (1)-(10) with potential (9) are displayed in the left panel of Fig. 9. Their coefficients are illustrated in the right panel of the same figure. These coefficients symmetrically decrease to approximations of at least 10^{-12} which means a reasonable accuracy of the method. We also have computed some *high-lying* eigenvalues namely λ_{100} , λ_{150} and λ_{200} , for $\nu := 1$ and $\mu := 500$. They have respectively the numerical values

$$199.001994801512, 301.001995781805, \text{ and } 403.001995224433.$$

They are five digits approximation for the corresponding harmonic oscillator eigenvalues $\lambda_n = 2n - 1$, $n = 1, 2, \dots$

In [31] the author solved this problem numerically for general ν and μ . He used a very elegant variational argument of Ritz type, based on Hermite functions, and observed that for large μ and fixed ν the eigenvalues of this problem approximate those of the harmonic oscillator. We have confirmed this observation even for higher index eigenvalues. In the left panel of Fig. 10 we display the relative drift of the first 200 eigenvalues of the problem. It is clear that approximately the first 70 eigenvalues are calculated with an accuracy better than 10^{-12} . Eigenvalues with index up to 150 remain at the same accuracy as $N \approx 500$. Above this index the accuracy decreases to 10^{-3} . Actually, over years, a lot of literature has gathered on this problem. Low order eigenvalues have accurately computed using Runge-Kutta type methods for instance in [32] and [33]. In [34] the author uses Hermite collocation in order to find only the first eigenvalues for some Schrödinger eigenproblem. With respect to the departure from orthogonality, i.e. the distance from zero of the scalar product of two eigenvectors, we display in the right hand side of Fig. 10, in a log linear plot, the absolute values of the of the scalar products of u_1 and u_j , $j = 2, \dots, 200$. It is again remarkable that this departure is less than 10^{-15} .

It is of some importance to justify our choice for SiC. Unlike all other methods of spectral collocation, where the differentiation matrices are highly non-normal, in SiC these matrices are symmetric or skew-symmetric for even respectively odd values of cut-off parameter N . And this is

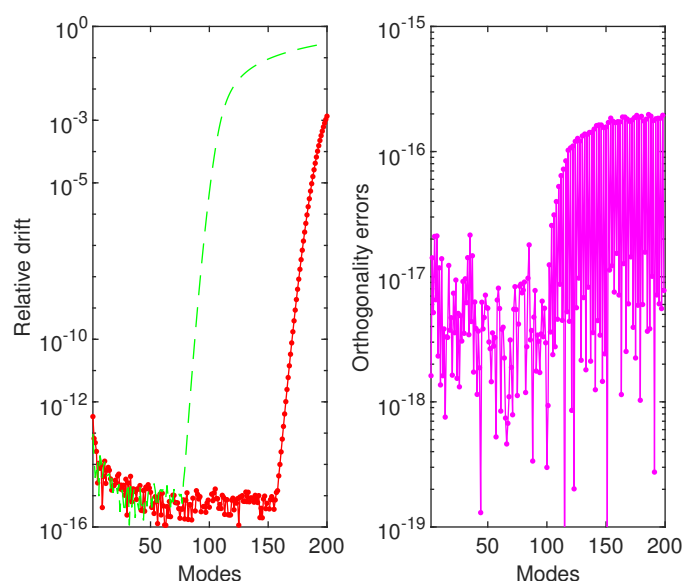


Figure 10. (a) The relative drift of the first 200 eigenvalues of problem (1)-(10) with potential (9), $N_1 := 500$ and $N_2 := 400$ -red dotted line and $N_1 := 300$ and $N_2 := 400$ - green line.(left panel). (b) In the right panel we display the orthogonality errors (deficiency) of the first eigenvector of the same problem with respect to the subsequent 199 of it.

an important numerical advantage. For instance in the MATLAB code below we use the routine *eigs* instead of *eig* which would have been more expensive and slower.

The following very simple MATLAB code has been used.

```
N=500; % order of approximation
h=0.1; % spacing (scaling factor)
[x,D]=sincdif(N,2,h); D2=D(:, :, 2); % 2nd SiC differentiation
nu=1; mu=500; % parameter of the problem
A=-D2+diag((x.^2)+nu*(x.^2)./(1+mu*(x.^2))); % the matrix
[V,D] = eigs(A,250,0); D=diag(D); % call MATLAB code eigs
[t,o]=sort(real(D)); D=D(o); V=V(:,o); % sort eigenvalues
```

This code is fairly similar with that from Section 4.2 with two differences. First, the Chebyshev differentiation matrices are replaced by sinc differentiation matrices and then the boundary conditions are absent. More exactly, the discrete sinc functions, on which the unknown solution is expanded, are defined by

$$S_k(x, h) := \frac{\sin\left[\frac{\pi}{h}(x - x_k)\right]}{\frac{\pi}{h}(x - x_k)}, \quad k = 1, 2, \dots, N, \quad (11)$$

and satisfy the boundary conditions (10). In (11) the nodes x_k are equidistant with spacing h and symmetric with respect to the origin.

5. Concluding remarks and open problems

Regarding the regular problems, Chebfun is unbeatable in terms of accuracy, computation speed, and the information they provide on the accuracy of computational process. It displays the optimal approximation order of unknowns (eigenvectors) and how and to what extent their Chebyshev coefficients decrease. It also specifies the degree to which some boundary conditions are satisfied.

As for the singular problems, the situation is not so offering. In this case, Chebfun leaves enough room for the application of usual (classical) spectral methods. For singular eigenproblems on

unbounded domains mapped ChC on the half line and SiC, for problems on the real line, perform better than Chebfun even for Chebfun applied on a mapped domain.

However, approaching these problems in parallel, with Chebfun as well as with the classical spectral methods, one can get greater confidence in the accuracy of numerical results. Regarding ChC method, using the so-called absolute or relative drift in terms of some parameters we ensure the numerical stability of the numerical process and can eliminate (numerically) spurious eigenvalues. In other words we get automatically and precisely the accuracy at which a specified set of eigenvalues is computed. The departure of orthogonality of a set of eigenvectors provides a useful hint for the accuracy of the numerical process. We have managed to correctly identify sets of multiple and high indices eigenvalues (triples) and even give some numerical meaning to the notion of continuous spectrum. This second issue obviously remains an open one.

All in all we can say that Chebfun as well as classical spectral methods in various forms, produce more accurate and comprehensive outcomes when solving singular and of course regular eigenproblems than classical methods. However, there remains an open problem, namely that of establishing (possibly automatically) the scaling factor.

Abbreviations

The following abbreviations are used in this manuscript:

c	scaling factor for unbounded domains
f.e.	finite element method
f. d.	finite difference method
GPS	generalized pseudospectral method
SL	Sturm-Liouville eigenproblem
ChC	Chebyshev collocation
LGRC	Laguerre Gauss Radau Collocation
SiC	sinc collocation
MATSLISE	Matlab package for SL and Schrödinger equations
MEP	Multiparameter Eigenvalue Problem
N	the order of approximation of spectral method (cutting-off parameter)
SLEDGE	SL Estimates Determined by Global Errors
SLEIGN	FORTTRAN package for numerical solution to SL eigenproblem
SLDRIVER	interactive package for the previous packages

1. Driscoll, T. A.; Bornemann, F.; Trefethen, L.N. The CHEBOP System for Automatic Solution of Differential Equations. *BIT* **2008**, *48* 701–723
2. Driscoll, T. A.; Hale, N.; Trefethen, L.N. Chebfun Guide. Pafnuty Publications, Oxford 2014
3. Driscoll, T. A.; Hale, N.; Trefethen, L.N. Chebfun-numerical computing with functions. <http://www.chebfun.org>. Accessed 15 November 2019
4. Olver, S.; Townsend, A. A fast and well-conditioned spectral method. *SIAM Rev.* **2013**, *55*, 462–489
5. Trefethen, L.N.; Birkisson, A.; Driscoll, T. A. Exploring ODEs. SIAM, Philadelphia 2018
6. Trefethen, L.N.: Approximation Theory and Approximation Practice, Extended Edition. SIAM, Philadelphia 2019
7. Gheorghiu, C.I. Spectral Methods for Non-Standard Eigenvalue Problems. Fluid and Structural Mechanics and Beyond. Springer-Verlag, Cham Heidelberg New-York Dordrecht London 2014
8. Gheorghiu, C.I. Spectral Collocation Solutions to Problems on Unbounded Domains. Casa Cărții de Știință Publishing House, Cluj-Napoca, Romania 2018
9. Weideman, J. A. C.; Reddy, S. C., A MATLAB Differentiation Matrix Suite. *ACM T. Math. Software* **2000**, *26*, 465–519
10. Roy, A.K. The generalized pseudospectral approach to the bound states of the Hulthén and the Yukawa potentials. *PRAMANA-journal of physics* **2005**, *65*, 1–15

11. Shizgal, B.D., Pseudospectral Solution of the Fokker-Planck Equation with Equilibrium Bistable States: the Eigenvalue Spectrum and the Approach to Equilibrium. *J. Stat. Phys.* **2016**, <https://doi.org/10.1007/s10955-016-1594-9>
12. Birkhoff, G.; Rota, G-C. Ordinary Differential Equations, Fourth Edition, John Wiley and Sons, New York Chichester Brisbane Toronto Singapore 1989; pp. 336–343
13. Pruess, S.; Fulton, C. T. Mathematical Software for Sturm-Liouville Problem. *ACM T. Math. Software* **1993**, *19*, 360–376
14. Pruess, S.; Fulton, C. T.; Xie, Y. An Asymptotic Numerical Method for a Class of Singular Sturm-Liouville Problems. *SIAM J. Numer. Anal.* **1995**, *32*, 1658–1676
15. Marletta, M.; Pryce, J.D. LCNO Sturm-Liouville problems computational difficulties and examples. *Numer. Math.* **1995**, *69*, 303–320
16. Pryce, J.D.; Marletta, M. A new multi-purpose software package for Schrödinger and Sturm-Liouville computations. *Comput. Phys. Comm.* **1991**, *62*, 42–54
17. Bailey, P. B.; Everitt, W. N.; Zettl, A. Computing Eigenvalues of Singular Sturm-Liouville Problems. *Results Math.* **1991**, *20*, 391–423
18. Bailey, P.B.; Garbow, B.; Kaper, H.; Zettl, A. Algorithm 700: A FORTRAN software package for Sturm-Liouville problems. *ACM T. Math. Software* **1991**, *17*, 500–501
19. Ledoux, V.; Van Daele, M.; Vanden Berghe, G. MATSLISE: A MATLAB Package for the Numerical Solution of Sturm-Liouville and Schrödinger Equations. *ACM T. Math. Software.* **2005**, *31*, 532–554
20. Solomonoff, A.; Turkel, E. Global Properties of Pseudospectral Methods. *J. Comput. Phys.* **1989**, *81*, 230–276
21. Hoepffner, J. Implementation of boundary conditions. <http://www.lmm.jussieu.fr/~hoepffner/boundarycondition.pdf>. Accessed 25 Aug. 2012
22. Gheorghiu, C.I., Pop, I.S. A Modified Chebyshev-Tau Method for a Hydrodynamic Stability Problem. Proceedings of the International Conference on Approximation and Optimization (Romania) - ICAOR Cluj-Napoca, July 29 - August 1, Vol. II, 119–126 (1996); <http://ictp.acad.ro>
23. Gheorghiu, C.I. On the numerical treatment of the eigenparameter dependent boundary conditions. *Numer. Algor.* **2018**, *77*, 77–93
24. Gheorghiu, C.I.; Hochstenbach, M.E.; Plestenjak, B.; Rommes, J. Spectral collocation solutions to multiparameter Mathieu's system. *Appl. Math. Comput.* **2012**, *218*, 11990–12000
25. Plestenjak, B.; Gheorghiu, C.I.; Hochstenbach, M.E. Spectral collocation for multiparameter eigenvalue problems arising from separable boundary value problems. *J. Comput. Phys.* **2015**, *298*, 585–601
26. Boyd, J. P. Traps and Snares in Eigenvalue Calculations with Application to Pseudospectral Computations of Ocean Tides in a Basin Bounded by Meridians. *J. Comput. Phys.* **1996**, *126*, 11–20
27. Ledoux, V.; Van Daele, M.; Vanden Berghe, G. Efficient computation of high index Sturm-Liouville eigenvalues for problems in physics. *Comput. Phys. Commun.* **2009**, *180*, 241–250
28. Ledoux, V.; Ixaru, L.Gr.; Rizea, M.; Van Daele, M.; Vanden Berghe, G. Solution of the Schrödinger equation over an infinite integration interval by perturbation methods, revisited. *Comput. Phys. Commun.* **2006**, *175*, 612–619
29. Schonfelder, J.L. Chebyshev Expansions for the Error and Related Functions. *Math. Comput.* **1978**, *32*, 1232–1240
30. von Winckel, G. Fast Chebyshev Transform (1D). <https://www.mathworks.com/matlabcentral/fileexchange/4591-fast-chebyshev-transform-1d>. Accessed 15 May 2015
31. Mitra, A.K. On the interaction of the type $\frac{vx^2}{1+\mu x^2}$. *J. Math. Phys.* **1978**, *19*, 2018–2022
32. Simos, T.E. Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. *J. Math. Chem.* **1998**, *24*, 23–37
33. Simos, T.E. An accurate finite difference method for the numerical solution of the Schrödinger equation. *J. Comput Appl. Math.* **1998**, *91*, 47–61
34. Trif, D. Matlab package for the Schrödinger equation. *J. Math. Chem.* **2008**, *43*, 1163–1176