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Numerical methods for solving radial Schrödinger equations

G. VANDEN BERGHE, V. FACK and H.E. DE MEYER
Laboratorium voor Numerieke Wiskunde en Informatica, Rijksuniversiteit Gent, Krijgslaan 281-S9, B9000 Gent, Belgium

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Abstract: An algorithm previously introduced by Brown et al. (1963) for solving radial Schrödinger equations is revisited and implemented in a more accurate way. The method is firstly applied to equations where potentials are present which are finite at the origin and which have an asymptotic behaviour $V(r) \to 0$ as $r \to \infty$. Typical examples of potentials belonging to that class are the Woods–Saxon and the Morse potential. Furthermore the method is also used for Coulomb-like potentials such as the Hulthén and the Hellmann potential. A comparison between the approximated numerical values and other available numerical and exact bound state energies is made.

Keywords: Two-point boundary, Schrödinger equation, shooting method, numerical.

1. Introduction

In the last decade a great deal of interest has been shown to the analytical as well as to the numerical study of the discrete spectrum of radial Schrödinger equations of the type

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - f(E, r)\right) u(r) = 0,$$

where

$$f(E, r) = \frac{l(l+1)}{r^2} - (E - V(r)). \tag{1.1}$$

In this paper we consider at first instance potentials $V(r)$ which are finite at the origin and which have an asymptotic behaviour $V(r) \to 0$ as $r \to \infty$. Following typical examples of potentials belong to that class:

- the Woods—Saxon potential

$$V_1(r) = \frac{u_0}{1+t} + \frac{u_1 t}{(1+t)^2}, \quad t = \exp\left[\frac{r - r_0}{a}\right]; \tag{1.2}$$

- the Morse potential

$$V_2(r) = D(\mathrm{e}^{-2\alpha x} - 2\,\mathrm{e}^{-\alpha x}), \quad x = \frac{r - r_0}{r_0}. \tag{1.3}$$

For $V_1(r)$ only approximate or numerical values for the eigenvalues E are available. In the last year many multistep algorithms were developed to obtain solutions of the radial equation (1.1)

with $V(r) = V_1(r)$. The first significant contribution amongst these came from Raptis and Allison [14], who on the basis of some information on the solution were able to write a two-step Numerov-like scheme. Ixaru and Rizea [11] compare three four-step methods and a piecewise constant perturbation method. For the Morse potential $V_2(r)$ closed expressions for bound-state eigenvalues with $l = 0$ are available [6]. For the states with $l \neq 0$ only approximate formulae for the eigenvalues are known.

Furthermore, we also consider potentials which are Coulomb-like at the origin and which have an asymptotic behaviour $V(r) \to 0$ as $r \to \infty$. Following typical examples of potentials belong to that class:

- the Hellmann potential [7]

$$V_3(r) = -\frac{A}{r} + \frac{B\, e^{Cr}}{r}, \tag{1.4}$$

with A and B the strengths of the constituent Coulomb and Yukawa potentials, respectively and C the so-called screening parameter;

- the Hulthén potential [9]

$$V_4(r) = \frac{-2Z}{\alpha} \frac{e^{-r}}{1 - e^{-r}}, \tag{1.5}$$

with α the screening parameter and where Z can be regarded as the charge of the nucleus.

The bound-state energies of (1.4) have been studied elaborately by Adamowsky [2], for various sets of values of B and C in a variational framework using ten variational parameters. The energy eigenvalues have been predicted for a wide range of the quantum numbers n and l. Dutt et al. [5] have investigated the bound-state properties of (1.4) using the shift $1/N$ expansion method. It appears that for certain regions of values of the B and C parameters convergence of the series expansion for the energy eigenvalues is in serious trouble for certain quantum states. The obtained results are not as accurate as the ones obtained by Adamowsky. Amongst the various methods which have been proposed in order to evaluate bound-state energies of the Hulthén potential (1.5) for $l \neq 0$, the Padé approximation method of Lai and Lin [12] and the dynamical group approach of Matthys and De Meyer [13] yield fairly accurate results.

In the present paper we like to extend a previously introduced algorithm [3] based upon an integration of the Schrödinger equation outwards from the origin to some matching-radius R_m and upon an integration inwards from some large distance R_∞, where the asymptotic solution is known.

In Section 2 the mathematical derivation of the method is reviewed, while in Section 3 the implementation of the method and discretized versions of occurring integrals, derivatives, etc. are introduced. In Section 4 a detailed numerical illustration is given and the accuracy of the introduced method will be discussed.

2. The numerical method

Starting from the radial Schrödinger equation we wish to find the discrete spectrum E for which the wave functions obey the Dirichlet boundary conditions

$$\lim_{r \to 0} u(r) \to 0, \qquad \lim_{r \to \infty} u(r) \to 0, \tag{2.1}$$

and also have the correct numbers of nodes. Since we shall integrate the equation outwards from the origin and likewise inwards from a large value R_∞ the asymptotic solution at the origin and at infinity has to be derived. For the potentials $V_1(r)$ and $V_2(r)$ finite at the origin, at small values of r, the term $l(l+1)/r^2$ dominates and (1.1) reduces to

$$\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2} + \left[(E - V(0)) - \frac{l(l+1)}{r^2}\right]u(r) = 0. \tag{2.2}$$

When $(E - V(0)) > 0$ the asymptotic solution reads $rj_l(Kr)$, where $j_l(z)$ is the spherical Bessel function and $K = \sqrt{E - V(0)}$. When $(E - V(0)) < 0$ one obtains as asymptotical solution $r\tilde{j}_l(K'r)$ with $\tilde{j}_l(z)$ a short notation for the modified spherical Bessel function and $K' = \sqrt{V(0) - E}$ [1].

The potential functions $V_3(r)$ and $V_4(r)$ have the following expansion in the vicinity of the origin:

$$V_i(r) = \frac{{}^{(i)}V_1}{r} + {}^{(i)}V_2 + {}^{(i)}V_3 r + \cdots, \quad i = 3, 4, \tag{2.3}$$

with

$${}^{(3)}V_1 = (-A + B), \qquad {}^{(3)}V_k = (-1)^{k-1}\frac{BC^{k-1}}{(k-1)!}, \quad k = 2, 3, \ldots, \tag{2.4}$$

and

$${}^{(4)}V_1 = \frac{Z}{\alpha}, \qquad {}^{(4)}V_2 = \frac{-Z}{6\alpha}, \qquad {}^{(4)}V_k = 0, \quad k \text{ odd},$$

$${}^{(4)}V_4 = \frac{Z}{15\alpha}\frac{1}{4!}, \qquad {}^{(4)}V_6 = -\frac{Z}{21\alpha}\frac{1}{6!}, \qquad {}^{(4)}V_8 = \frac{Z}{15\alpha}\frac{1}{8!}, \qquad {}^{(4)}V_{10} = -\frac{5Z}{33\alpha}\frac{1}{10!}. \tag{2.5}$$

The regular solution of (1.1) can then be expressed for sufficiently small r as

$$u(r) = r^{l+1}(a_1 + a_2 r + a_3 r^2 + \cdots). \tag{2.6}$$

By retaining a sufficient number of terms in the series expansion we can ensure the starting values in the vicinity of the origin are obtained with a suitable accuracy. The coefficients of (2.6) are given by:

$$a_1 = 1, \qquad 2(l+1)a_2 = V_1 a_1, \qquad 2(2l+3)a_3 = V_1 a_2 + (V_2 - E)a_1,$$

$$(i-1)(2l+i)a_i = V_1 a_{i-1} + (V_2 - E)a_{i-2} + \sum_{j=3}^{i-1} V_j a_{i-j}, \quad i > 3. \tag{2.7}$$

For the asymptotic behaviour at infinity, taking into account that $\lim_{r\to\infty} V(r) \to 0$, (1.1) reduces to

$$\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2} + E\,u(r) = 0, \tag{2.8}$$

delivering a solution $r\tilde{j}(K''r)$ with $K'' = \sqrt{|E|}$.

Integrating the equation outwards from the origin and inwards from R_∞, at any arbitrary radius R_m, if we have the correct eigenvalue E, the inner solution u_i and its derivative u_i' should

match the external solution u_e and its derivative u'_e. Since an arbitrary normalizing factor in the wave function is unimportant these conditions reduce to

$$L_i(E, R_m) = L_e(E, R_m), \tag{2.9}$$

with

$$L \equiv \frac{u'(E, r)}{u(E, r)} \equiv \frac{u'(r)}{u(r)}, \tag{2.10}$$

where we have explicitly indicated that the wave functions are E-dependent.

Starting with an initial guess for the unknown energy E, say $E + \Delta E$ we have on expanding in Taylor series around E,

$$\begin{aligned} L_e(E+\Delta E, R_m) - L_i(E+\Delta E, R_m) = {} & L_e(E, R_m) - L_i(E, R_m) \\ & + \Delta E\left(\frac{\partial L_e}{\partial E}(E, R_m) - \frac{\partial L_i}{\partial E}(E, R_m)\right) \\ & + \Theta\left((\Delta E)^2\right), \end{aligned} \tag{2.11}$$

where the first two terms on the right-hand side cancel because of (2.9). Taking into account the definition (2.10) for L one easily derives:

$$\begin{aligned} u^2(r)\frac{\partial L}{\partial E}(E, r) - u^2(r')\frac{\partial L}{\partial E}(E, r') &= \left[u(t)\frac{\partial u'}{\partial E}(t) - u'(t)\frac{\partial u}{\partial E}(t)\right]_{t=r'}^{t=r} \\ &= \int_{r'}^{r}\frac{\partial}{\partial t}\left[u(t)\frac{\partial u'}{\partial E}(t) - u'(t)\frac{\partial u}{\partial E}(t)\right] dt \\ &= \int_{r'}^{r}\left[u(t)\frac{\partial u''}{\partial E}(t) - u''(t)\frac{\partial u}{\partial E}(t)\right] dt. \end{aligned} \tag{2.12}$$

Since $u''(t) = f(E, t)u(t)$ (see (1.1)), it is easy to verify that

$$u(t)\frac{\partial u''}{\partial E}(t) - u''(t)\frac{\partial u}{\partial E}(t) = \frac{\partial f(E, t)}{\partial E}u^2(t) = -u^2(t). \tag{2.13}$$

Since $u(t) \to 0$ for $t \to 0$ and $t \to \infty$ one can derive from (2.11), taking into account (2.12) and (2.13), that

$$\begin{aligned} \Delta E \cong {} & -\left[L_e(E+\Delta E, R_m) - L_i(E+\Delta E, R_m)\right] \\ & \times\left[\frac{1}{u_i^2(R_m)}\int_0^{R_m} u_i^2(t)\, dt + \frac{1}{u_e^2(R_m)}\int_{R_m}^{\infty} u_e^2(t)\, dt\right]^{-1}. \end{aligned} \tag{2.14}$$

Thus starting with an initial guess E_0, we may find an approximated E-value by iterating

$$E_{n+1} = E_n - \Delta E, \tag{2.15}$$

checking at each iteration that the wave function has the correct number of nodes. If the initial guess is too far from the true value, the process may try to converge to a level for which the wave function has a different number of nodes from that required. In such a case the following empirical rule can be applied:

- if too many nodes, multiply the energy guess by 1.1;
- if too few nodes, multiply the energy guess by 0.9.

The iteration is stopped whenever $|\Delta E|$ is smaller than a given tolerance.

3. Implementation of the method

As matching-radius R_m, where the inner and outer solution should match, we have chosen the turning point, that is the point where $f(E, r)$ first changes in sign, when approaching from outside.

Several multistep methods can be used for the inner and outer integration of (1.1). The interval $[0, R_\infty]$ will be subdivided into equal parts of length h. Two types of so-called optimal multistep methods, one of order four, a second of order six, will be considered [8]. For second-order differential equations of the type

$$\frac{d^2y}{dx^2} = y'' = g(x, y) \tag{3.1}$$

they read:

$$y_{n+2} - 2y_{n+1} + y_n = \tfrac{1}{12}h^2(g_{n+2} + 10g_{n+1} + g_n) + \Theta(h^6) \tag{3.2}$$

and

$$y_{n+4} - 2y_{n+3} + 2y_{n+2} - 2y_{n+1} + y_n = \tfrac{1}{120}h^2\{9g_{n+4} + 104g_{n+3} + 14g_{n+2} + 104g_{n+1} + 9g_n\} + \Theta(h^8). \tag{3.3}$$

Herein y_k and g_k are short-hand notations for $y(x_k = kh)$ and $g(x_k, y(x_k))$, respectively. Applying (3.2) and (3.3) to (1.1) respectively results in:

$$u_{n+2} = \left[1 - \tfrac{1}{12}h^2 f(E, h(n+2))\right]^{-1} \times \left\{u_{n+1}\left(2 + \tfrac{5}{6}h^2 f(E, h(n+1))\right) - u_n\left(1 - \tfrac{1}{12}h^2 f(E, hn)\right)\right\} + \Theta(h^4) \tag{3.4}$$

and

$$u_{n+4} = \left[1 - \tfrac{3}{40}h^2 f(E, h(n+4))\right]^{-1} \times \left\{u_{n+3}\left(2 + \tfrac{13}{15}h^2 f(E, (n+3)h)\right) + u_{n+2}\left(-2 + \tfrac{7}{60}h^2 f(E, (n+2)h)\right) + u_{n+1}\left(2 + \tfrac{13}{15}h^2 f(E, (n+1)h)\right) + u_n\left(-1 + \tfrac{3}{40}h^2 f(E, nh)\right)\right\} + \Theta(h^6). \tag{3.5}$$

Starting from the origin or from R_∞ and using the asymptotic solutions discussed in Section 2, relations (3.4) and (3.5) reproduce stepwise the whole eigenfunction for a chosen E-value. The spherical and modified spherical Bessel functions occurring in the asymptotic solutions are derived by the first three terms of their series expansion, i.e., [1]:

$$j_l(z) \cong \frac{z^l}{1 \cdot 3 \cdot 5 \cdots (2l+1)}\left[1 - \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(2l+3)(2l+5)}\right] \tag{3.6}$$

and

$$\tilde{j}_l(z) \cong \frac{z^l}{1 \cdot 3 \cdot 5 \cdots (2l+1)}\left[1 + \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(2l+3)(2l+5)}\right]. \tag{3.7}$$

For $l = 0$ or 1 the following exact definitions have been used, respectively:

$$j_0(z) = \frac{\sin z}{z}, \qquad \tilde{j}_0(z) = \frac{\sinh z}{z}, \tag{3.8}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}, \qquad \tilde{j}_1(z) = -\frac{\sinh z}{z^2} + \frac{\cosh z}{z}. \tag{3.9}$$

If this stepwise constructed wave function has the correct numbers of nodes (2.14) gives in the turning point R_m a correction ΔE for E. For the calculation of the occurring terms again approximating formulae have to be introduced. For the calculation of L_e and L_i, one needs an approximation for the first derivative u' in R_m, making use of known results for u either in points to the left of R_m, or in points to the right of R_m. The lowest-order formulae for $u_i'(R_m)$ of that type read [4]

$$u_i'(R_m) = \tfrac{1}{2h}\left[3u(R_m) - 4u(R_m - h) + u(R_m - 2h)\right] + \Theta(h^2) \tag{3.10}$$

and

$$u_i'(R_m) = \tfrac{1}{12h}\left[25u(R_m) - 48u(R_m - h) + 36u(R_m - 2h) - 16u(R_m - 3h) + 3u(R_m - 4h)\right] + \Theta(h^4). \tag{3.11}$$

The formulae for $u_e'(R_m)$ are obtained from (3.10) and (3.11) by replacing h by $(-h)$.

The integrals occurring in the nominator of the right-hand side of (2.14) are replaced by composite quadrature formulae of the closed Newton–Cotes type [4]. Again making use of the intervals of length h, where $r_j = jh$ for each $j = 0, 1, 2, \ldots$ (with $r_{2k} = R_m$) one obtains as a first approximation (the composite Simpson's rule)

$$\int_0^{R_m} u_i^2(t)\,dt = \sum_{j=1}^{k} \int_{r_{2j-2}}^{r_{2j}} u_i^2(t)\,dt = \sum_{j=1}^{k} \left\{\tfrac{1}{3}h\left[u_i^2(r_{2j-2}) + 4u_i^2(r_{2j-1}) + u_i^2(r_{2j})\right]\right\} + \Theta(h^5) \tag{3.12a}$$

and

$$\int_{R_m}^{\infty} u_e^2(t)\,dt \cong \int_{R_m}^{R_\infty} u_e^2(t)\,dt = \sum_{j=k+1}^{m} \int_{r_{2j-1}}^{r_{2j}} u_e^2(t)\,dt = \sum_{j=k+1}^{m} \left\{\tfrac{1}{3}h\left[u_e^2(r_{2j-2}) + 4u_e^2(r_{2j-1}) + u_e^2(r_{2j})\right]\right\} + \Theta(h^5). \tag{3.12b}$$

As a better approximation for these integrals we also apply the composite 5-point closed Newton–Cotes quadrature rule. With now $r_{4k} = R_m$ one has

$$\int_0^{R_m} u_i^2(t)\,dt = \sum_{j=1}^{k} \int_{r_{4j-4}}^{r_{4j}} u_i^2(t)\,dt = \sum_{j=1}^{k} \left\{\tfrac{2}{45}h\left\{7\left(u_i^2(r_{4j-4}) + u_i^2(r_{4j})\right) + 32\left(u_i^2(r_{4j-3}) + u_i^2(r_{4j-1})\right) + 12u_i^2(r_{4j-2})\right\}\right\} + \Theta(h^7) \tag{3.13}$$

and an analogous formula for $\int_{R_m}^{\infty} u_e^2(t)\,dt$.

In the following we shall consider two different methods. In the first one, further called model I, the approximations of lower order ((3.4), (3.10) and (3.12)) are used, while in the second one (model II) the higher-order formulae ((3.5), (3.11) and (3.13)) are taken.

4. Numerical illustration

To illustrate the behaviour of the proposed models I and II on practical cases, we have chosen the potentials (1.2)–(1.5) mentioned in the introduction.

For the Woods–Saxon potential we introduce following parameter values:

$$u_0 = -50, \qquad a = 0.6, \qquad r_0 = 7, \qquad u_1 = -\frac{u_0}{a},$$

([10] and references therein). For this choice of parameters and a Schrödinger equation of the form (1.1) the discrete spectrum for $l = 0$ states has been studied in detail by Ixaru and Rizea [10]. The energies for such states with zero, two, four,..., twelve nodes are known with an accuracy of nine decimal digits. In a first instance the influence on the spectrum of the choice of R_∞ has been studied on both proposed models. By comparing results for several states with different n and l values we came to the conclusion that $R_\infty = 20$ is a general acceptable value. The influence of the step length h on the spectrum is illustrated in Table 1 for two $l = 0$ states, i.e., $n = 4$ and $n = 12$. We have stopped the iteration scheme (2.14) whenever $|\Delta E| < 10^{-10}$. Equidistant partitions were used at stepsizes of the form $h = 0.1 \times 2^{-n}$, $n = 0, 1, \ldots, 6$. As reference energies E^{ref} we have used the results reported by Ixaru and Rizea [11]. From Table 1 it is clear that model II is superior over model I. It is also evident that model II, choosing $h = 0.001$, guarantees results which are exact up to nine figures. In Table 2 we present the energy values for $n = 0, 2, 4, \ldots, 12$ and $l = 0$, 1 and 2 as evaluated within model II ($R_\infty = 20$, $h = 0.001$, $|\Delta E| < 10^{-10}$). The results for the $l = 0$ case confirm previously derived data; the other results are new.

For the Morse potential Flügge [6] gives a closed exact expression for the energy values of $l = 0$ states and an approximated expression for the other states. In order to make a comparison

Table 1
Absolute errors $|E - E^{\text{ref}}|10^9$ of eigenenergies of the Woods–Saxon potential for the $n = 4$, $l = 0$ and $n = 12$, $l = 0$ states as calculated for several step values; the reference eigenenergies are taken from [11], i.e., $E(n = 4) = -41.232607772$, $E(n = 12) = -8.676081670$

h	model I	model II	model I	model II
	$n = 4$, $l = 0$		$n = 12$, $l = 0$	
0.1	2458387	568891	31733904	7915794
0.05	302533	16379	2845738	190552
0.025	38589	737	283586	4815
0.0125	4781	45	30893	92
0.00625	598	3	3525	10
0.003125	74	0	423	1
0.0015625	9	0	52	0

Table 2
The eigenenergies of the Woods–Saxon potential derived within model II for the states with $n = 0, 2, 4, \ldots, 12$ and $l = 0$, 1 and 2

n	$l=0$	$l=1$	$l=2$
12	−8.676081670	−6.308097192	−3.972491432
10	−18.094688282	−15.812724871	−13.522303352
8	−26.873448916	−24.794185466	−22.689041510
6	−34.672313205	−32.868392986	−31.026820921
4	−41.232607772	−39.767208069	−38.253426539
2	−46.290753954	−45.237176986	−44.121537377
0	−49.457788728	−48.951731623	−48.349481052

possible, we have to bring the classical Schrödinger equation for that problem into a dimensionless form of the type (1.1), i.e., by substituting $r = r_0 z$ in (case $l = 0$)

$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2} + D\left[\exp\left(-2\alpha\left(\frac{r-r_0}{r_0}\right)\right) - 2\exp\left(-\alpha\left(\frac{r-r_0}{r_0}\right)\right)\right]u(r) = E'u(r), \quad (4.1)$$

and by multiplying the equation by the factor $(-2Mr_0^2/\hbar^2)$ one obtains

$$\frac{\mathrm{d}^2u(z)}{\mathrm{d}z^2} + \left\{E - \gamma^2\left(\mathrm{e}^{-2\alpha(z-1)} - 2\,\mathrm{e}^{-\alpha(z-1)}\right)\right\}u(z) = 0 \quad \text{with } E = \frac{2Mr_0^2E'}{\hbar^2},$$

$$\gamma^2 = \frac{2Mr_0^2D}{\hbar^2}. \quad (4.2)$$

Translated into our notation Flügge's result for the $l = 0$ energies reads:

$$E = -\gamma^2 + 2\alpha\gamma\left(n+\tfrac{1}{2}\right) - \alpha^2\left(n+\tfrac{1}{2}\right)^2, \quad n = 0, 1, 2, \ldots, \text{ with } n_{\max} < \frac{1}{2}\left(\frac{2\gamma}{\alpha} - 1\right). \quad (4.3)$$

His approximation of the energies for $l \neq 0$ states is given by

$$E = -\gamma^2 + 2\alpha\gamma\left(n+\tfrac{1}{2}\right) - \alpha^2\left(n+\tfrac{1}{2}\right)^2 + l(l+1) - \frac{3(\alpha-1)}{\alpha\gamma}\left(n+\tfrac{1}{2}\right)l(l+1) - \frac{9(\alpha-1)^2}{4\alpha^4\gamma^2}l^2(l+1)^2. \quad (4.4)$$

For specific choices of the parameters γ and α, (4.3) takes on very simple values. Choosing $\gamma^2 = m^2$, $m = 1, 2, \ldots$, results in:

$$E = -\left(\alpha\left(n+\tfrac{1}{2}\right) - m\right)^2. \quad (4.5)$$

For α an even integer, (4.5) reproduces negative integer values. In Table 3 we compare the theoretical energy values (4.4) and (4.5) with numerical ones, derived within model II with $m = 10$, $\alpha = 2$, $h = 0.001$, $R_\infty = 20$ and $|\Delta E| < 10^{-10}$ for states with $n = 0$, 1, 2, 3 and 4 and $l = 0$, 1 and 2. For the $l = 0$ case model II reproduces the exact results as correctly as possible. By comparing the other data one can observe that Flügge's approximations are not very accurate for the parameter value used.

Table 3
Eigenenergies of the Morse potential (with parameters $m = 10$, $\alpha = 2$) as derived within model II and as predicted by Flügge [6] for $n = 0, 1, \ldots, 4$ and $l = 0$, 1 and 2

n	$l=0$		$l=1$		$l=2$	
	E^{th}	E^{num}	E^{th}	E^{num}	E^{th}	E^{num}
0	−81	−81.000000000	−79.155	−79.161799963	−75.500	−75.544697966
1	−49	−49.000000000	−47.455	−47.482803567	−44.400	−44.508123798
2	−25	−25.000000000	−23.755	−23.827466489	−20.400	−21.543363518
3	−9	−9.000000000	−8.055	−8.204425593	−6.200	−6.679971857
4	−1	−0.999999999	−0.355	−0.648872427	–	–

For the potentials $V_3(r)$ and $V_4(r)$ we have performed all calculations with steplength $h = 0.001$ and R_∞ three times the value of the turning point which has been determined numerically. A tolerance of 10^{-8} has been used in all cases. The model II approximations have been introduced.

For the numerical work we have taken in (1.4) $A = 1$. By this we use the same scaling for B and the energy eigenvalues as in Adamowsky's paper [2]. As an example we have computed the bound state energies E of the lowest-lying states, $1s$ to $3d$ for $B = 5$ and for various values of C. These results are compared with those of Adamowsky in Table 4. One can observe that for small C-values discrepancies occur between our results and the ones of Adamowsky. Possibly this has to do with the trial functions, describing the energy wave functions, introduced by Adamowsky. A limitation to a $N = 10$ element basis is perhaps too restrictive in the case of positive B-values and small C-values.

Table 4
Energy eigenvalues in atomic units of states $1s - 3d$ for the Hellmann potential as a function of the screening parameter C for $B = 5$; the first row represents our results, the second one denotes Adamowsky's results [2]

State	$B=5$					
	$C=0.05$	$C=0.1$	$C=0.2$	$C=0.5$	$C=2.0$	$C=10.0$
$1s$	−0.010994	−0.020832	−0.038587	−0.082804	−0.218772	−0.421975
	−0.01099	−0.02083	−0.03858	−0.08280	−0.21877	−0.42197
$2s$	−0.008589	−0.014822	−0.024318	−0.042634	−0.079594	−0.114641
	−0.00857	−0.01481	−0.02432	−0.04263	−0.07959	−0.11464
$2p$	−0.010754	−0.019936	−0.035378	−0.067367	−0.115630	−0.124919
	−0.01075	−0.01993	−0.03538	−0.06736	−0.11563	−0.12492
$3s$	−0.00681	−0.010919	−0.016455	−0.025639	−0.040697	−0.052423
	−0.00670	−0.01090	−0.01645	−0.02564	−0.04069	−0.05238
$3p$	−0.008406	−0.014217	−0.022488	−0.036099	−0.052458	−0.055527
	−0.00838	−0.01421	−0.02249	−0.03610	−0.05246	−0.05552
$3d$	−0.010293	−0.018298	−0.030017	−0.046941	−0.055432	−0.055556
	−0.01029	−0.01830	−0.03001	−0.04694	−0.05543	−0.05555

Table 5
Energy eigenvalues of $1s-3d$ states for the Hulthén potential ($Z=1$) in atomic units as a function of the screening parameter α; the first row represents our results and the second one denotes the group dynamical approach results of Matthys and De Meyer [13]; in the last row are given for the s-states the exact eigenvalues and for the other states the Padé approximation results of Lai and Lin [12]

	0.025	0.050	0.100	0.150	0.200	0.300
$1s$	−0.48757814	−0.47531250	−0.45125000	−0.42781250	−0.40500000	−0.36125000
	−0.4875777	−0.4753121	−0.4512490	−0.4278107	−0.4049935	−0.3612317
	−0.48757814	−0.47531250	−0.45125000	−0.42781250	0.405000000	−0.36125000
$2s$	−0.11281250	−0.10125000	−0.08000000	−0.06124999	−0.04499999	−0.02000000
	−0.1128115	−0.1012485	−0.0799969	−0.0612453	−0.0450014	−0.0200014
	−0.11281250	−0.10125000	−0.08000000	−0.06125000	−0.04500000	−0.02000000
$2p$	−0.11276047	−0.10104245	−0.07917943	−0.05944152	−0.04188605	−0.01379003
	−0.1127604	−0.1010425	−0.0791794	−0.0594415	−0.0418860	−0.0137900
		−0.1010443	−0.079179		−0.041886	
$3s$	−0.04375868	−0.03336805	−0.01680556	−0.00586806	−0.00055556	
	−0.0437589	−0.0333687	−0.0168070	−0.0058797	−0.0005607	
	−0.04375868	−0.03336805	−0.01680556	−0.00586806	−0.00055556	
$3p$	−0.04370689	−0.03316450	−0.01605373	−0.00446631		
	−0.0437071	−0.0331650	−0.0160535	−0.0044664		
	−0.043707	−0.033165	−0.016054	−0.004466		
$3d$	−0.04360305	−0.03275318	−0.01448423	−0.00139659		
	−0.0436030	−0.0327532	−0.0144842	−0.0013965		
	−0.043603	−0.032753	−0.014484	−0.001391		

In Table 5 the results for the bound-state energies obtained by the present technique for the Hulthén potential (with $Z=1$) are listed and compared either with exact values (s-states) or with the results obtained by a Padé approximation method [12] and with a dynamical group approach method [13]. Although our method generates, due to the chosen dimensionless form of (1.1), energy eigenvalues which are rescaled with respect to the classical expression for E in atomic units, we present for simplicity in Table 5 numerical values in atomic units as a function of the screening parameter α. In these units, for s-states the bound state energies for $Z=1$ are known to be given by the simple formula [6]

$$E=-\tfrac{1}{8n^2}(2-\alpha n^2)^2.$$

As can be observed our method reproduces for s-states the energies as accurate as possible. For the other states we confirm the results of the previous papers but with a better accuracy.

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