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# An algebraic method to solve the radial Schrödinger equation

M. Gadella<sup>a,\*</sup>, L.P. Lara<sup>b,c</sup>

<sup>a</sup> Departamento de Física Teórica, Atómica y Optica, Facultad de Ciencias, 47011, Valladolid, Spain

<sup>b</sup> Departamento de Física, FCEIA, UNR, Av. Pellegrini 250, 2000 Rosario, Argentina

<sup>c</sup> Departamento de Sistemas, FRRO, UTN, Zevallos 1341, 2000 Rosario, Argentina

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#### ABSTRACT

We propose a method of numerical integration of differential equations of the type  $x^2y'' + f(x)y = 0$  by approximating its solution with solutions of equations of the type  $x^2y'' + (ax^2 + bx + c)y = 0$ . This approximation is performed by segmentary approximation on an interval. We apply the method to obtain approximate solutions of the radial Schrödinger equation on a given interval and test it for two different potentials. We conclude that our method gives a similar accuracy than the Taylor method of higher order.

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# 1. Introduction and outline of the method

As we all know, many relevant fundamental laws in physics, chemistry, social sciences or economics are formulated in terms of differential equations, which are the basis to solve a great number of problems on these disciplines. And we also know that many of these important differential equations cannot be solved analytically. Therefore, many methods for obtaining numerical solutions have been developed [1].

The aim of the present article is to introduce a method for numerical integration of second order non homogeneous non autonomous ordinary differential equations of the type  $x^2y''(x) + f(x)y(x) = 0$ . We propose an algebraic method of integration with initial values and without singular points in the interval of integration. As usual, the method can be also used as a basis for the numerical integration of equations with boundary conditions.

One of the most interesting applications of our method is indeed the radial Schrödinger equations with potentials of different types. There are some other methods in the literature dealing with the numerical solution of the one dimensional Schrödinger equation. Among them, we should mention the so-called "piecewise perturbation method" (PPM), which is based on a perturbative decomposition of the potential [2]. In the case of the radial Schrödinger equation, previous numerical studies including PPM have been applied to a certain class of radial potentials which includes the Coulomb case [3].

In our method, described below in the second part of the present introduction, we find numerical solutions of the radial Schrödinger equation using another piecewise method based on the approximation of the original equation by another for which the solutions are well known. In our case, the radial potential could be arbitrary with no other singularity than the origin. The numerical integration is then performed on an interval of the form  $[\epsilon, H]$  with  $\epsilon > 0$  and H finite, so that we can compare our results with those given by the Taylor method. As particular examples of application, we have chosen the Wood–Saxon potential and the spherical oscillator.

For the numerical integration, we have used identical mesh intervals and this choice was motivated by its simplicity. Here, we have used a step size h = 0.1 and have checked that the use of variable step sizes does not improve the efficiency of the calculation and, in addition, requires another algorithm that increases CPU times. There are some other methods using different mesh intervals widths [4]. Our method is simple and improves the precision of the Taylor method. However, it is necessary to say that it requires more CPU times, as we have checked in the two examples studied on Sections 3.1 and 3.2.

<sup>\*</sup> Corresponding author. Tel.: +34 983 423145; fax: +34 983 423013. *E-mail address:* manuelgadella1@gmail.com (M. Gadella).

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Our numerical test and computations have been performed with the help of the Mathematica package.

The remainder of the paper is organized as follows: right below in the second part of this section, we briefly described our method. In the next section, we develop the method and discuss the uniform convergence of the proposed solution. Then, we show the local error. In Section 3, we present some applications in quantum mechanics, particularly to the radial Schrödinger equation with two types of potentials: the Woods–Saxon and the spherical oscillator. The paper ends with some concluding remarks.

## 1.1. Outline of the method

We start with a method of numerical integration valid for equations of the following type:

$$x^{2}y''(x) + f(x)y(x) = 0,$$
(1)

with initial conditions given by  $y(x_0) = y_0$ ,  $y'(x_0) = y'_0$ , where  $y_0, y'_0$  are real numbers. The function f(x) is an analytic function of one real variable on the interval  $x_0 < x < x + H$  and eventually  $x_0$  may be a singular point.

Our method uses the general solution of the following equation

$$x^{2}y''(x) + (ax^{2} + bx + c)y(x) = 0,$$
(2)

which is often written in terms of the Whittaker functions *M* and *W* as follows [5,6]:

$$y(x) = c_1 M_{\alpha,\beta} (2i\sqrt{a}x) + c_2 W_{\alpha,\beta} (2i\sqrt{a}x), \tag{3}$$

where  $\alpha = -ib/(2\sqrt{a})$  and  $\beta = -\frac{1}{2}\sqrt{4c-1}$ . Then, we approximate the coefficient f(x) of y(x) in (1) by a quadratic polynomial on the variable x [7]. Consider the initial value problem of (3) on the interval  $(x_0, x_0 + H)$  and divide it into *n* disjoint intervals each of length  $h_n := H/n$ . On the *k*th interval ( $x_k, x_k + h$ ), k = 0, 1, ..., n - 1, we approximate f(x) by the polynomial  $p_{n,k}(x) := a_{n,k}x^2 + b_{n,k}x + c_{n,k}$ . In each interval, the values  $\{a_{n,k}, b_{n,k}, c_{n,k}\}$  depend on the optimal method to approximate f(x): either the Taylor method, the minimal squares or the quadratic segmentary interpolation. Taking into account (3), the approximate solution of (1) on the kth interval is

$$y_{k}(x) = c_{1,k} M_{\alpha_{k},\beta_{k}}(2i\sqrt{a_{k}} x) + c_{2,k} W_{\alpha_{k},\beta_{k}}(2i\sqrt{a_{k}} x),$$

$$x_{k} < x < x_{k} + h_{n} = x_{n+1}, \quad k = 0, 1, ..., n,$$
(4)

with  $\alpha = -ib_k/(2\sqrt{a_k})$  and  $\beta_k = -\frac{1}{2}\sqrt{4c_k-1}$ .

The integration constants  $c_{1,k}$  and  $c_{2,k}$  are determined as follows: take the first interval  $(x_0, x_1)$  (recall that  $x_{k+1} = x_k + h_n$ ) and the known initial values  $y(x_0)$ ,  $y'(x_0)$ . Carrying these two initial values into (4) with k = 0, we can obtain  $c_{1,0}$  and  $c_{2,0}$ , since the functions  $M_{\alpha_k,\beta_k}(2i\sqrt{a_k}x)$  and  $W_{\alpha_k,\beta_k}(2i\sqrt{a_k}x)$  are linearly independent. Then,  $y(x_1)$  and  $y'(x_1)$  are determined. We can use these values as initial values for the interval  $(x_1, x_2)$  to obtain  $c_{1,1}$  and  $c_{2,1}$  and so on. The result is obviously an approximate solution for (1).

# 2. On the convergence of the method

The objective of the present section is to show that this method works in the sense that we can construct an approximate solution so that it converges uniformly to the exact solution. The fact that we are using a quadratic interpolation demands some extra conditions on the coefficients defining the interpolating functions. As we shall see these conditions would not have been required should the interpolation have been linear.

To this end, let us rewrite (1) in matrix form as

$$\Phi' = F(x) \cdot \Phi, \qquad \Phi(x_0) = \Phi_0 \tag{5}$$

with

$$\Phi = \begin{pmatrix} y \\ z \end{pmatrix} \text{ and } F(x) = \begin{pmatrix} 0 & 1 \\ \frac{f(x)}{x^2} & 0 \end{pmatrix}$$
(6)

and z(x) = y'(x).

Then, we use the function  $y_k(x)$  as obtained in (4) to construct the segmentary solution on  $[x_k, x_{k+1}]$  given by  $\begin{pmatrix} y_k(x) \\ z_k(x) \end{pmatrix}$  again with  $z_k(x) = y'_k(x)$ , k = 1, 2, ..., n - 1. Since this solution has been constructed by dividing the interval  $[x_0, x_0 + H]$  into n parts of length  $h_n$ , we shall denote the solution constructed on this manner as  $\Phi_n$ . Note that  $[x_k, x_{k+1}] = [x_k, x_k + h_n]$ .

It is well known that the existence and uniqueness of solutions on a neighborhood of  $x_0$ , with the given initial conditions, is guaranteed by classical results [5]. However, we need to show that the approximate solution  $\Phi_n$  to (6) converges uniformly to the exact solution in order to legitimate our procedure.

We construct the approximate solution of  $\Phi_n(x)$  being the solution on each interval of the form  $[x_k, x_k + h_n]$ , k = 0, 1, ..., n - 1, of the equation

$$\Phi_n'(x) = G_{n,k}(x) \,\Phi_n(x),\tag{7}$$

with

have

$$G_{n,k}(x) = \begin{pmatrix} 0 & 1\\ \frac{a_{n,k}x^2 + b_{n,k}x + c_{n,k}}{x^2} & 0 \end{pmatrix}.$$
 (8)

In what follows, we assume that  $0 \notin [x_0, x_0 + H]$ . We denote by  $\varphi_n(x)$  the function equal to  $\frac{1}{x^2}(a_{n,k}x^2 + b_{n,k}x + c_{n,k})$  on each interval of the form  $[x_k, x_k + h_n]$ . Since  $\varphi_n(x)$  interpolates  $\varphi(x) := f(x)/x^2$ , we have that  $\varphi(x_k) = \varphi_n(x_k)$  for all k = 1, 2, ..., n and for each value of n. From now on, we shall denote the functions of the sequence  $\{\varphi_n(x)\}$  as interpolating functions. In the next result, we shall discuss the convergence of the sequence of interpolating functions to the exact function  $\varphi(x)$ .

**Lemma.** Assume that the coefficients  $a_{k,n}$  and  $b_{k,n}$  as in (8) were uniformly bounded for any n = 1, 2, ..., and k = 1, 2, ..., n. This means that there exists two positive constants  $\alpha$  and  $\beta$  such that  $|a_{k,n}| \leq \alpha$  and  $|b_{k,n}| \leq \beta$ . Then, the sequence of interpolating functions  $\varphi_n(x)$  converges uniformly to  $\varphi(x)$  on the closed interval  $[x_0, x_0 + H]$ .

**Proof.** It is enough to show that the sequence  $f_n(x)$  of continuous functions on  $[x_0, x_0 + H]$  such that are equal to  $a_{n,k}x^2 + b_{n,k}x + c_{n,k}$  on each interval of the form  $[x_k, x_k + h_n]$  converges uniformly to the function f(x).

The function f(x) is continuous on the interval  $[x_0, x_0 + H]$  and therefore uniformly continuous on the interval. This means that given an  $\varepsilon > 0$ , there exists a  $\delta > 0$  such that if  $x, y \in [x_0, x_0 + H]$  with  $|x - y| < \delta$ , then,  $|f(x) - f(y)| < \varepsilon$ . Since  $h_n \mapsto 0$  as  $n \mapsto \infty$ , we can choose n such that,  $\varepsilon > 0$ ,  $h_n < \delta$  being fixed. Then for any  $x \in [x_k, x_k + h_n]$ , we

$$|f(x) - f_n(x)| \le |f(x) - f(x_k)| + |f(x_k) - f_n(x_k)| + |f_n(x_k) - f_n(x)|.$$
(9)

Since  $|x - x_k| < h_n < \delta$ , then  $|f(x) - f(x_k)| < \varepsilon$ . Uniform continuity guarantees the independence on the interval  $[x_k, x_k + h_n]$  under consideration. The fact that  $f_n(x)$  is an interpolating function for f(x) with interpolating points  $x_k$ , k = 1, 2, ..., n shows that  $f(x_k) = f_n(x_k)$ . Furthermore,

$$\begin{aligned} |f_n(x_k) - f_n(x)| &= |a_{k,n}x_k^2 + b_{k,n}x_k + c_{k,n} - a_{k,n}x^2 - b_{k,n}x - c_{k,n}| \\ &= |a_{k,n}(x_k^2 - x^2) + b_{k,n}(x_k - x)| = |x_k - x| |a_{k,n}(x_k + x) + b_{k,n}| \\ &\leq h_n \{ |a_{k,n}|h_n + |b_{k,n}| \} < h_n \{ \alpha H + \beta \}. \end{aligned}$$

$$(10)$$

In consequence,  $|f(x) - f_n(x)| \le \varepsilon + h_n C$ , where  $C = \alpha H + \beta$  is a fixed constant. Obviously, for any m > n the same inequality holds and remains independent of the chosen point  $x \in [x_0, x_0 + H]$ . Then, the uniform convergence of the sequence  $\{f_n(x)\}$  to f(x) follows. Now, the uniform convergence of the sequence  $\{\varphi_n(x)\}$ , where each of the  $\varphi_n(x)$  is defined on each subinterval  $[x_k, x_k + h_n]$  as  $\frac{1}{x^2}(a_{n,k}x^2 + b_{n,k}x + c_{n,k})$ , to  $\varphi(x) := f(x)/x^2$  follows immediately. The lemma is proven.  $\Box$ 

**Remarks.** 1. In the previous result, we have excluded the origin for technical reasons. Should we choose  $x_0 = 0$ , then we have to make a slightly different fitting in the interval  $[0, x_1]$  (on the other intervals we keep the same procedure), as we shall explain in the next paragraph. Nevertheless, we shall not use this approach in the examples given in here, where we shall always choose  $x_0 > 0$ , although small.

Let us assume that the function f(x) is analytic on a neighborhood of the origin. Let us choose h smaller than the radius of convergence of f(x). Then, all we have to do is to prove the uniform convergence of  $\varphi_n(x)$  to  $\varphi(x)$  on the interval [0, H]. The proof on the interval [h, H] has been provided by the lemma. Then, we have to show this uniform convergence on the interval  $[0, x_1], x_1 = h$ . We recall that

$$\varphi(x) = \frac{f(x)}{x^2}, \qquad \varphi_n(x) = \frac{ax^2 + bx + c}{x^2},$$
(11)

where we have omitted the subindices for simplicity. No confusion should arise as we are focusing our attention on the interval  $[0, x_1]$ . Due to our hypothesis of analyticity and our choice of *h*, for any  $x \in [0, x_1]$ , we have:

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + x^2F(x),$$
(12)

where F(x) is analytic on the same neighborhood of the origin with F(0) = 0.<sup>1</sup> Consequently, for any  $x \in [0, x_1]$ , we have

$$|\varphi_n(x) - \varphi(x)| = \left| \frac{f(0)}{x^2} + \frac{f'(0)}{x} + \frac{f''(0)}{2} + F(x) - \frac{c}{x^2} - \frac{b}{x} - a \right|.$$
(13)

<sup>&</sup>lt;sup>1</sup> Note that the hypothesis of analyticity can be relaxed. It is sufficient that  $f^{(n)}(x)$  be continuous on an open interval including [0, h], with n = 0, 1, 2, 3. In this case, the Taylor theorem, and consequently (12), hold with  $F(x) = [xf^{(3)}(\xi)]/3!, \xi \in (0, h)$ .

If we choose c := f(0) and b := f'(0), we still need a to be fixed. This can be done with the condition  $\varphi_n(x_1) = \varphi(x_1)$ . Consequently,

$$a := \frac{f''(0)}{2} + F(x_1). \tag{14}$$

Note that *c* and *b* are constants, although *a* depends on *n*, since  $x_1$  depends on *n* (recall that h = H/n). Then, (13) gives

$$|\varphi_n(x) - \varphi(x)| = |F(x) - F(x_1)|, \tag{15}$$

which can be arbitrarily small for any  $x \in [-0, h]$ . This shows the uniform convergence on the interval [0, H].

This procedure gives  $f(x_1) = ax_1^2 + bx_1 + c$  and f(0) = c, so that the continuity is guaranteed. However,  $f'(x_1) \neq 2ax_1 + b$ . 2. If instead of a quadratic type interpolation we take a linear interpolation, no restrictions in the coefficients are necessary. Assume that we interpolate f(x) by the sequence  $g_n(x)$  where on each interval of the form  $[x_k, x_k + h_n]$ ,  $g_n(x)$  is given by  $a_{k,n}x + b_{k,n}$ . Then, under the conditions of the lemma, we have for any  $x \in [x_k, x_k + h_n]$ , k = 1, 2, ..., n,

$$|f(x) - g_n(x)| \le |f(x) - f(x_k)| + |f(x_k) - g_n(x_k)| + |g_n(x_k) - g_n(x)| \le \varepsilon + 0 + |g_n(x_k) - g_n(x_k + h_n)| \le \varepsilon + |f(x_k) - f(x_k + h_n)| \le 2\varepsilon,$$
(16)

so that  $\max_{x \in [x_0, x_0+H]} |f(x) - g_n(x)| \le 2\varepsilon$ . Obviously, the same result is true for the same  $\varepsilon$  for any m > n. Thus, uniform convergence holds without the need of any extra condition for the coefficients  $a_{k,n}$  and  $b_{k,n}$ .

Note that the condition  $\{g_n(x)\}$  is an interpolating sequence for f(x), automatically gives the values for the coefficients  $a_{k,n}$  and  $b_{k,n}$ . This is not true for the quadratic interpolation, so we need an extra condition to assure the uniform convergence.

3. The function  $f_n(x)$  equal to  $a_{n,k}x^2 + b_{n,k}x + c_{n,k}$ , which depends on three parameters on each of the intervals  $[x_k, x_k + h_n]$ , is obviously not determined with the two interpolation conditions  $f_n(x_k) = f(x_k)$ ;  $f_n(x_k + h_n) = f(x_k + h_n)$ , k = 1, 2, ..., n. If one of the parameters, say  $a_{k,n}$ , is determined by a constant a on all intervals, then  $b_{n,k}$  and  $c_{n,k}$  are fixed. This procedure gives uniquely a quadratic interpolation of f(x), but then one needs to be sure that  $f_n(x)$  converges uniformly to f(x). This comes up if f'(x) exists and is continuous on the interval  $[x_0, x_0 + H]$  (and therefore bounded), where the right derivative at  $x_0$  and the left derivative at  $x_0 + H$  are defined as usual.

In fact, at each node  $x_k$ , we have

$$f(x_k + h_n) = a(x_k + h_n)^2 + b_{k,n}(x_k + h_n) + c_{k,n}$$
  

$$f(x_k) = ax_k^2 + b_{k,n}x_k + c_{k,n}.$$
(17)

The system given in (17) gives

$$b_{k,n} = \frac{1}{h_n} \begin{vmatrix} f(x_k + h_n) - a(x_k + h_n)^2 & 1 \\ f(x_k) - ax_k^2 & 1 \end{vmatrix}$$
  
=  $\frac{f(x_k + h_n) - f(x_k)}{h_n} - \frac{a(x_k + h_n)^2}{h_n}.$  (18)

The first term in the second row of (18) is approximately equal to  $f'(x_k)$ , while the second term is close to  $-2ax_k$ . Thus,  $b_{k,n}$  is bounded and the conditions on the lemma are satisfied.

The uniform convergence is required in order to show that the solutions of the sequence of equations given by (7) converge to the exact solution of (5) as will be shown in our next result.

**Theorem.** The sequence of approximate solutions  $\{\Phi_n(x)\}$ , defined as above, with initial values  $\Phi(x_0) = \Phi_0$  converges uniformly to the exact solution of (5) on the interval  $[x_0, x_0 + H], x_0 \ge 0$ .

**Proof.** Let us rewrite (7) as

$$\Phi'_{n}(x) = F(x) \,\Phi_{n}(x) + R_{n}(x), \tag{19}$$

where on each interval  $[x_k, x_k + h_n]$ 

$$R_n(x) \coloneqq (G_k(x) - F(x)) \, \Phi_n(x). \tag{20}$$

Let us integrate (19) with the integration interval  $(x_k, x)$ ,  $x_k \le x \le x_k + h_n$ . This gives along the initial condition  $\Phi_n(x_k) = \Phi_k$ , n = 1, 2, ...,

$$\Phi_n(x) = \Phi_k + \int_{x_k}^x F(x') \,\Phi_n(x') \,\mathrm{d}x' + \int_{x_k}^x R_n(x') \,\mathrm{d}x', \tag{21}$$

where *n* is a positive integer. If *m* is another positive integer, we have

$$\Phi_{n+m}(x) = \Phi_k + \int_{x_k}^x F(x') \,\Phi_{n+m}(x') \,\mathrm{d}x' + \int_{x_k}^x R_{n+m}(x') \,\mathrm{d}x'.$$
(22)

Let us subtract (21) from (22). The norm of this difference satisfies this obvious inequality:

$$\|\Phi_{n+m}(x) - \Phi_n(x)\| \le \int_{x_k}^x \|F(x')\| \|\Phi_{n+m}(x') - \Phi_n(x')\| dx' + \int_{x_k}^x \|R_{n+m}(x')\| dx' + \int_{x_k}^x \|R_n(x')\| dx'.$$
(23)

Since F(x) is a continuous function on the interval  $[x_0, x_0 + H]$ , then it is bounded in this compact interval. Let us denote by N the supreme of the norm of F(x) in such interval,  $M = \max ||F(x)||, x \in [x_0, x_0 + H]$ . Then, (23) yields,

$$\|\Phi_{n+m}(x) - \Phi_n(x)\| \le M \int_{x_k}^x \|\Phi_{n+m}(x') - \Phi_n(x')\| \, \mathrm{d}x' + \int_{x_k}^x \|R_{n+m}(x')\| \, \mathrm{d}x' + \int_{x_k}^x \|R_n(x')\| \, \mathrm{d}x'.$$
(24)

Let us denote by  $f_n(x)$  the function which coincides with  $a_{kn}x^2 + b_{kn}x + c_{kn}$  on each of the intervals  $[x_k, x_k + h_n]$  (with the restrictions imposed in the previous lemma and subsequent remarks), and assume that  $f_n(x)$  converges uniformly to f(x) on  $[x_0, x_0 + H]$ . As we have remarked, this is true if and only if  $\varphi_n(x) := \frac{1}{x^2}f_n(x)$  converges uniformly to  $\varphi(x) := \frac{1}{x^2}f(x)$ . The latter means that for any  $\varepsilon > 0$ , there exists N > 0 such that if n > N, then,

$$\||\varphi_n(\mathbf{x})| - |\varphi(\mathbf{x})|\| \le \|\varphi_n(\mathbf{x}) - \varphi(\mathbf{x})\| < \varepsilon,$$
(25)

where  $\|\psi(x)\| := \max |\psi(x)|$ . From (25) one gets,

$$\|\varphi_n(x)\| \le \|\varphi(x)\| + \varepsilon = \left\|\frac{f(x)}{x^2}\right\| + \varepsilon \le \frac{1}{x_0^2} \|f(x)\| + \varepsilon =: K.$$
(26)

Next, let us consider the homogeneous linear equation

$$L(y) = y^{(n)}(x) + a_1(x)y^{(n-1)}(x) + \dots + a_n(x)y(x) = 0$$
(27)

with solutions on an interval *I*. Assume that there exist *n* non negative constants  $b_1, b_2, \ldots, b_n$  such that

$$\max_{x \in I} |a_j(x)| \le b_j, \quad j = 1, 2, \dots, n.$$
(28)

Let  $C := 1 + b_1 + b_2 + \cdots + b_n$ . Then for any  $x_0 \in I$  and for any solution  $\phi(x)$  of (27), we have

$$\|\Phi(x)\| \le \|\Phi(x_0)\| \exp\{C|x - x_0|\},\tag{29}$$

for all  $x \in I$  and

$$\Phi(\mathbf{x}) := \begin{pmatrix} \phi(\mathbf{x}) \\ \phi'(\mathbf{x}) \\ \vdots \\ \phi^{(n-1}(\mathbf{x}) \end{pmatrix}.$$
(30)

The norm of the vector  $\Phi(x)$  in (30) is given by

$$\|\Phi(x)\| \coloneqq \{|\phi(x)|^2 + |\phi'(x)|^2 + \dots + |\phi^{(n-1)}(x)|^2\}^{1/2}.$$
(31)

In our case, the equation is  $y''_n(x) + \varphi_n(x)y(x) = 0$ ,  $I = [x_0, x_0 + H]$ , C = K + 1 and  $x_0 \in I$ . Thus, if n > N

$$\|\Phi_n(x)\| \le \|\Phi_0\| \exp\{C|x - x_0|\} \le \|\Phi_0\| \exp\{CH\} =: A,$$
(32)

and, hence, solutions (21) of Eq. (7) are uniformly bounded.

Now, let us go back to Eq. (15). Since we are operating on a finite dimensional space, all linear operators are bounded and therefore (20) implies

$$\|R_n(x)\| \le \|G_k(x) - F(x)\| \|\Phi_n(x)\| \le A \|G_k(x) - F(x)\|.$$
(33)

The space of real 2 × 2 matrices is finite dimensional and hence the norms on this space are all equivalent. Let *G* be an arbitrary 2 × 2 matrix with entries  $g_{ij}$ . Let us use the notation  $||G||_1 := \max_{1 \le i,j \le 2} |g_{ij}|$ . Then, the property of equivalence of norms shows that there exists a positive real number a > 0 such that  $||G|| \le a ||G||_1$ . Thus,

$$\|R_n(x)\| \le A \|G_k(x) - F(x)\| \le A \|G_k(x) - F(x)\|_1$$
  
=  $A |\varphi_n(x) - \varphi(x)|,$  (34)

since

$$G_k(x) - F(x) = \begin{pmatrix} 0 & 0\\ \varphi_n(x) - \varphi(x) & 0 \end{pmatrix}.$$
(35)

For n > N, (32) gives

$$\|R_n(x)\| \le A \max_{x \in [x_0, x_0+H]} |\varphi_n(x) - \varphi(x)| < A\varepsilon,$$
(36)

valid for any  $x \in [x_0, x_0 + H]$ . Since n + m > N, we also have in the same interval that

$$\|R_{n+m}(x)\| < A\varepsilon. \tag{37}$$

Then,

$$\int_{x_0}^x \|R_n(x')\| \, \mathrm{d}x' \le A\varepsilon(x-x_0) \le AH\,\varepsilon, \quad \text{and} \quad \int_{x_0}^x \|R_{n+m}(x')\| \, \mathrm{d}x' \le AH\,\varepsilon. \tag{38}$$

Also,

$$\int_{x_{k}}^{x} \| \Phi_{n+m}(x') - \Phi_{n}(x') \| dx' \leq \int_{x_{k}}^{x} \max_{x \in [x_{0}, x_{0}+H]} \| \Phi_{n+m}(x) - \Phi_{n}(x) \| dx'$$

$$\max_{x \in [x_{0}, x_{0}+H]} \| \Phi_{n+m}(x) - \Phi_{n}(x) \| \int_{x_{k}}^{x} dx' \leq (x - x_{k}) \max_{x \in [x_{0}, x_{0}+H]} \| \Phi_{n+m}(x) - \Phi_{n}(x) \| h_{n}$$

$$\times \{ \max_{x \in [x_{0}, x_{0}+H]} \| \Phi_{n+m}(x) - \Phi_{n}(x) \| \}.$$
(39)

Combining (24) with (38) and (39), we get

$$\|\Phi_{n+m}(x) - \Phi_n(x)\| \le h_n M \max_{x \in [x_0, x_0+H]} \|\Phi_{n+m}(x) - \Phi_n(x)\| + 2AH\varepsilon,$$
(40)

which readily implies that

$$\max_{x \in [x_0, x_0 + H]} \| \Phi_{n+m}(x) - \Phi_n(x) \| \le h_n M \max_{x \in [x_0, x_0 + H]} \| \Phi_{n+m}(x) - \Phi_n(x) \| + 2AH \varepsilon,$$
(41)

or

$$\max_{x \in [x_0, x_0 + H]} \| \Phi_{n+m}(x) - \Phi_n(x) \| \le \frac{2AH}{1 - h_n M} \varepsilon,$$
(42)

which is arbitrarily small, since  $h_n \mapsto 0$ . Note that (42) is valid for any  $x \in [x_0, x_0 + H]$ , since any x in this interval lies in some subinterval of the form  $[x_k, x_k + h_n]$ . Then, the sequence  $\Phi_n(x)$  is Cauchy uniform and therefore converges uniformly to its limit. Let us call this limit  $\Psi(x)$ :

$$\Psi(x) = \lim_{n \to \infty} \Phi_n(x) = \Phi_0 + \lim_{n \to \infty} \int_{x_0}^x F(x') \, \Phi_n(x') \, \mathrm{d}x' + \lim_{n \to \infty} \int_{x_0}^x R_n(x') \, \mathrm{d}x'.$$
(43)

Due to the uniform convergence of the sequence  $\Phi_n(x)$ , we have

$$\lim_{n \to \infty} \int_{x_0}^{x} F(x') \, \Phi_n(x') \, \mathrm{d}x' = \int_{x_0}^{x} F(x') \{ \lim_{n \to \infty} \Phi_n(x') \} \, \mathrm{d}x'.$$
(44)

Also, Eq. (36) implies that

$$\lim_{n\to\infty}\int_{x_0}^x R_n(x')\,\mathrm{d}x'=0. \tag{45}$$

Therefore, (43) and (44) together imply that

$$\Psi(\mathbf{x}) = \Phi_0 + \int_{x_0}^{x} F(\mathbf{x}') \,\Psi(\mathbf{x}') \,\mathrm{d}\mathbf{x}',\tag{46}$$

which shows that the limit of the sequence  $\Phi_n(x)$  is indeed a solution of the exact system (5)–(6).

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## 2.1. Remark: local error

It is well known that the local error depends on the form one approaches the function f(x). In our case, we have used a fitting by means of a second order Taylor polynomial around x<sub>k</sub>. Since the equation  $x^2y''(x) + f(x)y(x) = 0$  and its approximation  $x^2y''(x) + (ax^2 + bx + c)y(x) = 0$ , with initial values given by  $y(x_k)$  and  $y'(x_k)$  satisfy the existence and uniqueness theorems, then the solutions are analytic at  $x_{\nu}$ . Expanding both functions in Taylor series we can determine the local error  $e_k = |y(x_k) - y_k|$ . A simple operation gives

$$e_{k+1} = \frac{1}{120} \frac{1}{x_k^2} |y(x_k) f^{(3)}(x_k)| h_n^5, \quad k = 0, \dots,$$
(47)

which shows that the local error is of the order of  $O(h_n^5)$ , with  $h_n = H/n$ .

## 3. The radial Schrödinger equation

In this section, we consider the Schrödinger equation in spherical coordinates

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \psi \right) + \frac{1}{r^2} \nabla_{\theta, \varphi} \psi + \frac{2\mu}{\hbar^2} \left( E - V \right) \psi = 0, \tag{48}$$

corresponding to a particle with reduced mass  $\mu$  subject to the spherically symmetric potential V(r). If we denote the angular momentum operator as  $\ell$ , we can write (48) as

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \psi \right) - \frac{1}{\hbar^2} \frac{\ell^2}{r^2} \psi + \frac{2\mu}{\hbar^2} \left( E - V \right) \psi = 0.$$
(49)

If we now use separation of variables  $\psi(r, \theta, \varphi) = R(r)Y_{lm}(\theta, \varphi)$  and take into account that  $\ell^2 Y_{lm} = \hbar^2 l(l+1)Y_{lm}$ , we obtain

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} R \right) + \frac{2\mu}{\hbar^2} \left( E - V - \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} \right) R = 0.$$
(50)

By performing the change of radial wave function given by  $\chi(r) = rR(r)$ , the radial part of the wave equation can be written as

$$\frac{d^2}{dr^2}\chi + \frac{2\,\mu}{\hbar^2}\left(E - V - \frac{\hbar^2}{2\,\mu}\frac{l\,(l+1)}{r^2}\right)\chi = 0,\tag{51}$$

where we choose the boundary conditions given by  $\chi(0) = 0$ . In order to simplify the expression given in (51), we define

$$a = \frac{\hbar^2}{\mu e^2}, \qquad \rho = \frac{r}{a}, \qquad E_0 = \frac{\hbar^2 e^2}{\mu}, \qquad \epsilon = \frac{E}{E_0}, \qquad v = \frac{V}{E_0}.$$
 (52)

Then, (51) can be written as

$$\rho^2 \chi''(\rho) + f_{\epsilon,l}(\rho)\chi(\rho) = 0,$$
(53)

where,

$$f_{\epsilon,l}(\rho) = 2\epsilon \rho^2 - 2v\rho^2 - l(l+1).$$
(54)

The prime denotes derivation with respect to the variable  $\rho$ .

Our goal is to solve (53) with (54) using the ideas outlined in Section 1 and study the advantages that our procedure could have in relation to the Taylor method (see other methods in [8]). Let us consider an interval of the form  $[\eta, H]$ , where  $\eta > 0$ can be taken arbitrarily small. Let us divide this interval into *n* equally spaced subintervals and on each of these subintervals, we have a second order approximant polynomial of the type

$$\chi_k = c_{1,k} M_{\alpha_k,\beta_k} (2i\sqrt{a_k} \rho) + c_{2,k} W_{\alpha_k,\beta_k} (2i\sqrt{a_k} \rho), \tag{55}$$

with  $\rho_k < \rho < \rho_{k+1} = \rho_k + h_n$ , k = 1, 2, ..., n. We have  $\alpha_k = -i\frac{b_k}{2\sqrt{a_k}}$ ,  $\beta_k = -\frac{i}{2}\sqrt{4c_k - 1}$ . This method is exact if the radial potential is equal either to  $\rho^{-2}$ ,  $\rho^{-1}$  or  $\rho^0$  (constant). For potentials  $V(\rho)$  with the property  $\rho^2 V(\rho) \mapsto 0$  as  $\rho \mapsto 0$ , Eq. (48) can be approximated for small  $\rho$  as  $\rho^2 \frac{d^2 \chi}{d\rho^2} - l(l+1)\chi = 0$ . Thus, in a small interval close to the origin it can be exactly integrated by our method. The result is approximately equal to  $\rho^{l+1}$  as expected. On the other hand, if  $V(\rho) \mapsto 0$  as  $\rho \mapsto \infty$ , the asymptotic expression results to be  $\rho^2 \chi'' + 2\epsilon \rho^2 \chi = 0$  (here  $x_0$  has to be large enough) and also admit exact numerical integration. In particular, the local error of  $\chi$ , when f(x) is approximated by a Taylor quadratic polynomial is given by

$$e_{k+1} = \frac{1}{10} \frac{|\chi_k|}{\rho_k^2} \left| v'(\rho_k) + \rho_k v^{(2)}(\rho_k) + \frac{1}{6} \rho_k^2 v^{(3)}(\rho_k) \right| h^5, \quad k = 0, \dots.$$
(56)

In what follows, we shall present our results for two types of potentials: the Woods–Saxon and the quadratic potential.

#### 3.1. Woods-Saxon potential

The Woods–Saxon potential is a mean field potential for the nucleons inside the atomic nucleus, which is widely used by nuclear physicists [9]. This has the following form:

$$v = -\frac{v_0}{1 + \exp\left(\frac{\rho - R}{\alpha}\right)},\tag{57}$$

where R,  $\alpha$  and  $v_0$  are parameters. We want to determine the solution of Eq. (53) for the particular case l = 0. To do it, we perform the following change of variables:

$$y := \left(1 + \exp\left\{\frac{\rho - R}{\alpha}\right\}\right)^{-1}.$$
(58)

Thus, Eq. (53) can be rewritten as:

$$y^{2}(y-1)\frac{d^{2}\chi}{dy^{2}} + y(y-1)(2y-1)\frac{d\chi}{dy} + 2\alpha^{2}(\epsilon + v_{0}y)\chi = 0.$$
(59)

Its general solution is given in terms of the arbitrary constants  $c_i$ , i = 1, 2 as

$$\chi(y) = (-1+y)^{i\alpha} \sqrt{2(v_0+\epsilon)} \{ c_1 y^{-\delta} F_{2,1}(-\gamma_-, 1-\gamma_-, 1-2\delta, y) + c_2(-1)^{2\delta} y^{\delta} F_{2,1}(\gamma_+, 1+\gamma_+, 1+2\delta, y) \},$$
(60)

where  $\gamma_{\pm} = i\alpha\sqrt{2}(\sqrt{\epsilon} \pm \sqrt{v_0 + \epsilon})$ ,  $\delta = i\alpha\sqrt{2\epsilon}$  and  $F_{2,1}(a, b, c, x)$  are the well-known hypergeometric functions. If we replace *y* in (60) by its value in terms of  $\rho$  given in (59), we finally obtain the general solution  $\chi(\rho)$  of (53) with *v* given by the Woods–Saxon potential. We shall use this exact solution in order to determine the accuracy of the discrete solution as obtained by our method.

To this end, let us consider the case,  $v_0 = 1$ ,  $\alpha = 1/2$ , R = 5. If we impose the condition that  $\chi(\rho)$  be square integrable, then,  $\epsilon$  is an eigenvalue of the Schrödinger equation. Using (60), we can obtain an eigenvalue numerically and we obtain the value  $\epsilon^* = -0.81133937019$ . Its corresponding eigenfunction is given by:

$$\chi(\rho) = -i \frac{1 + \exp(-10 + 2\rho)}{\exp(-5 + \rho)} \left(\frac{1}{1 + \exp(-10 + 2\rho)}\right)^{1.13692} \left(-1 + \frac{1}{1 + \exp(-10 + 2\rho)}\right)^{0.5 + 0.307132i} \times F_{2,1}\left(0.636922 + 0.307132\,i, \ 1.63692 + 0.307132\,i, \ 2.27384, \ \frac{1}{1 + \exp(-10 + 2\rho)}\right).$$
(61)

In order to quantify the accuracy of our method, we define the following index:

$$d^{2} = \frac{1}{n} \sum_{j=1}^{n} (\chi(\rho_{j}) - \chi_{j})^{2}.$$
(62)

For the next numerical results relative to each interval  $(\rho_j, \rho_j + h)$ , the coefficient  $2\epsilon\rho^2 - 2v\rho^2$  (with l = 0) of Eq. (53) was fitted by means of a quadratic polynomial determined by the least square method. In the case of the chosen parameters, we see that when  $\rho > 10$ , then  $\chi(\rho)$  is negligible. Then, we use h = 0.1 and the interval  $0.1 \le \rho \le 10$  and we obtain  $d^2 = 3.1 \times 10^{-15}$ . Let us compare this result with the integration of Eq. (53) by means of the Taylor method of order *n*. The result is shown in the following table:

From this table, we conclude that the Taylor method requires a sixth order in order to improve our result. For the choice h = 0.5 and  $0.1 \le \rho \le 10$ , we obtain  $d^2 = 4.3 \times 10^{-10}$ . On the other hand, the Taylor method gives

We see from the above table that one needs an eighth order to improve our degree of accuracy.

Finally, we may consider h = 1.0, which is a quite big value for most of the integration methods, and as usual  $0.1 \le \rho \le 10$ , we obtain  $d^2 = 1.6 \times 10^{-6}$ . For the Taylor method,

In this case, a fourteenth order is required to improve our result.

However, concerning CPU times, the Taylor method is still more efficient than ours. For instance, for h = 0.1 (first table), our method takes 4.7 s, while using Taylor, one needs 0.23 s.

#### 3.2. Spherical oscillator

The second example of physical interest is given by the spherical oscillator, which can be exactly solved, which will be a basis for testing the accuracy of our method. In this case, the potential is given by  $v(\rho) = \rho^2/2$ . Then, Eq. (53) has the following form in this case:

$$\rho^2 \chi'' + (2\epsilon \rho^2 - \rho^4 - l(l+1))\chi = 0.$$
(63)

If we define a new unknown function  $f(\rho) := \exp(\rho^2/2) \chi(\rho)$ , we have

$$f''(\rho) - 2\rho f'(\rho) + \left(2\epsilon - 1 - \frac{l(l+1)}{\rho^2}\right) f(\rho) = 0.$$
(64)

Note that  $\rho = 0$  is a singular regular point. Then, the solution on a neighborhood of the origin must have the form

$$f(\rho) = \rho^s \sum_{k=0}^{\infty} a_k \rho^k.$$
(65)

In order to get a solution of (64), we have to replace (65) into (64) and find a recurrence among the  $a_k$ . However, the function  $\chi(\rho)$ , solution of (63) should be square integrable, since we are looking for the eigenvalues (bound states) of our physical problem. Then, the series in (65) must be truncated. Thus, we obtain the following relation among the coefficients  $a_k$ :

$$a_{q+2} = \frac{-2k + 2q}{(q+2)(q+2l+3)} a_q, \quad q = 0, \dots, k,$$
  

$$a_{j+2} = 0, \quad j = k+2, \dots, \infty,$$
  

$$\epsilon_{k,l} = \frac{1}{2}(2k+2l+3),$$
  

$$s = l+1.$$
(66)

Thus, the square integrable solution of (63) is given by

$$\chi_{k,l} = c_{k,l} \exp\left(-\frac{\rho^2}{2}\right) \rho^{l+1} \sum_{q=0}^k a_q \rho^q$$
(67)

where  $c_{k,l}$  is a normalization constant.

In order to compare exact and numerical solutions, we fix  $a_0 = 0$  and  $a_1 = 1$ . To conclude, we want to present two examples for which in each interval  $(\rho_j, \rho_j + h)$ , the coefficient  $(2\epsilon\rho^2 - \rho^4 - l(l+1))$  is fitted by means of a quadratic polynomial determined through the least squares method.

**Example 1.** Take l = 0 and k = 2. Then, the eigenvalue is given by  $\epsilon_{2,0} = 7/2$  and its corresponding eigenfunction by  $\chi_{2,0} = \rho(1 - \frac{2}{3}\rho^2) \exp(-\frac{1}{2}\rho^2)$ . We use our method with h = 0.1 and range of integration  $0.1 \le \rho \le 5$ . For  $\rho > 5$ , one sees that  $\chi_{2,0} \cong 0$ . Then, we get  $d^2 = 1.4 \times 10^{-14}$ .

In the next table, we compare this value to the value obtained using the Taylor method of order *n*:

The accuracy of our method is then similar to the Taylor method of order seventh. If we now use h = 0.5 and  $0.1 \le \rho \le 5$ , we get  $d^2 = 3.3 \times 10^{-8}$ . The result given by the Taylor method is now:

Here, the Taylor method requires an eleventh order to improve our accuracy. However, Taylor is more efficient in terms of CPU times. For h = 0.1, our method requires 5 s, while the Taylor's 0.1 s.

**Example 2.** Let us choose l = 2 and k = 4. In this case,  $\epsilon_{4,2} = 15/2$  and the corresponding exact eigenfunction is given by

$$\chi_{4,2} = \rho^3 \left( 1 - \frac{4}{7} \, \rho^2 + \frac{4}{63} \, \rho^4 \right) \, \exp\left( -\frac{1}{2} \, \rho^2 \right).$$

We use our method with h = 0.1 within the range  $0.1 \le \rho \le 6$ . Note that for  $\rho > 6$ , we have that  $\chi_{2,0} \cong 0$ . In this case,  $d^2 = 1.1 \times 10^{-17}$ . Let us compare our result with that given by the Taylor method of order *n*, which is given in the next table:

We see that our method behaves like the Taylor method of eighth order.

Let us take now h = 0.5 and again  $0.1 \le \rho \le 6$ . Then,  $d^2 = 7.7 \times 10^{-9}$ . The Taylor method gives:

We see that we need a twelfth order to improve our accuracy in this latter case.

# 4. Concluding remarks

We have developed a method for the numerical solution of equations of the form  $x^2y''(x) + f(x)y(x) = 0$ , using the well-known solutions of the equation  $x^2y''(x) + (ax^2 + bx + c)y(x) = 0$ . The method uses segmentary approximation. We have shown the uniform convergence of the approximate solutions to the exact solutions as the number of segments, all of equal length, goes to infinity.

Then, we apply our results to the numerical solution of the radial Schrödinger equation on an interval. We use two potentials to test the power of our method and compare it with the well-known Taylor method. For the Woods–Saxon potential, our method clearly improves the Taylor method and its accuracy improves, as compared with the Taylor method, when the length h of the interpolating segments increases from 0.1 through 1.0. A similar result is obtained in our second example in which we use a potential of the spherical oscillator type. This shows a coincidence with the previous results [10,11].

In terms of CPU times, the Taylor method is still one order of magnitude more efficient, as our examples show.

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