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Error Sources in the Standard Numerical Integration of the Schrödinger Equation: An Improved Method

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A numerical study of the standard Numerov method for the solution of the Schrödinger equation is done by looking at the errors of the solution and the limits of precision for this method. Comparison is made with the results of an improved method that traces back all sources of errors, minimizing them and making the error of each of the sources of comparable magnitude to the others in order to optimize the computing time. A reduction factor of more than 100 is found for the computing time, given a certain accuracy. On the other hand, fixing a certain computational time, a substantial increase in accuracy is gained. The improved method proves particularly suitable for the study of weakly bound states, potentials with discontinuities, singular potentials, or those mixing atomic and nuclear degrees of freedom.

1. INTRODUCTION

In the present paper we analyze the popular shooting method which uses the Numerov procedure to integrate numerically the Schrödinger equation. In doing so we point out the different sources of error of the numerical procedure, then make a numerical study of the error induced from those sources and the limits to precision that the method has as a consequence.

A brief exposition is then made of an improved method, which traces back all sources of error in the numerical integration and carefully selects in a coordinated way the initial conditions for the integration of the equation, as well as the step, to have all sources of error of the same order of magnitude.

In the standard method the step h and the maximum value of the radius r_M, where we stop the integration, are taken independently without much knowledge of which of the two sources of error is larger: the numerical errors accumulated in the integration because of the finiteness of h, or the errors propagated to the numerical solution because of the approximate solution taken at h or r_M. As a consequence it is not clear how to proceed most efficiently to improve the solution, nor we have much idea of the accuracy of the solution in a general case.

The new method developed has a scale of precision, given by an integer number p

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and provides a solution with increasing accuracy as the index of precision is increased. The method optimizes the solution since all sources of error are required to be of the same order of magnitude, and the initial conditions, as well as the step, are simultaneously changed, when more accuracy is required, in such a way as to have all sources of error decreasing in the same proportion.

The efficiency gained is remarkable. As a general rule we can say that if the standard method gives a certain accuracy in a certain time, the improved method provides three to four significant digits more in the same time. Conversely, given a certain precision, the improved method requires from 100–1000 times less time than the standard method for current potentials. In particular cases of weakly bound states and others, the improved method provides seven significant figures when the standard method fails to provide even one. Also when the standard method reaches the limit of precision, indepedently of how small the step h is made or how far r_M goes, the improved method normally provides 3–4 more significant digits.

The new method proves to be especially suited for the study of weakly bound states (~ 10 orders of magnitude smaller than the scale of energies) or for calculating thresholds of coupling constants in order to have a bound state. The method is equally suited to investigate corrections to atomic properties from the presence of the nucleus as an object with internal structure (finite size effects, etc.).

2. The Standard Numerov Method

We briefly review the Numerov method [1] and its application to the eigenvalue problem of the Schrödinger equation [2] to see the sources of error. Let us start with the radial Schrödinger equation,

$$\frac{d^2u(r)}{dr^2} = \left(v(r) + \frac{l(l+1)}{r^2} - \varepsilon \right) u(r) = g(r)\, u(r), \tag{1}$$

where

$$\begin{aligned} &u(r) = rR(r), \qquad && \varepsilon = \frac{2mE}{\hbar^2}, \\ &v(r) = \frac{2mV(r)}{\hbar^2}, \qquad && g(r) = v(r) + \frac{l(l+1)}{r^2} - \varepsilon. \end{aligned} \tag{2}$$

The Numerov method provides an algorithm that, given the solution in the points $n-1$, n of a given regular partition of step h, allows us to calculate the solution at the point $n+1$. Concretely,

$$u_{n+1} = \frac{(2 + (10/12)\, h^2 g_n)\, u_n - (1 - (h^2/12)\, g_{n-1})\, u_{n-1}}{1 - (h^2/12)\, g_{n+1}} + O(h^6), \tag{3}$$

where the error in u_{n+1} is given by

$$\delta u \propto u_n^{vi} h^6 = h^6[(g^{iv} + 7g''g + 4g'^2 + g^3)u + (4g''' + 6gg')\,u']. \tag{4}$$

To determine the eigenvalues of the problem, we integrate from $r=0$ up to a matching point $r=r_c$ (out integration) and from a maximum value of the radius r_M inwards, up to r_c (in integration). With the boundary conditions $u(r)_{r\to 0} \to 0$, $u(r)_{r\to\infty} \to 0$, the values of ε for which the two solutions coincide at $r=r_c$ (up to an arbitrary normalization constant) give the eigenvalues of the problem. To determine these eigenvalues we introduce the function $G(\varepsilon)$,

$$G(\varepsilon) = \frac{u'_{\text{out}}}{u_{\text{out}}}\bigg|_{r_c} - \frac{u'_{\text{in}}}{u_{\text{in}}}\bigg|_{r_c}. \tag{5}$$

Hence the zeros of $G(\varepsilon)$ give us the eigenvalues of the problem. To speed up the numerical procedure the Newton method is used to refine the eigenvalue when we are close to a zero of $G(\varepsilon)$. If $G(\varepsilon)\approx 0$, then $\delta\varepsilon$ such that $G(\varepsilon+\delta\varepsilon)=0$ is given by

$$\delta\varepsilon = -\frac{G(\varepsilon)}{G'(\varepsilon)} + O((\delta\varepsilon)^2). \tag{6}$$

The value of $G'(\varepsilon)$ is provided by the same numerical integration by means of the standard formula

$$\frac{dG(\varepsilon)}{d\varepsilon} = -\frac{1}{u_{\text{out}}^2(r_c)}\int_0^{r_c} u_{\text{out}}^2(r)\,dr - \frac{1}{u_{\text{in}}^2(r_c)}\int_{r_c}^{\infty} u_{\text{in}}^2(r)\,dr. \tag{7}$$

To start the out integration at $r=0$, we choose the approximate solution $u(0)=0$, $u(h)=h^{l+1}$, based on the asymptotic behaviour $u(r)\propto r^{l+1}$ for $r\to 0$ and standard potentials [3, 4]. At large values of r, starting at r_M, we normally approximate the solution by a standard first-order WKB solution, provided that r_M is beyond the last turning point. The choice is not unique, but we must always rely on approximate solutions to start the numerical integration.

This short review allows us to see the sources of error in this numerical integration:

(1) Error from the Numerov method: From one point to another we introduce an uncertainty of order $O(h^6)$. By accumulation of errors this turns out to be an error of $O(h^4)$ for the solution, because it is a second-order differential equation [11].

(2) The solution $u(0)=0$, $u(h)=h^{l+1}$ can be considered exact, up to an irrelevant normalization contant. However, we note that the Numerov method can produce troubles by starting from these two points. Indeed, imagine $l\geqslant 5$, then $u(2h)$ from (3) will be approximately $(2h)^{l+1}$; but the error, $u^{vi}h^6$, is also of order $O(h^{l+1})$ and hence the error induced in $u(2h)$ can be of the same order of

magnitude as the solution itself. These errors will inevitably propagate to the solution at larger r.

(3) The WKB solution at $r \approx r_M$ is also approximate and the errors of this solution will have some repercussion in the accuracy of the method.

(4) The evaluation of ε by means of (6) requires the knowledge of $G'(\varepsilon)$ calculated by means of (7). The numerical integration of (7) will also introduce some errors. On the other hand, we only know the solution up to r_M and not up to ∞ as required there. The contribution $\int_{r_M}^{\infty} u_{\text{in}}^2(r)\, dr$, which is not included in $G'(\varepsilon)$, is another source of error to be taken into account.

(5) When the number of points taken in the integration becomes appreciable, then we must also consider the rounding errors of the computer.

(6) If the potential has a discontinuity, when we go in the numerical integration from two points to the left of the discontinuity to another one to the right of it, the Numerov method assumes a continuity of the function and its derivatives, and hence takes the values of u'' of the left to calculate the function to the right of the discontinuity. The error induced is of order $O(h^2)$ (odd derivatives do not appear in the Numerov method) instead of $O(h^6)$.

3. Improved Method

We have carefully analyzed all these sources of error and made useful corrections to minimize the errors and have a proper control of their magnitudes. The selection of the initial conditions, the step and the other corrections are done in such a way that errors induced from each one of these sources are all of the same order of magnitude. All these modifications are implemented in a computer program that for a given input precision (index $p = 1 - 7$, (8); 7, (8) for maximum precision) automatically sets up those conditions and gives as a result the eigenfunctions and eigenvalues to the desired precision.

The details of the corrections are rather lengthy and have been published elsewhere [5]. The aim of this paper is not to show the details of the new method, but rather to prove the limits in the precision of the standard method, which have been normally overlooked, with the implicit assumption that more precision can be gained by simply making the step h smaller; the only limitation being the precision of the computer.

For these purposes, we have selected a few potentials and studied the precision of the eigenvalues by changing h and r_M. The results are then compared to those obtained with the improved method.

However, to understand the reasons for the improvement we will summarize briefly the ingredients of the new method:

(1) The method splits the region of integration in a minimum of ten different regions. In each one of them, according to (4) we choose g^3h^6u as representative of

the error induced from one step to the other . The accumulative errors in u_n will be of order of $O(h^4)$. We introduce an index of precision p, such that

$$|g|\, h^2 \leqslant 5^{-p}, \tag{8}$$

and then h is chosen in each region such that $|g|_{\max} h^2 = 5^{-p}$. This allows the use of different steps in different regions, thus economizing work without loss of precision. The relative error in the wave function from the accumulative errors is of the order of $(gh^2)^2$ and hence of order 5^{-2p}. With values of $p = 8$, the errors fall inside the last two digits of a 16 digit computer, which will be generally lost due to the computer rounding errors. Hence $p = 7$, 8 normally gives the optimal precision with this method.

(2) We could choose r_M and the initial conditions such that

$$\delta u(r_M)/u(r_M) \sim O(h^4) \sim 5^{-2p}. \tag{9}$$

However, this would grossly overestimate the errors from this source and force us unnecessarily and dangerously into the classically forbidden region, where the wave function decreases very fast. The reason for this is that it neglects the healing properties of the solution. To see this, consider the Schrödinger equation written in the form

$$S'(r) + S^2(r) = g(r), \tag{10}$$

where

$$S(r) = \frac{u'(r)}{u(r)}, \tag{11}$$

which is the Ricatti form of the radial equation.

$S(r)$ also has an accumulative error of $O(h^4)$, as has been proved in [5]. If the good solution $S(r)$, for a certain eigenvalue, has an error $\delta S(r)$, Eq. (10) will then give

$$\delta S'(r) + 2S(r)\, \delta S(r) + \delta S(r)^2 = 0. \tag{12}$$

We can now impose that

$$\left(\frac{\delta S(r_M)}{S(r_M)}\right)^2 \sim O(h^4), \tag{13}$$

which is much less restrictive than (9). Thus the last term in (12) can be neglected and the integration of the equation leads us to

$$\delta S(r) = \delta S(r_M)\, \frac{u(r_M)^2}{u(r)^2}, \tag{14}$$

which shows the propagation of the errors and the healing properties. If $r < r_M$, then $|\delta S(r)| < |\delta S(r_M)|$ since $u(r)$ grows very fast in the classically forbidden region when r decreases. The matching point r_c for the in and out integrations is relevant for the evaluation of the eigenvalues, as shown in Section 2. Thus, we wish $\delta S(r) \sim O(h^4)$ for r relatively close to r_c. A compromise is made at a point r_b to the right of the turning point, close enough to r_c, but which allows an easy evaluation of (14) in terms of the WKB approximation. Thus r_M is chosen such that the conditions (13) and $\delta S(r_b) \sim O(h^4)$ are fulfilled. By doing that, the smallness of the error $\delta S(r_b)$ is equally tied to the smallness of the initial error (13), that provides $O(h^2)$ for $\delta S(r_M)/S(r_M)$, and the healing factor in (14) that provides an extra $O(h^2)$. This, of course, forces an automatic change of r_M when h is changed to have both conditions fulfilled. We also choose the WKB approximation for the solution at r_M, with terms up to 4th order. The formulas used for the WKB method up to 4th order can be seen in the Appendix.

(3) At short distances, $r \to 0$, we make a change of variable and function [6, 7] given by

$$r = e^x, \qquad u(r) = e^{x/2} \varphi(x). \tag{15}$$

With this change, the Schrödinger equations is

$$\varphi''(x) = \bar{g}(x)\, \varphi(x) \tag{16}$$

with

$$\bar{g}(x) \equiv (v - \varepsilon)\, e^{2x} + (l + 1/2)^2. \tag{17}$$

When $x \to -\infty$ $(r \to 0)$, the function $\bar{g}(x)$ has a finite positive limit, and thus for $x \to -\infty$, we will have a classically forbidden region in this new variable. This allows us to use similar techniques to those exposed before, with explicit account of the healing properties, and a special treatment of the approximate solution at small r that goes beyond the r^{l+1} approximation.

(4) As we have seen in Eqs. (6) and (7), we need the function $G'(\varepsilon)$ to evaluate the eigenvalues. Thus, we need the integral

$$I_{in}(r_M) = \frac{1}{u_{\text{in}}(r_M)^2} \int_{r_M}^{\infty} u_{\text{in}}^2(r)\, dr, \tag{18}$$

but we have not evaluated $u_{\text{in}}(r)$ beyond r_M. We can express (18) in terms of $S(r)$ as

$$I_{\text{in}}(r_M) = \int_{r_M}^{\infty} dr \exp \int_{r_M}^{r} 2S_{\text{in}}(r')\, dr', \tag{18'}$$

and then use an iterative part integration to express (18') in terms of known quan-

tities at r_M. By differentiating (18') with respect to r_M and reordening terms we can now write formally

$$I_{\text{in}}(r_M) = \left[1 + \frac{1}{2S_{\text{in}}}\frac{d}{dr}\right]^{-1} \left(\frac{-1}{2S_{\text{in}}}\right)\Bigg|_{r_M} \tag{18''}$$

which allows for a series expansion in terms of the derivation operator, formally equivalent to a repeated part integration. The interest of this expansion lies in the fact that each term of this expansion is of the order of S_0, S_1, S_2,..., of the WKB expansion. By keeping four terms in (18'') the error induced is again of order $O(h^4)$ in G'. A similar thing is done for short distances to account for the missing integral from 0 to x_0, where we start the out integration in the variable x. The rest of the integration in (7) is done by using Bode's formula [8], which has an accumulated error of order $O(h^6)$.

(5) Discontinuities are specially treated by considering them as boundaries of some of the regions in which we divide the integration domain. If we reach the point n (the discontinuity) from the left, we calculate S_n and then use this S_n to start the integration in the right. Since we need two points to start the Numerov integration, we have to generate u_{n+1}, which is done appropriately by using techniques similar to the Numerov method to generate u_{n+1} to the accuracy of $O(h^6)$.

(6) The method allows for an estimate of the total error, since $G(\varepsilon)$ which involves u' will be of order $O(h^4)$, thus the dimensionless variable $G(\varepsilon)\cdot G'(\varepsilon)$ will be of order $O(h^4)$, and hence by means of (6) we can obtain an estimate of the error. This estimate is normally conservative, being, as a general rule, about one order of magnitude larger than the actual error.

4. Results and Discussion

We have selected a few potentials and compared the results of the standard method to those of our method.

(a) Coulomb potential:

$$V(r) = -\frac{a}{r}, \qquad a > 0 \tag{19}$$

with the spectrum

$$\varepsilon_{k,l} = -\frac{a^2}{4(k+l)^2}, \qquad l = 0, 1,..., \quad k = 1, 2,..., \tag{20}$$

where k counts the number of nodes (the origin included), and l is the angular momentum.

In Table I we show the results for $a = 10$. We select a few eigenvalues and write the corresponding value of r at the turning point together with the accuracy of the

TABLE I

Coulomb Potential

				Standard			Optimized			
l	k	Turning point	Exact eigenvalue	R_{max}	Number of points	Relative error	p	R_{max}	Number of points	Relative error
				1.	10^3–10^5	10^{-3}				
				2.	2×10^4	10^{-7}				
0	1	0.4	−25.0	5.	10^5	10^{-8}	7	2.9	6×10^4	10^{-12}
				2.	7×10^3	10^{-5}	4	1.6	6×10^3	10^{-9}
				5.	5×10^5	10^{-9}	5	1.9	10^4	10^{-10}
							6	2.9	2.5×10^4	10^{-11}
				56.	2×10^5	10^{-7}	7	38.	10^5	10^{-13}
0	5	10.	−1.0				4	27.	2×10^4	10^{-9}
							5	29.	4×10^4	10^{-10}
				30.	3×10^6	10^{-10}	6	32.	7×10^4	10^{-12}
				50.	10^5	10^{-12}	7	32.	10^5	10^{-12}
5	1	15.	−0.694	30.	3×10^6	10^{-9}	4	21.	10^4	10^{-9}
				40.	4×10^6	10^{-11}	6	27.	5×10^4	10^{-11}
				139.	4×10^3	10^{-4}	2	130.	4×10^3	10^{-8}
				163.	2×10^4	10^{-7}	4	150.	2×10^4	10^{-10}
19	1	100.	−0.0625	200.	2×10^5	10^{-11}	7	250.	4×10^5	10^{-13}
				200.	2×10^6	10^{-10}				
				300.	3×10^5	10^{-11}				

standard method for given couples of r_M ($R_{\max}$) and h (in the table we write instead the number of points). We should note that in the improved method, we select only the index of precision p, and then everything is determined automatically. The first line for $l=0$, $k=1$ shows that the standard method (SM), for $r_M=1.0$, has a limit of precision at a relative error of 10^{-3}, independent of the number of points. This clearly illustrates the error coming from the initial conditions, which cannot be overcome in spite of the smallness of the step h. If we increase r_M, we gain some precision. However, note that with even a smaller r_M and a larger h (third line), the optimized method (OM) provides four more significant digits. If we compare the SM to the OM in the fourth line, we see again that for about the same r_M and h, the OM provides three more significant digits. The fifth line tells us instead that for a given precision, i.e., 10^{-9}, the OM requires 50 times fewer points (hence an economy of a factor 50 in time) to get the eigenvalue to even more precision. A similar consequence is obtained from comparison of the third line of the SM with the second one of the OM. We should note, however, that the combination of r_M and the number of points in the SM is already optimized since we have used the results of our OM as a guideline. This is certainly an aid that we cannot use in general; hence it is very unlikely that the right couple is used in a general problem, which would have as a consequence unnecessary computational time without any gain in precision.

The second block shows results for $l=0$, $k=5$. The first line shows that with a smaller r_M and larger h the OM gives 6 more significant digits than the SM. Comparison of the first line of the SM with the second line of the OM shows that with a factor 10 less time, the OM still offers two more significant digits than the SM. Comparison of the second line of the SM with the third one of the OM shows that with 100 times less points, we get about the same precision.

The third block corresponds to $l=5$, $k=1$. The second line shows that the OM gives the same precision as the SM in a factor 300 less time. The third line shows again than the OM gives the same precision with a factor 100 less time.

The good results of the SM in the first line are rather accidental. In spite of what we said in point (2) of Section 2, values of $l=5$ do not seem to introduce much extra error than smaller values of l, which should be attributed to the excellent healing properties of the wave function at small r for l large.

The fourth block shows the results for $l=19$, $k=1$. The first and second lines show that with about the same r_M and h the OM provides 3 to 4 more significant digits than the SM. However, if we increase the number of points, as in line 3, we only gain two significant digits from the OM to the SM. The problems associated with $l \geqslant 5$ thus seem more serious for small values of the step h, where the optimized method provides a much better result in the same computing time. However, if the step is small, the healing properties of the equation increase the accuracy of the SM. Comparison of line 3 and 4 of the SM shows that a decrease of h does not lead to a better result but makes it actually worse. Comparison of lines 3 and 5 shows that no extra precision is gained by increasing r_M, telling us that the absolute limit of precision of the SM is at 10^{-11}.

Apart from all considerations taken into account so far, an inspection of the table shows that the OM has a maximal precision with two to three more significant figures than the SM. Since we rarely require so many significant digits in physical problems, it is clear that the best asset of the OM for this simple problem is that it can provide a certain accuracy with $\frac{1}{100}$ of the time of the SM without having to worry about the selection of r_M and h, which are done automatically for a given precision p.

(b) Yukawa potential:

$$V(r) = -2g\frac{e^{-r}}{r}, \qquad g > 0. \tag{21}$$

The results are shown in Table II. The first block shows results for the eigenvalue corresponding to $g = 0.9$, $l = 0$, $k = 1$. Once again the first line shows that the OM provides the same accuracy as the SM in 100 times less time than the SM. Comparison of lines 1 and 2 of the SM shows again that an increase in the number of points does not provide better precision, but the contrary, and comparison of lines 1 and 3, that an increase in r_M does not lead to a more accurate result either. The precision of the SM saturates at 10^{-7} while the OM does it at 10^{-9} in one tenth of the time. The fact that we get fewer significant digits here than in the Coulomb case is due to the fact that the state studied here is weakly bound.

The second block shows results for $g = 2.0$, $l = 0$, $k = 1$. The first line shows once more that for a certain time the OM provides three more significant digits. Comparison of lines 2 and 3 of the SM shows that an increase in r_M does not give a better result, while comparison of lines 3 and 4 clearly shows that an increase in the number of points leads actually to worse results, indicating that we have reached the saturation level of the precision. The OM method still provides two more significant digits in less computing time. For the "exact" eigenvalues we have used the OM and calculated the eigenvalue several times, starting from differential trial energies. All figures that appear repeated are considered good. This procedure proved, to be extremely reliable when applied to analytically soluble potentials [5].

(c) Hulthen potential:

$$V(r) = U(1 - e^{r/a})^{-1}, \qquad U,\ a > 0 \tag{22}$$

with exact solution for the s wave [3],

$$\varepsilon_{k,0} = -\frac{(k^2 - a^2U)^2}{4a^2k^2}, \qquad k \leqslant [a\sqrt{U}]. \tag{23}$$

The results are shown in Table III. The case studied here is the case of a very weakly bound state, of order $\varepsilon \sim 10^{-10}$, when the potential is of order of 10^{-1}. A quick inspection of the results with the SM shows clearly that this method is unable to provide a single significant figure realiably, while the OM provides seven

TABLE II

Yukawa Potential

					Standard			Optimized			
g	l	k	Turning point	Exact eigenvalue	R_{max}	Number of points	Relative error	p	R_{max}	Number of points	Relative error
					35.	4×10^5	10^{-7}				
0.9	0	1	8.	-0.002847[a]	35.	4×10^6	10^{-5}	4	28.	6×10^3	10^{-6}
					50.	5×10^5	10^{-7}				
								5	30.	10^4	10^{-7}
								7	34.	3×10^4	10^{-9}
					7.	7×10^3	10^{-5}	4	7.	7×10^3	10^{-8}
2.0	0	1	1.	-1.18436	20.	2×10^5	10^{-9}	5	7.	1×10^4	10^{-9}
					50.	5×10^5	10^{-9}				
					50.	5×10^6	10^{-8}				
								6	9.	2.5×10^4	10^{-10}
								7	11.	6×10^4	10^{-11}

[a] Weakly bound state.

TABLE III

Potential	l	k	Turning point	Exact energy	Standard			Optimized ($p=7$)		
					R_{max}	Number of points	Relative error	R_{max}	Number of points	Relative error
Hulthén					200.	10^3-10^6	10^{4b}			
					300.	3×10^5	10^{-1}			
	0	3	196.	-2.7×10^{-10a}	300.	10^7	$1.^b$			
					400.	4×10^5	10^{-1}			
$\frac{0.09001}{1.-e^{r/10.}}$					400.	2×10^7	$1.^b$			
					600.	2×10^5	1.	500.	8×10^4	10^{-7}
Square well					2.2	2×10^5	10^{-6}			
	0	1	2.	2.213435	2.2	2×10^7	10^{-3}			
$81.\theta(r-2)$					2.3	5×10^4	10^{-5}	2.2	3×10^4	10^{-12}
					7.	7×10^5	5×10^{-2}			
$-\frac{0.24}{r^2}-\frac{1.2}{r}$	0	1	1.5	-1.0	30.	3×10^6	5×10^{-2}			
					32.	10^5	10^{-1}	17.	10^5	10^{-10}

[a] Weakly bound state.

[b] The guessed improved eigenvalue was positive.

significant digits in this case. The OM thus proves very efficient in the evaluation of very weakly bound states and in the related problem of evaluating threshold coupling constants of a certain potential to have just one bound state, a problem that has received some attention in the literature [9]. Our results for this problem [5] provide the coupling constants with relative error 10^{-9}, while the special perturbative methods [9], based on Padé approximants, or the variational methods [10] give a relative error of 10^{-1}–10^{-2}.

(d) Square well: In the second block of Table III we illustrate the case of a square well potential to show the errors involved in the case of discontinuities of the potential. The results of the SM show a ceiling of precision at 10^{-6} when we use 2×10^5 points. An increase of the number of points leads to less accurate results. The OM provides 6 more significant digits with one tenth of the time.

(e) Singular potential: We have chosen a potential that goes as r^{-2} for small radia and which has an exact eigenvalue for $l=0$, $k=1$. In this case the ceiling of precision of the SM is 5×10^{-2}, while the OM provides 8 to 9 more significant figures in about one tenth of the time.

In the standard method we have taken a constant step h in the whole range of the integration. However, one of the benefits of the OM is that we have taken a different step h in different regions, hence economizing in computing time. We may wonder how much of the success of the OM is due to the use of this variable step. To find the answer we have used an improved SM (ISM) with the same partition of the integration range as the OM and the same choice for h in each one of the regions of the partition. Hence the ISM method and the OM only differ in the

TABLE IV

Coulomb Potential

					OM	ISM	SM
l	k	p	R_{max}	N	(Significant digits)		
0	1	4	1.6	6300	9	6	6
		5	1.9	11000	10	7	6
		6	2.3	24000	11	8	7
		7	2.9	62000	12	8	8
0	5	4	27	17000	9	6	5
		5	29	34000	10	7	5
		6	32	70000	12	8	6
		7	38	160000	13	8	6
5	1	4	21	8000	9	6	5
		6	27	47000	11	10	8
		7	32	130000	12	12	11
19	1	2	130	3500	8	5	4
		4	150	19000	10	7	6
		7	250	370000	13	13	12

choice of the initial conditions. Thus the ISM still benefits from some of the improvements of the OM.

In Tables IV and V we show the comparative results for the SM, OM, and ISM. In Table IV, for the Coulomb potential, we can see in the first and second blocks that, with the same number of points and equal choice for R_{max}, the ISM provides about one more significant digit than the SM, while the OM provides about 4 more significant digits than the SM, thus stressing the role played by the initial conditions.

The third and fourth blocks show again that for large values of l the OM is far more efficient than the ISM or SM for a small number of points, while when this number is increased, all methods give accurate results.

In Table V we show the results for the Yukawa, Hulthén, square, and singular potentials. In the first and second blocks for the Yukawa potential we see again that the ISM provides about one more significant digit than the SM while the OM provides from three to four more signicant digits than the SM. In the case of a weakly bound state of the Hulthén potential, the ISM provides a substantial improvement over the SM but the OM still provides three more significant digits than the ISM. In the case of the square-well potential the ISM provides no improvement over the SM while the OM provides 7 more significative digits than the SM. In this case the appropriate matching at the discontinuity of the potential, used in the OM is the essential factor in the precision of the OM. Finally for the singular potential the improvement of the ISM over the SM is small while the OM provides 9 more significant digits than the SM.

Study of Tables IV and V reveals that the proper care of the initial conditions taken in the OM is the major factor in the improvements offered by the method.

TABLE V

Yukawa and Other Potentials

						OM	ISM	SM
g	l	k	p	R_{max}	N	Significant digits		
0.9	0	1	4	28	5700	6	4	4
			5	30	8900	7	5	4
			7	34	36000	9	7	5
2.0	0	1	4	7	6900	8	6	5
			5	7	11000	9	7	6
			6	9	25000	10	7	6
			7	11	61000	11	8	7
Hulthén	0	3	7	500	83000	7	4	1.5
Square well	0	1	7	2.2	36000	12	5	5
Singular potential	0	1	7	17	92000	10	1.5	1

5. Conclusions

In this paper we have shown the limits of precision of the standard method for the integration of the Schrödinger equation and compared the results to an optimized method that has been recently developed.

The errors of the integration come essentially from the finiteness of the step h and from the propagation of the errors of the approximate initial conditions. Because of these errors the SM reaches a ceiling of precision at a certain point independently of the smallness of h (in fact, the solution becomes worse for smaller values of h because of the rounding errors of the computer), while the OM still provides two to three more significant digits.

For particular problems, like weakly bound states, potentials with discontinuities or singular potentials that go, such as ar^{-2} for small r ($a > -\frac{1}{4}$), the OM provides from 6 to 8 more significant digits.

Apart from the higher precision reached by the OM, for potentials of general use, such as the Coulomb potential or Yukawa, given a certain computer time, the OM generally provides 3 to 4 more significant digits than the SM. Conversely, if a certain precision is required, the OM reaches it in $\frac{1}{100}$ of the time of the SM as an average. For the special potentials quoted before the gain in efficiency is even higher. All these factors are found in the most favorable situation for the SM when an optimal choice of h and r_M is done that requires the smallest computational time. In general we do not have a precise idea of which combination to take. Generally, the computer will do unnecessary work that does not result in a gain of precision. The OM selects instead the initial conditions and the step automatically, according to the precision required.

In summary the OM provides a substantial gain in efficiency in the numerical solution of the Schrödinger equation with a remarkable reduction of computer time for a given precision of the solution, or a much more accurate solution, with the same computational time than the SM. The OM method proves especially suited to the study of particular problems such as weakly bound states, potentials with discontinuities, singular potentials, thresholds of coupling constants, or potentials with two parts where one is a small correction to the other as would be the case in problems that mix atomic with nuclear degrees of freedom [5].

APPENDIX: WKB Formulas up to 4th Order

In the WKB method the variable S is expanded as a series of terms

$$S(r) = \sum_{n=0}^{\infty} S_n(r) \tag{A1}$$

with

$$S_0(r) = -\sqrt{g(r)} \equiv -p(r) \tag{A2}$$

in the classically forbidden region. A recurrent relation is fulfilled by the terms S_n,

$$S'_{n-1}(r) + \sum_{k=0}^{n} S_k(r)\, S_{n-k}(r) = 0, \qquad n > 0. \tag{A3}$$

If we define

$$\varphi_n(r) \equiv \frac{1}{g(r)} \frac{d^n}{dr^n} g(r), \tag{A4}$$

then we have

$$\varphi'_n(r) = \varphi_{n+1} - \varphi_n \varphi_1, \tag{A5}$$

hence in terms of the φ's,

$$\begin{aligned} S_1 &= -\frac{1}{4}\varphi_1, \\ S_2 &= \frac{1}{2^5 p}(5\varphi_1^2 - 4\varphi_2), \\ S_3 &= \frac{1}{2^6 p^2}(18\varphi_1\varphi_2 - 15\varphi_1^3 - 4\varphi_3) \\ S_4 &= \frac{1}{2^{11} p^3}(1105\varphi_1^4 - 1768\varphi_1^2\varphi_2 + 448\varphi_1\varphi_3 + 304\varphi_2^2 - 64\varphi_4). \end{aligned} \tag{A6}$$

The derivatives involved can be calculated numerically. If we define

$$\tilde{g}_n = \frac{g(r+nh)}{g(r)}, \qquad n = -2, -1, \ldots, 2, \tag{A7}$$

then we have

$$\begin{aligned} h\varphi_1 &= (\tilde{g}_{-2} - 8\tilde{g}_{-1} + 8\tilde{g}_1 - \tilde{g}_2)\tfrac{1}{12} + O(h^5), \\ h^2\varphi_2 &= (-\tilde{g}_{-2} + 16\tilde{g}_{-1} + 16\tilde{g}_1 - \tilde{g}_2)\tfrac{1}{12} - \tfrac{10}{4} + O(h^5), \\ h^3\varphi_3 &= (-\tilde{g}_{-2} + 2\tilde{g}_{-1} - 2\tilde{g}_1 + \tilde{g}_2)\tfrac{1}{2} + O(h^5), \\ h^4\varphi_4 &= (\tilde{g}_{-2} - 4\tilde{g}_{-1} - 4\tilde{g}_1 + \tilde{g}_2 + 6) + O(h^5). \end{aligned} \tag{A8}$$

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