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Numerov Method Maximally Adapted to the Schrödinger Equation

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We construct and investigate the two-step scheme which is maximally specialized for the Schrödinger equation. The new scheme is found to preserve all attractive features of the standard Numerov method (ease in programming, flexibility in application, speed in run, etc.) with the important advantage of being more efficient for problems involving high values of energy. Its efficiency is actually found to be close to that of the piecewise perturbation methods, a fact which strongly recommends it for further applications. © 1987 Academic Press, Inc.

1. INTRODUCTION

The method of Numerov is very popular among the people who are interested in solving the Schrödinger equation and the reason for its popularity is mainly due to the fact that it is the simplest and the easiest to program of all the existing methods of the same order.

It was the top method in the sixties, when it was intensively investigated mathematically (see, e.g., [1]) and frequently applied to current problems; but afterwards it gradually lost its position in favor of other methods, notably the piecewise perturbation methods. For a recent review of the latter see [2, Chap. 3].

The fact that the method of Numerov is weaker than the piecewise pertubation methods (especially when high values of energy are involved) is quite normal; whereas the latter methods were specially tailored for the Schrödinger equation, the Numerov method was not. It follows that this method may join the competition again only after it is adapted for a particular form of a second-order differential equation, viz. the Schrödinger equation.

As a matter of fact, the problem of deriving multistep methods adapted to special equations is not new but for many years the investigations were more or less sporadic and focused on very particular cases (see, e.g., [3]). These efforts were first systematized and brought on a rigorous mathematical basis by Lyche [4] in 1972.

The theory of Lyche opened the possibility of trying to adapt the Numerov method to the Schrödinger equation and the first adaptations for successive degrees

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of completeness were reported in [5, 6]. Adaptations of four-step methods were also considered [7].

It is important to point out that the algorithms proposed in [5, 6] exhaust the potentialities offered by Lyche's theory, that is, they are the only possible adaptations whose convergence is secured by this theory. Yet, they do not saturate the criterion formulated in [6, 8] to produce the maximally adapted algorithm, since such an algorithm would be of a form whose convergence is no longer secured in that frame.

The purpose of this paper is to derive the maximally adapted algorithm, to investigate its convergence, and to show how it behaves in practice. We will find that it is convergent indeed, that it is as easy to implement as the standard Numerov method, and that its results are not only much better than those of the latter but almost as good as the results of the piecewise perturbation methods of the same order.

For the mentioned qualities the new algorithm is again placing the method of Numerov in the class of high efficient methods.

2. Derivation of the New Scheme

We here consider the one-dimensional Schrödinger equation

$$y'' = f(x)y, \qquad f(x) = V(x) - E, \qquad x \in [a, b] \tag{2.1}$$

with nonsingular potential $V(x)$ and focus on the two-step (or three-point) schemes to solve it, that is, on schemes of the form

$$\begin{aligned} &a_0\, y(x+h) + a_1\, y(x) + a_2\, y(x-h) \\ &\quad = h^2[b_0\, y''(x+h) + b_1\, y''(x) + b_2\, y''(x-h)]. \end{aligned} \tag{2.2}$$

In practice the values of the second-order derivative at $x-h$, x, and $x+h$ must be replaced here as indicated in Eq. (2.1). Equation (2.2) becomes an algebraic equation connecting the solution values $y(x+h)$, $y(x)$, and $y(x-h)$ from which, if two are known, the third results directly.

The method of Numerov is the scheme with the weights

$$a_0 = a_2 = 1, \qquad a_1 = -2, \qquad b_0 = b_2 = \tfrac{1}{12}, \qquad b_1 = \tfrac{5}{6}, \tag{2.3}$$

and these weights were obtained on the basis of the simple condition that Eq. (2.2) integrates polynomials whose degree is as high as possible. Equation (2.2) with weights (2.3) actually integrates the following set of functions

$$1, \qquad x, \qquad x^2, \qquad x^3, \qquad x^4, \qquad \text{and} \qquad x^5, \tag{2.4}$$

or, equivalently, any polynomial of the fifth degree. In other words, the method of Numerov is a scheme valid for *any* differential equation of the form

$$y'' = F(x, y), \qquad x \in [a, b], \tag{2.5}$$

provided h is small enough to ensure that the solution of this equation is well approximated by a fifth degree polynomial over any elementary subinterval of width $2h$ of $[a, b]$. In short, this method is an *unspecialized* method.

To generate a two-step scheme specialized to the Schrödinger equation (SE) means to construct the weights a_i and b_i on the basis of some conditions which explicitly account for the particularity that $F(x, y)$ which occurs in Eq. (2.1) is linear in y and a systematic way to accomplish this task was proposed in [6, 8] and further detailed in [2, Section 3.8]. If, over some elementary range of width $2h$, we approximate $V(x)$ by some constant $\bar{V}$ and denote $\bar{f} = \bar{V} - E$, then the solution of Eq. (2.1) is well represented by a linear combination of the hierarchized set of functions

$$\exp[\pm \bar{f}^{1/2} x], \qquad x \exp[\pm \bar{f}^{1/2} x], \qquad x^2 \exp[\pm \bar{f}^{1/2} x], \ldots. \tag{2.6}$$

The general criterion to generate a method specialized for SE thus consists of constructing the weights a_i and b_i on the basis of a reference set of functions which includes pairs from the natural set (2.6) and the more pairs included, the more specialized the algorithm.

The total number of functions admitted in the reference set remains the same as in the case of the original option (2.4), that is, six. Three further options thus become available viz.:

$$1, \quad x, \quad x^2, \quad x^3, \quad \exp[\pm \bar{f}^{1/2} x], \tag{2.7}$$

$$1, \quad x, \quad \exp[\pm \bar{f}^{1/2} x], \quad x \exp[\pm \bar{f}^{1/2} x], \tag{2.8}$$

and

$$\exp[\pm \bar{f}^{1/2} x], \qquad x \exp[\pm \bar{f}^{1/2} x], \qquad x^2 \exp[\pm \bar{f}^{1/2} x]. \tag{2.9}$$

In short, the two-step scheme (2.2) admits four levels of specialization for SE, where each level is identified by the number of pairs from the natural set. Specifically, the standard Numerov method is a zeroth level scheme because the set (2.4) embeds no such pair, while the methods based on sets (2.7), (2.8), and (2.9) will be in order first, second, and third level schemes. Hereinafter these will be identified as S_k, $k = 0, 1, 2, 3$. All these versions exhibit the common feature of being symmetric, that is, $a_0 = a_2$ and $b_0 = b_2$. Without going into detail we only note that this is a natural consequence of the particularity of the space spanned by each of the four sets (2.4), (2.7), (2.8), and (2.9) of being invariant to reflection $x \to -x$, to translation $x \to x + \Delta x$, and of remaining closed with respect to the second-order differentiation.

Versions S_1 and S_2 have been investigated in [5] and in [6], respectively, and the theoretical and experimental results reported there show that S_1 is more efficient than S_0 and that S_2 is more efficient than both S_0 and S_1. The version S_3 is examined in this paper and, as it will be seen later on, it confirms the expectation of being the most efficient of all.

Construction of the Weights of S_3

Equation (2.2) is homogeneous in the weights and thus it is defined up to an arbitrary scale factor. For this reason there is no loss in generality if from the very beginning we take $a_0 = a_2 = 1$. Equation (2.2) reads

$$y(x+h) + a_1 y(x) + y(x-h) = h^2[b_0 y''(x+h) + b_1 y''(x) + b_0 y''(x-h)] \tag{2.10}$$

and its weights are determined below upon the condition that Eq. (2.10) is identically satisfied by all functions of set (2.9).

On introducing $y(x) = \exp[\bar{f}^{1/2}x]$ into Eq. (2.10) we get

$$a_1 + E^+(1, Z) = ZE^+(1, Z)b_0 + Zb_1 \tag{2.11}$$

and the same equation results also when we introduce $y(x) = \exp[-\bar{f}^{1/2}x]$. Here $Z = \bar{f}h^2$ and

$$E^{\pm}(n, Z) = \exp[nZ^{1/2}] \pm \exp[-nZ^{1/2}], \qquad n = 1, 2, 3, \ldots. \tag{2.12}$$

Likewise, the introduction of $y(x) = x\exp[\pm\bar{f}^{1/2}x]$ gives

$$E^-(1, Z) = Z^{1/2}[2E^+(1, Z) + Z^{1/2}E^-(1, Z)]b_0 + 2Z^{1/2}b_1 \tag{2.13}$$

and the introduction of $y(x) = x^2\exp[\pm\bar{f}^{1/2}x]$ gives

$$E^+(1, Z) = [2E^+(1, Z) + 4Z^{1/2}E^-(1, Z) + ZE^+(1, Z)]b_0 + 2b_1. \tag{2.14}$$

Equations (2.11), (2.13), and (2.14) form a linear algebraic system for the three unknowns a_1, b_0, and b_1 with the solution

$$a_1(Z) = -(2 + \Delta A(Z)/D(Z)), \qquad b_0(Z) = B_0(Z)/D(Z), \qquad b_1(Z) = B_1(Z)/D(Z), \tag{2.15}$$

where

$$\Delta A(Z) = -(1/8Z^{1/2})[6E^-(1, Z) + 2Z^{1/2}E^+(1, Z) - 3E^-(2, Z) + Z^{1/2}E^+(2, Z) - 6Z^{1/2}], \tag{2.16}$$

$$B_0(Z) = (1/8Z^{3/2})[Z^{1/2}E^+(1, Z) - E^-(1, Z)], \tag{2.17}$$

$$B_1(Z) = (1/8Z^{3/2})[E^-(2, Z) + Z^{1/2}E^+(2, Z) - 6Z^{1/2}], \tag{2.18}$$

$$D(Z) = (1/8Z^{1/2})[3E^-(1, Z) + Z^{1/2}E^+(1, Z)]. \tag{2.19}$$

Equation (2.10) with weights (2.15) defines the S_3 scheme; for accurate numerical computation of $\Delta A(Z)$, $B_0(Z)$, $B_1(Z)$, and $D(Z)$, as well as for other technical details, see Appendix A. The deviations of $a_1(Z)$, $b_0(Z)$, and $b_1(Z)$ from the constant values -2, $\frac{1}{12}$, and $\frac{5}{6}$ corresponding to S_0 are plotted in Fig. 1 for $-3 < Z < 3$. It is seen that each of the three curves passes through zero when $Z = 0$, i.e., S_0 is the particular case $Z = 0$ of S_3. This conclusion is also supported by the series expansions given in Appendix A.

3. Convergence of S_3

The importance of expressions (2.16), (2.17), (2.18), and (2.19) for the weights (similar expressions were also reported by Raptis in [10]) is only academic unless it is proved that the resultant S_3 is indeed a convergent method.

The main difficulty in proving the convergence of S_3 comes from the fact that both its b weights and one of its a weights are h-dependent; remember that $Z = \bar{f}h^2$. In fact, none of the existing approaches of convergence of multistep methods [4, 9]

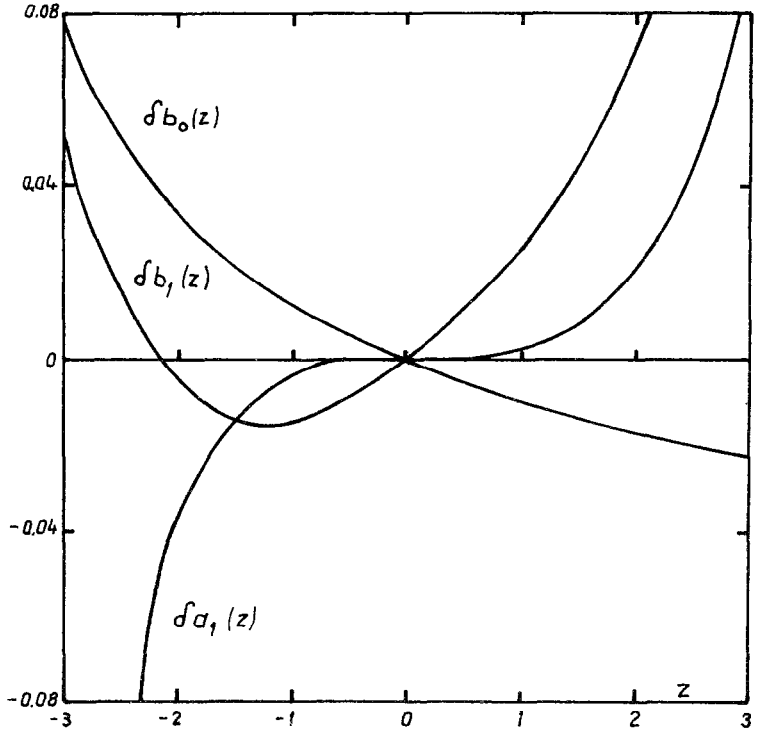

FIG. 1. Deviations of the Z dependent weights $a_1(Z)$, $b_0(Z)$ and $b_1(Z)$ of S_3 from the corresponding constant weights of the standard Numerov method, i.e., $\delta a_1(Z) = a_1(Z) + 2 = -\Delta A(Z)/D(Z)$, $\delta b_0(Z) = B_0(Z)/D(Z) - \frac{1}{12}$, $\delta b_1(Z) = B_1(Z)/D(Z) - \frac{5}{6}$.

is here applicable ad litteram and the reason is obvious for Henrici's approach because this was constructed for methods with constant weights.

Less transparent is the reason in the case of Lyche's approach [4] since this has been constructed for methods with h dependent weights. An attentive examination shows, however, that when investigating the two necessary and sufficient conditions for convergence, that is, consistence and stability, Lyche treats the former in full generality but leaves the latter essentially as in [9]. Lyche's approach is thus found to cover only the methods with h-dependent b and constant a, a class to which method S_3 does not belong.

Altogether, when examining the convergence of S_3 we can follow [4] for consistency but we must treat the stability separately.

Local Truncation Error and Consistency

Since, by its very construction, S_3 integrates exactly the six functions under Eq. (2.9) it follows that the leading term of the local error of S_3 (we denote it as $\varepsilon_3(x)$) is of the form

$$\varepsilon_3(x) = KR(x) \tag{3.1}$$

where $R(x) = 0$ is a sixth-order linear differential equation of Euler's type whose solutions are just the mentioned six functions. Its characteristic equation thus is $(z^3 - \bar{f})^3 = 0$, so

$$R(x) = y^{(6)} - 3\bar{f}y^{(4)} + 3\bar{f}^2y^{(2)} - \bar{f}^3y. \tag{3.2}$$

The factor K is determined on the basis that, on one hand, the leading term of the local truncation error of S_0 is

$$\varepsilon_0(x) = h^6 \Delta_0(x), \qquad \Delta_0(x) = -\frac{1}{240}\, y^{(6)}(x); \tag{3.3}$$

and that, on the other hand, S_0 is the particular case of S_3 corresponding to $Z = 0$; i.e., $\bar{f} = 0$. It follows that Eqs. (3.1) and (3.3) must be identical when $\bar{f} = 0$, so $K = -h^6/240$.

In conclusion, the leading term of the local truncation error of S_3 is

$$\begin{aligned} \varepsilon_3(x) &= h^6 \Delta_3(x), \\ \Delta_3(x) &= -\frac{1}{240}\left[y^{(6)}(x) - 3\bar{f}y^{(4)}(x) + 3\bar{f}^2y^{(2)}(x) - \bar{f}^3y(x)\right], \end{aligned} \tag{3.4}$$

and it shows that S_3 is consistent.

Stability

In the following we will refer to the general two-step scheme (2.10) where the only assumption is that all the written weights are h-dependent. In other words we cover *all* methods of this type, S_3 included.

In general, the stability of a multistep method to solve differential equations of order r is identified as the property of being convergent for the simplest equation $y^{(r)}=0$. In particular, the investigation of the stability of scheme (2.10) means simply searching for whether it is convergent for $y''=0$ and, at this point, it is perhaps useful to first briefly review the content of the concept of convergence for this particular case. We thus consider the problem

$$y''=0, \qquad x\in[a,b], \qquad y(a)=A, \qquad y'(a)=B, \tag{3.5}$$

where A and B are arbitrary constants, with the exact solution $y(x)=A+B(x-a)$. We take some arbitrary value $X\in(a,b]$ and further divide $[a,X]$ into n equally spaced subintervals through the mesh points $x_0=a$, $x_1=a+h$, ..., $x_n\equiv X=a+nh$. As a matter of fact, it is important to keep in mind that this implies a direct connection between n and h, viz. $nh=X-a$, so that the larger the n, the smaller the h.

These mesh points are used to propagate the solution of Eq. (3.5) by means of algorithm (2.10), that is, by means of the recurrence relation

$$y_k+a_1(h)\,y_{k-1}+y_{k-2}=0, \qquad k=2,3,\ldots,n. \tag{3.6}$$

This needs two starting values y_0 and y_1. The value of y_0 is simply $y_0=y(a)=A$, while for y_1 we may take any value such that

$$\lim_{h\to 0}(y_1-y_0)/h=B, \tag{3.7}$$

a condition which is satisfied if we put $y_1=A+Bh+\Delta y_1$ with $\Delta y_1=\delta h^s$, where δ is arbitrary and $s>1$.

Clearly, the final value y_n depends on the number of steps we take and the definition of the convergence refers to the behavior of y_n when n tends to infinity. Specifically, scheme (3.6) is called convergent if y_n tends to $y(X)=A+(X-a)B$ for any A, B, X, δ, and $s>1$.

These points in mind, we have the following

THEOREM. *If* $a_1(h)$ *is of form*

$$a_1(h)=-(2+\Delta a(h)) \tag{3.8}$$

with

$$\Delta a(h)=O(h^{2+q}), \qquad q>0 \tag{3.9}$$

then scheme (2.10) *is stable.*

Proof. The idea of the proof consists of showing that if $a_1(h)$ satisfies the two conditions (3.8) and (3.9) then the recurrence relation (3.6) is convergent.

The latter is simple enough to be treated by hand. If we assume that $y_k = d^k$, $d \neq 0$, Eq. (3.6) becomes

$$d^2 - (2 + \Delta a(h))d + 1 = 0, \tag{3.10}$$

an algebraic equation with two roots d_+ and d_-. These can be written compactly as

$$d_\pm = \tfrac{1}{2}(2 + \Delta a \pm (4\Delta a + \Delta a^2)^{1/2}) = \exp[\pm Q^{1/2}], \tag{3.11}$$

where

$$Q(h) = \Delta a(h)(1 - \tfrac{1}{12}\Delta a(h)) + O((\Delta a)^{5/2}). \tag{3.12}$$

Condition (3.9) guarantees that $Q(h) = O(h^{2+q})$, $q > 0$, so that we can write

$$Q(h) = h^{2+q}\,\Delta Q(h), \qquad q > 0, \tag{3.13}$$

where $\Delta Q(h)$ is a bounded function of h.

The general form of y_k is a linear combination of d_+^k and d_-^k,

$$y_k = C_+ d_+^k + C_- d_-^k, \tag{3.14}$$

and the coefficients C_+ and C_- are readily fixed in terms of the starting values via conditions $y_0 = C_+ + C_-$ and $y_1 = C_+ d_+ + C_- d_-$.

We are interested in the error at $k = n$ and this is

$$E_n \equiv y(x_n) - y_n = A \cdot C_A + B \cdot C_B + \delta \cdot C_\delta \tag{3.15}$$

with

$$\begin{aligned} C_A &= S(n-1, Q) - S(n, Q) + 1, \qquad C_B = -h(S(n, Q) - n), \\ C_\delta &= -h^s S(n, Q), \qquad S(p, Q) = E^-(p, Q)/E^-(1, Q). \end{aligned} \tag{3.16}$$

Now, since $Q(h)$ is of form (3.13), we can use a truncated series of the exponential functions which occur in $S(p, Q)$. For $p = n$ we have, in order,

$$\begin{aligned} S(n, Q) &= \frac{\exp[nQ^{1/2}] - \exp[-nQ^{1/2}]}{\exp[Q^{1/2}] + \exp[-Q^{1/2}]} \\ &= \frac{\exp[(X-a)(h^q\,\Delta Q)^{1/2}] - \exp[-(X-a)(h^q\,\Delta Q)^{1/2}]}{\exp[h(h^q\,\Delta Q)^{1/2}] - \exp[-h(h^q\,\Delta Q)^{1/2}]} \\ &= \frac{X-a}{h} \cdot \frac{1 + (1/6)\,h^q(X-a)^2\,\Delta Q + \ldots}{1 + (1/6)\,h^{2+q}\,\Delta Q + \ldots} \\ &\simeq \frac{X-a}{h}\left[1 + \frac{1}{6}((X-a)^2 - h^2)\,h^q\,\Delta Q\right] \end{aligned} \tag{3.17}$$

and, similarly, we find that

$$S(n-1, Q)=\frac{X-a-h}{h}\left[1+\frac{1}{6}((X-a-h)^2-h^2)\,h^q\,\Delta Q\right]. \tag{3.18}$$

The following expressions for the coefficients thus result:

$$\begin{aligned} C_A &\simeq -\tfrac{1}{2}h^q(X-a)(X-a-h)\,\Delta Q(h), \\ C_B \simeq \tfrac{1}{3}(X-a+h)C_A, &\qquad C_\delta \simeq -h^{s-1}(X-a); \end{aligned} \tag{3.19}$$

and we see that all these tend to zero when h is decreased. In other words, if conditions (3.8) and (3.9) are satisfied, the recurrence relation is convergent and then scheme (2.10) is stable. Q.E.D.

For the particular case of S_3, Eqs. (A.1) and (A.2) show that

$$\Delta a=\Delta A(Z)/D(Z) \simeq -\tfrac{1}{240}Z^3=-\tfrac{1}{240}\bar{f}^3h^6, \tag{3.20}$$

i.e., conditions (3.8) and (3.9) are satisfied with $q=4$ and S_3 is then stable.

4. Quantitative Theoretical Estimate of the Efficiency of S_3

The expressions of the local truncation error for the standard and the maximally specialized Numerov schemes are given in Eqs. (3.3) and (3.4), respectively, but these formulas do not yet make it clear how much better is S_3 than S_0. To obtain this information we must work out these expressions in terms of the very Schrödinger equation.

We first write $f(x)$ of Eq. (2.1) in a form in which the energy dependence is conveniently separated. We thus define $g(x)=V(x)-\bar{V}$, where $\bar{V}$ is the previously mentioned constant approximation of $V(x)$, and $\bar{f}=\bar{V}-E$. We have

$$f(x)=g(x)+\bar{f}, \tag{4.1}$$

where $g(x)$ reflects the quality of the constant approximation of $V(x)$ and $\bar{f}$ embeds the energy dependence. Further we express the derivatives $y^{(2)}$, $y^{(4)}$, and $y^{(6)}$ which enter $\Delta_0(x)$ and $\Delta_3(x)$ in terms of the very equation $y''=fy$. We also account for that $g^{(n)}=V^{(n)}$ for any nth order derivative with respect to x and organize the terms as polynomials in the energy dependent $\bar{f}$:

$$y^{(2)}=\bar{f}y+gy \tag{4.2}$$

$$y^{(4)}=\bar{f}^2y+2\bar{f}gy+[(V^{(2)}+g^2)\,y+2V'y'] \tag{4.3}$$

$$\begin{aligned} y^{(6)}=\bar{f}^3y+3\bar{f}^2gy+\bar{f}[(3g^2+7V^{(2)})\,y+6V'y'] \\ +(g^3+4V'^2+7V^{(2)}g+V^{(4)})y+(4V^{(3)}+6V'g)y'. \end{aligned} \tag{4.4}$$

The latter multiplied by $-\frac{1}{240}$ is exactly $\Delta_0(x)$, while for $\Delta_3(x)$ we get

$$\Delta_3(x) = -\frac{1}{240}[4V^{(2)}\bar{f}y + (g^3 + 4V'^2 + 7V^{(2)}g + V^{(4)})y + (4V^{(3)} + 6V'g)y'] \tag{4.5}$$

To compare $\Delta_3(x)$ and $\Delta_0(x)$ we distinguish two situations according to the value of E.

When E is close to the potential, i.e., when $\bar{f} = \bar{V} - E \simeq 0$, only the free terms in these polynomials in $\bar{f}$ are numerically relevant and these are identical in the two Δ's. S_0 and S_3 are then expected to exhibit similar accuracies.

The picture is changing when E is substantially displaced from $\bar{V}$, either above, i.e., $\bar{f} \ll 0$, or below, i.e., $\bar{f} \gg 0$. In both cases $|\bar{f}|$ is a big number and thus the first term becomes dominating in the polynomials (4.4) and (4.5). For large $|\bar{f}|$ we actually obtain the (asymptotic) behaviors

$$\Delta_0(x) \simeq -\tfrac{1}{240}\bar{f}^3 y, \tag{4.6}$$

$$\Delta_3(x) \simeq -\tfrac{1}{60}\bar{f}V^{(2)}y, \tag{4.7}$$

i.e., the error of the standard Numerov method increases as the third power of $\bar{f}$ while that of the new, maximally specialized method S_3 increases with $\bar{f}$ only linearly, a striking difference indeed.

5. User-Oriented Issues

In the following we will repeatedly refer to S_3 in the form (A.5) which is the most convenient for practical use, viz.:

$$\begin{aligned} &D(Z)\,y(x+h) - (2D(Z) + \Delta A(Z))\,y(x) + D(Z)\,y(x-h) \\ &\quad = h^2[B_0(Z)f(x+h)\,y(x+h) + B_1(Z)f(x)\,y(x) \\ &\qquad + B_0(Z)f(x-h)\,y(x-h)]. \end{aligned} \tag{5.1}$$

If we put here $Z = 0$ we obtain the standard Numerov scheme S_0 so that, except for the explicit computation of the Z-dependent weights, S_3 is as easy to apply as is S_0.

Some issues of practical interest are reviewed below.

Accumulated Truncation Error

If S_0 is used in the forward integration regime, then, as resulted from the general theory of Henrici [9], the truncation error accumulated at each mesh point $x_k = a + kh$, i.e.,

$$E_k \equiv y(x_k) - y_k \tag{5.2}$$

is of the form

$$E_k = h^4 e(x_k) + O(h^6), \tag{5.3}$$

where $e(x)$ is the solution of the initial value problem

$$e'' = f(x)e + \Delta_0(x), \qquad e(a) = e'(a) = 0, \tag{5.4}$$

called the error equation, where $\Delta_0(x)$ is given by Eq. (3.3).

This theory can be repeated with minor changes to S_3 and the result is the same as above with the only exception that now the error equation is

$$e'' = f(x)e + \Delta_3(x), \qquad e(a) = e'(a) = 0, \tag{5.5}$$

i.e., with $\Delta_3(x)$ given by Eq. (3.4) in place of $\Delta_0(x)$.

The conservation of form (5.3) implies that the order of S_3 and S_0 is the same and equal to four. The real difference for the efficiency of the two methods then resides only in the different magnitudes of $e(x)$ which, in turn, is dictated in terms of the different behaviors of $\Delta_0(x)$ and $\Delta_3(x)$; the latter issue was discussed in the previous section.

In practice, Eq. (5.5) is useful only insomuch as $\Delta_3(x)$ can be generated numerically. The case of large values of E offers such a possibility since the asymptotic expression (4.7) is available. For such a case Eq. (5.5) may be effectively used (for solving it numerically one can apply just S_3 in form (A.5)) to decide on the step size adjustment, for instance. An alternative, simpler technique for the step size adjustment can be derived on the basis of Eq. (B.5) given in Appendix B.

Round-off Error Propagation and the Summed Form

It is known that the round-off error accumulated through S_0 increases as h^{-2} and, also, that this dependence can be reduced to a more decent behavior, i.e., h^{-1}, if a special form, called the summed form, is used (see, e.g., [9]).

The same remains true, also, for S_3. To derive its summed form we denote

$$z(x) = [D(Z) - h^2 B_0(Z) f(x)]\, y(x) \tag{5.6}$$

to write Eq. (5.1) as

$$z(x+h) - 2z(x) + z(x-h) = h^2 g(x, z; h) \tag{5.7}$$

with

$$g(x, z; h) = \frac{1}{h^2} \cdot \frac{\Delta A(Z) + h^2(2B_0(Z) + B_1(Z))f(x)}{D(Z) - h^2 B_0(Z) f(x)}\, z(x). \tag{5.8}$$

Equation (5.7) is further treated as in [2, p. 78] to obtain the desired summed form. It is the set of the following two equations:

$$z(x+h) = z(x) + S(x), \tag{5.9a}$$

$$S(x+h) = S(x) + \frac{\Delta A(Z) + h^2(2B_0(Z) + B_1(Z))f(x+h)}{D(Z) - h^2 B_0(z) f(x+h)} z(x+h), \tag{5.9b}$$

with the starting values $z(a)$ and $S(a) = z(a+h) - z(a)$. If here we put $Z = 0$, we obtain the familiar summed form of S_0.

Application of S_3 to Systems of Coupled Equations

The matrix extension of Eq. (3.1), viz.

$$\mathbf{y}'' = \mathbf{f}(x)\mathbf{y}, \tag{5.10}$$

or, on components,

$$y_i'' = \sum_{j=1}^{j=N} f_{ij}(x)\, y_j, \qquad f_{ij} = V_{ij}(x) - E\delta_{ij}, \qquad i = 1, 2, \ldots, N, \tag{5.11}$$

is known as the coupled channel equation.

It can be solved directly by scheme (5.1) which, of course, is now a matrix equation. Also $\Delta\mathbf{A}$, $\mathbf{B}_0$, $\mathbf{B}_1$, and $\mathbf{D}$ are now N by N diagonal matrices of weights.

Specifically, let $\bar{V}_{ii}$ be an approximation to $V_{ii}(x)$ over $[x-h, x+h]$. We form $Z_i = (\bar{V}_{ii} - E)h^2$ and use it to generate the weights of S_3 in channel i. The diagonal matrices with these weights, viz.

$$\begin{aligned} \Delta\mathbf{A}_{ij} &= \delta_{ij}\, \Delta A(Z_i), \qquad & \mathbf{B}_{0_{ij}} &= \delta_{ij} B_0(Z_i), \\ \mathbf{B}_{1_{ij}} &= \delta_{ij} B_1(Z_i), & \mathbf{D}_{ij} &= \delta_{ij} D(Z_i) \end{aligned} \tag{5.12}$$

are the ones to be used in the matrix equation (5.1).

6. Numerical Illustration

To compare experimentally S_0 and S_3 we have chosen the Woods–Saxon potential

$$V(x) = u_0/(1+t) + u_1 t/(1+t)^2, \qquad t = \exp[(x - x_0)/a_0], \tag{6.1}$$

where $u_0 = -50$, $a_0 = 0.6$, $x_0 = 7$, and $u_1 = -u_0/a_0$ (see [6] and references therein). The domain of numerical integration is $[a = 0, b = 15]$ and both schemes have been programmed in summed form.

For the value of $\bar{V}$ which occurs in S_3 we use three choices: *Choice* 1 is

$$\bar{V} = \begin{cases} -50 & 0 \leqslant x \leqslant 6.5 \\ 0 & 6.5 < x \leqslant 15, \end{cases} \tag{6.2}$$

originally proposed in [6, 8] as representing a reasonable step-function approximation to $V(x)$ of Eq. (6.1). *Choice* 2 is the result of the application of the procedure proposed in Appendix B. *Choice* 3 consists of changing $\bar{V}$ at each iteration step; specifically, at the step which involves x_{i-1}, x_i, and x_{i+1} we take simply $\bar{V} = V(x_i)$.

Our test refers to the eigenvalue problem associated to Eq. (2.1). To compute the eigenvalues, that is, bound states when $E<0$ and resonances when $E>0$, we adapted the program described in [2, Chap. 5], with the only notable exception that now backward integration is used at each test E which occurs in the shooting process.

All computations were carried out on an IBM 370/135 in double precision arithmetic and the accuracy gain with S_3 over S_0 was found to gradually increase with the energy, in full agreement with the theoretical predictions of Section 4. A representative selection of the results is given in Table I, where we also added data from the CPM(1), which is the best placed piecewise perturbation method of the fourth order.

If the three versions of S_3 are compared it is seen that the verion corresponding to Choice 1 is weaker than the other two. The comparison of the latter two versions allows us to acquire some experimental evidence on the range of validity of the procedure proposed in Appendix B. We see that the two versions are of similar accuracy except for the last resonance at $h = \frac{1}{16}$ and $\frac{1}{32}$. The reason for the

TABLE I

Absolute Errors $\Delta = E^{\text{ref}} - E^{\text{calc}}$ of the Resonances Calculated by Methods S_0 and S_3 with Three Choices for $\bar{V}$ and CPM(1)

Reference resonance	h	S_0	S_3 Choice 1	S_3 Choice 2	S_3 Choice 3	CPM(1)
$E = 53.588872$	$\frac{1}{16}$	−230727	586(2)	107(8)	58(239)	60
	$\frac{1}{32}$	−14110	35(2)	2(10)	3(479)	4
	$\frac{1}{64}$	−879	2(2)	0(10)	0(959)	0
$E = 163.215341$	$\frac{1}{16}$	−9106839	716(2)	83(6)	103(239)	123
	$\frac{1}{32}$	−479227	44(2)	10(7)	8(479)	10
	$\frac{1}{64}$	−29500	2(2)	0(7)	0(959)	0
$E = 341.495874$	$\frac{1}{16}$		1594(2)	99(5)	28(239)	163
	$\frac{1}{32}$	−7536068	127(2)	12(5)	14(479)	17
	$\frac{1}{64}$	−436825	7(2)	1(5)	1(959)	1
$E = 989.701916$	$\frac{1}{16}$		−1443(2)	2070(4)	−5147(239)	−42
	$\frac{1}{32}$		412(2)	114(4)	17(479)	36
	$\frac{1}{64}$		24(2)	3(4)	3(959)	3

Note. The errors are given in 10^{-6} units. Empty areas indicate that the error there exceeds the format allowed in the table. For the S_3 versions the number of calculations of the weights at each test energy in the shooting process is given in parentheses.

discrepancy is that in these cases the terms proportional to powers of h higher than six, which are disregarded in Eq. (3.4) and also in our procedure, are still numerically important.

It is quite instructive to compare the methods for computational effort. This can be done theoretically by examining their formulas in the same way as in [2, Chap. 5] for several methods, S_0 and CPM(1) included. The result is that, if the weights were already calculated at some previous step of the recurrence procedure, the execution time step is the same for S_0 and S_3 and approximately five times smaller than for CPM(1). If the weights must be calculated anew at that step, the time for S_3 becomes approximately equal to that for CPM(1).

In Table I we give in parentheses the number of changes of $\bar{V}$ on $[a, b]$ or, equivalently, the number of calculations of the weights at each test energy. Since these numbers are small for Choices 1 and 2 and much smaller than that for Choice 3, the times are expected to be roughly equal for S_0 and S_3 with Choices 1 and 2 and about five times smaller than for S_3 with Choice 3 and for the CPM(1), a prediction fairly confirmed experimentally.

The comparison of the best placed S_3 versions with CPM(1) suggests that, for one and the same h, they are of comparable accuracy. However, such a conclusion is not typical because it happens that the Woods–Saxon potential somewhat favors S_3. Technically, the reason is that the second derivative of the potential here (note that this occurs in Eq. (4.7)) is significantly different from zero only in a very narrow subinterval of the integration domain. Our experimental tests on other potentials indicate that, at high energies, CPM(1) performs generally better than S_3.

7. Conclusions

The method developed in this paper represents the maximal adaptation of a two-step scheme to the Schrödinger equation. Our method, abbreviated as S_3, is found to enjoy the following main properties:

(i) It retains all the features of the standard Numerov method as, for instance, easy to program, flexibility in application, possibility of being extended for coupled equations and also for complex potentials.

(ii) Its order is four.

(iii) Its error increases *linearly* with energy (for comparison, it is recalled that the increase is cubic for the standard Numerov method) and thus it can be successfully applied also for problems involving high values of E.

(iv) If, for the latter problems, S_3 is compared with the piecewise perturbation methods on one and the same partition, the advantages are seen to be shared. In fact, on one hand, the errors from S_3 are typically larger than from the piecewise perturbation methods but, on the other hand, the computation time is often much shorter.

APPENDIX A: READY-TO-PROGRAM FORMULAS OF THE WEIGHTS

Equation (2.10) with the weights (2.15)–(2.18) is not yet convenient to be implemented as an efficient code and the two main reasons are:

(i) For small values of $|Z|$ the computation of functions $\Delta A(Z)$, $B_0(Z)$, $B_1(Z)$, and $D(Z)$ through Eqs. (2.16)–(2.18) is extremely sensitive to the near cancellation of like terms.

(ii) Some values in the range of real, negative Z exist at which $D(Z)$, the common denominator of all weights, vanishes and the weights would become infinite at these values.

To cure difficulty (i) a threshold $T>0$ is introduced and series expansions in powers of Z are used for $\Delta A(Z)$, $B_0(Z)$, $B_1(Z)$, and $D(Z)$ for $|Z|<T$, viz.,

$$\Delta A(Z)=-Z^3\sum_{k=0}^{k_{\max}}\Delta A_k Z^k, \qquad B_i(Z)=\sum_{k=0}^{k_{\max}}[B_i]_k Z^k, \qquad i=0,1,$$
$$D(Z)=\sum_{k=0}^{k_{\max}} D_k Z^k, \tag{A.1}$$

where

$$\Delta A_k=\frac{1}{(2k+7)!}[16\cdot 2^k(2k+1)+k+5], \qquad [B_0]_k=\frac{k+1}{2(2k+3)!},$$
$$[B_1]_k=\frac{2^{2k}(2k+5)}{(2k+3)!}, \qquad D_k=\frac{k+2}{2(2k+1)!}. \tag{A.2}$$

$k_{\max}$ depends on the value of T and also on the accuracy required in the results. In our computations we have used $T=1$ and the value $k_{\max}=10$ was found sufficient to obtain 14 exact figures.

To speed up the computation it is recommended that coefficients (A.2) are generated once, at the beginning of the whole program, and simply called from the memory whenever the case $|Z|<T$ is active.

Note also that if we put $Z=0$ in Eq. (A.1) we obtain $\Delta A(0)=0$, $B_0(0)=\frac{1}{12}$, $B_1(0)=\frac{5}{6}$, and $D(0)=1$, which are just the weights of the standard Numerov method.

When Z is real and $|Z|\geqslant T$ we introduce $p=|Z|^{1/2}$, $q=8p$, $t=1/(qZ)$, and

$$c=\begin{cases}2\cosh p & \text{if } Z\geqslant T\\ 2\cos p & \text{if } Z\leqslant -T,\end{cases}$$
$$s=\begin{cases}2\sinh p & \text{if } Z\geqslant T\\ 2\sin p & \text{if } Z\leqslant -T,\end{cases} \tag{A.3}$$

to get the following ready-to-program formulas:

$$\begin{aligned} \Delta A(Z) &= -[pc(c+2) - 3s(c-2) - q]/q, \\ B_0(Z) &= (pc - s)t, \\ B_1(Z) &= [c(pc+s) - q]t, \\ D(Z) &= (3s + pc)/q. \end{aligned} \tag{A.4}$$

In short, Eqs. (A.1)–(A.4) enable safe and fast computation of the weights for any real Z and only real arithmetic is used in the program.

There are also cases when $V(x)$ and/or E are complex, as, for instance, when investigating quantum absorbtion problems. In such a case, Z is also complex. Series (A.1)–(A.2) remain valid for $|Z| < T$ but the original functions (2.16)–(2.18) must be programmed for $|Z| \geqslant T$. Naturally the computer will now work with complex arithmetic.

Difficulty (ii) is readily avoided if Eq. (2.10) with weights (2.15) is first multiplied by the common denominator $D(Z)$:

$$\begin{aligned} &D(Z)\, y(x+h) - (2D(Z) + \Delta A(Z))\, y(x) + D(Z)\, y(x-h) \\ &\quad = h^2[B_0(Z)\, y''(x+h) + B_1(Z)\, y''(x) + B_0(Z)\, y''(x-h)]. \end{aligned} \tag{A.5}$$

Indeed, since the zeros of $\Delta A(Z)$, $B_0(Z)$, and $B_1(Z)$ are different from the zeros of $D(Z)$, Eq. (A.5) works equally well for any Z.

APPENDIX B: Choosing a Suitable $\bar{V}$

We first consider the behavior of $y(x)$ and $y'(x)$ in various regions of the integration interval. Standard WKB arguments show that in a classically allowed region, $y(x)$ is of the form

$$y(x) \simeq A(x) \sin\left[\int^x |f(x')|^{1/2}\, dx' + \varphi(x)\right], \tag{B.1}$$

where the amplitude $A(x)$ and the phase shift $\varphi(x)$ are typically almost constant. Thus we can write $|y(x)| \leqslant A(x)$ and $|y'(x) \leqslant |f(x)|^{1/2} A(x)$. In a classically forbidden region, similar arguments indicate that $y(x)$ and $y'(x)$ behave such as $|y'(x)|/|y(x)| \simeq f(x)^{1/2}$ so that, upon introducing

$$D(x) = \begin{cases} |y'(x)|/A(x) & \text{in allowed regions} \\ |y'(x)|/|y(x)| & \text{in forbidden regions,} \end{cases} \tag{B.2}$$

we can write compactly

$$D(x) \leqslant |f(x)|^{1/2}. \tag{B.3}$$

Strictly speaking, the WKB arguments cease to be valid if x is in the vicinity of a turning point. Since, however, for typical potentials such regions happen to be very narrow, anyway much narrower than the regions where the WKB approximation is valid, we feel justified in disregarding the less frequent situations and so we simply admit that Eq. (B.3) is valid for any value of x.

These points in mind we are ready to tackle the problem of describing numerically the local accuracy of S_3. We choose the scaled absolute error in the classically allowed regions and relative error in the forbidden regions, that is,

$$\mathrm{Acc}(x) = \begin{cases} |\varepsilon_3(x)|/A(x) & \text{in allowed regions} \\ |\varepsilon_3(x)|/|y(x)| & \text{in forbidden regions,} \end{cases} \tag{B.4}$$

and apply Eqs. (3.4), (3.5), and (B.3) to get that

$$\mathrm{Acc}(x) \leqslant \tfrac{1}{240} h^6 A^c(x; \bar{V}) \leqslant \tfrac{1}{240} h^6 A^1(x; \bar{V}), \tag{B.5}$$

where

$$A^c(x; \bar{V}) = |V^{(4)}(x) + 4V^{(2)}(x) f(x) + 4V'^2(x) + g^3(x) + 3V^{(2)}(x) g(x)| + |4V^{(3)}(x) + 6V'(x) g(x)| \cdot |f(x)|^{1/2}, \tag{B.6}$$

$$A^1(x; \bar{V}) = B(x) + Q(x; \bar{V}), \tag{B.7}$$

$$B(x) = |V^{(4)}(x) + 4V^{(2)}(x) f(x) + 4V'^2(x)| + 4\,|V^{(3)}(x)| \cdot |f(x)|^{1/2} \tag{B.8}$$

and

$$Q(x; \bar{V}) = |g(x)| \cdot [|g^2(x) + 3V^{(2)}(x)| + 6\,|V'(x)|\,|f(x)|^{1/2}]. \tag{B.9}$$

Upper labels c and 1 were here used to distinguish between a close and a larger bound.

These formulas can be exploited in various ways, in particular, for finding a suitable value for $\bar{V}$. If, for instance, we decide to change $\bar{V}$ at each mesh point, Eqs. (B.7) and (B.9) tell us that $\bar{V} = V(x)$ is the optimal choice irrespective of the energy; with this choice of maximal value of $\mathrm{Acc}(x)$ over $[a, b]$ is $\bar{A} = h^6 \|B\|/240$, where $\|B\| = \max_{x \in [a,b]} |B(x)|$. Such an option is however unpractical since it implies the computation of the weights of S_3 at each local application and this strongly increases the computation effort. Also the accuracies are by no means uniformly distributed over $[a, b]$.

More attractive is to construct a constant piecewise $\bar{V}$,

$$\bar{V} = \bar{V}_k, \qquad x \in I_k \equiv [\bar{x}_k, \bar{x}_{k+1}),$$
$$k = 0, 1, 2, \ldots, k_{\max}, \qquad \bar{x}_0 = a, \qquad \bar{x}_{k_{\max}+1} = b \tag{B.10}$$

consisting of subintervals which are as broad as possible on the condition that the maximal accuracy over each I_k is maintained at some level around $\bar{A}$. In our

practical procedure this level is 1.1 $\bar{A}$ and we rely on the mesh points $x_n = a + nh$ as the natural reservoir from which the ends of each I_k are selected.

We focus on one such subinterval, that identified by $k = K$, say, and also assume that its left-hand end is known, $\bar{x}_K = x_p$. To find the other end and also $\bar{V}_K$, we successively investigate the intervals $[x_p, x_{p+n}]$, $n = 1, 2, 3, \ldots$. At each n the investigation consists of a two step process:

Step 1. We construct $\bar{V}$ as

$$\bar{V} = \frac{1}{x_{p+n} - x_p} \int_{x_p}^{x_{p+n}} V(x)\, dx. \tag{B.11}$$

Step 2. We calculate $A^c\ (x_{p+q}; \bar{V})$ (standard finite difference representation is used to calculate the derivatives of $V(x)$) and compare to 1.1 $\|B\|$. We cover in order $q = 1, 2, \ldots, n$ and the process is stopped at the first q, at which it is detected that $A^c(x_{p+q}; \bar{V})$ exceeds 1.1 $\|B\|$. In such a case (i) the value x_{p+n-1} is assigned to $\bar{x}_{K+1}$ and $\bar{V}_K$ is taken as

$$\bar{V}_K = \frac{1}{x_{p+n-1} - x_p} \int_{x_p}^{x_{p+n-1}} V(x)\, dx \tag{B.12}$$

if $n > 1$ and (ii) $\bar{x}_{K+1} = x_{p+1}$ and $\bar{V}_K = V(x_p)$ if $n = 1$. If the test is successful for all q, the procedure is repeated from Step 1 with the new $n = n + 1$.

Some final remarks follow:

1. A salient property of the inequalities under (B.5) is that they do not imply an explicit knowledge of $y(x)$. The immediate practical consequence is that the accuracy can be appraised well before the Schrödinger equation is solved, in contrast to the usual techniques where the solution and the accuracy appraisal advance simultaneously.

2. The energy dependence of $A^c(x; \bar{V})$ is of the form

$$A^c(x; \bar{V}) = |a(x; \bar{V}) + b(x)E| + c(x; \bar{V})\, |V(x) - E|^{1/2}$$

with obvious identifications for a, b, and c. This formula can be used in practice to easily check for the range of energies for which $\bar{V}$, originally constructed on the basis of some test energy E_t, still remains acceptable.

3. Inequalities (B.5) are also valid for versions S_1 and S_2 provided A^c and A^1 are correspondingly modified. An inequality of the form

$$\mathrm{Acc}(x) \leqslant \tfrac{1}{240} h^6 A^c(x)$$

can also be derived for the standard Numerov method. As a matter of fact, the step size adjustment technique recently proposed by Oset and Salcedo in [11] is consistent with such an inequality but the approximation of $A^c(x)$ used there is quite crude.

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