JOURNAL OF COMPUTATIONAL PHYSICS 72, 70–77 (1987)

An Algorithm for Integrating the Schrödinger Equation*

A. E. THORLACIUS AND E. D. COOPER†

TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, Canada V6T 2A3

Received November 18, 1985; revised August 18, 1986

Presented here is an algorithm tailored to solve the radial Schrödinger equation for the case of proton scattering from an optical potential. The algorithm is straightforward to use and results in a significant increase in speed, around a factor of 2 at least, over the conventional Numerov algorithm.

INTRODUCTION

Integration of radial Schrödinger equations and their ilk has received much attention in the last few years. In the interest of brevity, the reader is referred to the references in Ref. [1 et seq.].

The Schrödinger equation, and also many other equations in physics, may be reduced to the form

$$y''(x) = f(x)\, y(x), \tag{1}$$

where x is some dimensionless parameter. Often $y(x)$ will be a column vector of functions and $f(x)$ a square matrix, in which case Eq. (1) represents a set of coupled equations. There are many algorithms available for solving Eq. (1), and some justification is required before presenting yet another. The algorithm presented here is especially useful for doing optical model fits to proton elastic scattering data. Such fits entail solving Eq. (1) many times over with slightly different parameters each time. Any gain in speed is quite desirable since it can save several hours of computer time. We have two goals in mind in this work: to develop an algorithm which is both simple to implement and which allows a significant gain in speed over a modification of the Numerov method due to Raynal [2, 3] Raynal's algorithm is chosen here as a standard since it appears to be the simple, most widely used algorithm, to date, for the optical model problem.

The method, hereafter referred to as the enhanced Numerov algorithm (ENA), is presented and tested here in the context of high-energy proton scattering in the

* Work supported by U.S. DOE Grant ACO2 81ER 0047 and the Natural Sciences and Engineering Research Council of Canada.

† Present address: McGill University, 3600 University St., Montreal, P.Q. H3A 2T8.

0021-9991/87 $3.00

optical model; however, the algorithm is appropriate for any system of equations (1) which have the property:

$$y(x)\, f'(x) \ll f(x)\, y'(x). \tag{2}$$

In the optical model example $f(x)$ is of the form

$$f(x) = \left(-1 + U(r) + \frac{l(l+1)}{x^2} \right) \tag{3a}$$

$$x = kr, \qquad l = 0, 1, 2, \ldots, \tag{3b}$$

where k is the wave vector in the center-of-mass frame and r is the radius coordinate. We note that the Dirac equation for proton–nucleus scattering may also always be reduced to the form in Eq. (1).

To solve the scattering problem, all that is needed is the regular solution to Eq. (1) at two points, called the matching radii, at a large enough value of x so that the potential $U(r)$ has become negligible. Phase shifts are then extracted by matching to appropriate asymptotic forms (Bessel functions or Coulomb functions). The algorithm presented here is for obtaining just these two points, although extraction of the complete wave function is quite straightforward.

The Enhanced Numerov Method

Using Taylor's expansions for $y(x)$ and $f(x)$ it is straightforward to show that (1) implies

$$\begin{aligned} &y(x+h)(1 - T(x+h)) + y(x-h)(1 - T(x-h)) - (2 + 10T(x))\, y(x) \\ &\quad = \frac{1}{3} \sum_{m=3}^{\infty} \frac{h^{2m} y^{(2m)}(x)(2m+3)(2-m)}{(2m)!} \end{aligned} \tag{4}$$

where

$$T(x) = \frac{h^2}{12} f(x). \tag{5}$$

The usual prescription [4] is to notice that the r.h.s. of Eq. (4) is $o(h^6)$ and may be neglected if h is small enough.

It has been pointed out [1] that if we approximate $f(x)$ by its asymptotic form (i.e., -1), then the series on the r.h.s. of Eq. (4) may be summed exactly. In practice this device allows a large step size when the potentials are very weak and l/x is small. However, if the potentials are weak, then, since nuclear potentials drop exponentially for large x, we are close to the matching radii and there is little more integration to do. If the potentials are not weak, then the modification gives little improvement, in fact if $l \neq 0$ then $f(x)$ will change sign for small x, and for these

values the correction actually worsens the algorithm. However, in the case of electromagnetic potentials which do not drop exponentially, there is a large region where this modification gives a significant increase in speed over the Cowell method [4].

The next logical step is to calculate the r.h.s. of Eq. (4) at each point by assuming that $f(x)$ is slowly varying compared to $y(x)$. By this we mean

$$f^{(m)}(x)\, y^{(n)}(x) \ll f^{(n)}(x)\, y^{(m)}(x), \qquad m > n. \tag{6}$$

In our optical model example, $y(x) \sim \sin(x + \ldots)$, so differentiating $y(x)$ with respect to x is going to leave it of the same order and magnitude. We take $f(x)$ to be the Fermi form

$$f(x) \sim \left(U_0 \Big/ 1 + \exp\left\{ \frac{r - R}{a} \right\} \right) - 1, \tag{7}$$

where R is taken to be 5 fm and a is around 0.6 fm. The approximation is expected to be at its worst around the nuclear surface, where this function is most rapidly varying.

Successive uses of Eqs. (6) and (1) lead us to the approximation:

$$y^{(2m)}(x) \simeq (f(x))^m\, y(x). \tag{8}$$

By using Eq. (8) to approximate the terms of the r.h.s. of Eq. (4) we can analytically sum the series and obtain a formula which is exact whenever $f(x)$ is locally constant. If, following Numerov [4], we define

$$w(x) = (1 - T(x))\, y(x), \tag{9}$$

then we obtain the formula

$$w(x + h) + w(x - h) = (2 \cosh \sqrt{12T(x)})\, w(x). \tag{10}$$

In Eq. (10) T is a small quantity and we may do a power series expansion, keeping only terms $o(h^4)$ to get

$$w(x + h) + w(x + h) = (2 + 12T(x) + 12T(x)^2)\, w(x). \tag{11}$$

This constitutes what we refer to as Raynal's algorithm, although Raynal's original derivation is somewhat different; Raynal took the Numerov formula [5],

$$w(x + h) + w(x - h) = \left\{ \frac{2 + 10T(x)}{1 - T(x)} \right\} w(x) \tag{12}$$

and expanded the denominator in powers of $T(x)$, keeping the first 2 powers of $T(x)$ to obtain Eq. (11). The formula (10) has the property that it is correct to order h^6 for all $f(x)$'s, and is exact whenever $f(x)$ is locally constant.

Numerical Tests

Numerical tests have been performed on Eq. (10) for values of l between 0 and 100, and also for $U_0 = 0$, 0.4, 4, which in the optical model example would correspond to proton scattering with energies of $\sim\infty$, 125, and 12 MeV from a 50 MeV potential. As a criterion to judge the algorithm we considered what step size was required to produce a relative error 10^{-6} in the final phase shifts. In all cases, not just the smallest value of U, the ENA allowed the step size to be increased by a factor of 3 over the Raynal algorithm. Often the algorithm allowed an increase of a factor of 5. By testing the accuracy of Eq. (10) on a point-by-point basis we found that (10) offered no improvement whatsoever over Raynal's algorithm until we reached the classical turning point, $T(x) = 0$; thus we propose using Raynal's algorithm up to the turning point and Eq. (10) from then on. This proposal constitutes what we refer to as the enhanced Numerov algorithm.

There is one drawback to this algorithm which is important for partial waves which have $l = 1$. At the original Raynal algorithm must be modified since $\lim_{x\to 0} f(x)\, y(x)$ does not vanish. In the Raynal method this is accomplished in an approximate way by assuming $y(x)$ to be a parabola. For a given step size this introduces an error which turns out to be of the same order of magnitude as the error margin using the Raynal method over the range of integral. Since our method, for a given step size, is significantly better there, then we must start our integration more carefully using a spherical Bessel-like fit to the function to obtain the value of $\lim_{x\to\infty} f(x)\, y(x)$. We would like to also add the caveat that the $l = 0$ partial waves will have a problem self-starting if the potential is irregular at the origin; however, with a suitable parametrization this can always be avoided.

Figure 1 shows the accumulation of error for the case $U_0 = 0.4$, $l = 4$, $k = 2.5$. The curves shown reflect the errors in the phase of the wave function accumulated as the

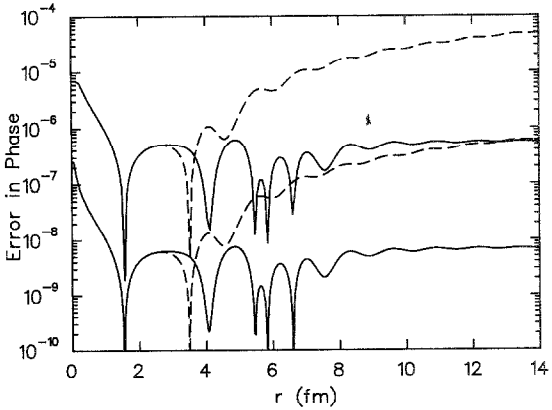

FIG. 1. The accumulation of error in the phase of the wave function as the outward integration is done. The solid curves are calculated using the ENA, the dashed curves with Raynal's algorithm. The upper two curves are calculated using a step size (Δx) of 0.1875, the lower two curves with a step size a third as big, 0.0625.

outward integration is done, using two step sizes, $h = 0.0625$ and 0.1875. The solid curves are obtained using the ENA, with the same step size both inside and outside the turning point. The dashed curves are the result of using the Raynal algorithm everywhere. The Raynal algorithm appears to be accumulating less error at large distances than near the turning point; however, this is an artifact of using a logarithmic scale. The ENA does not appear to introduce an error at all into the phase once the turning point is passed, and this leads one to suspect that the step size in this region may be larger than absolutely necessary. A method for doubling the step size is called for, and this requires an estimate of the local error. This is discussed later. We have not closely examined step size doubling, as it conflicts with one of our philosophies in this paper, namely simplicity.

We are left with one problem, namely that while Eq. (10) is straightforward, it involves a square root and a hyperbolic cosine evaluation at each step. Since $T(x)$ in general will be complex, this entails many machine operations which will slow the integration down significantly. Specifically on a VAX 8600 the ENA has roughly six times as many operations per step as the Raynal algorithm, meaning that the new algorithm as indicated in Eq. (10) is actually slower. However, we do not have to work this hard to evaluate the r.h.s. of Eq. (10).

Since $T(x)$ is small, of order h^2, we may evaluate the hyperbolic cosine by a power series. Specifically, if we define

$$S(x) \equiv 12T(x) = h^2 f(x), \tag{13}$$

then

$$\cosh \sqrt{S} \simeq 1 + \frac{S}{2!} + \frac{S^2}{4!} + \frac{S^3}{6!} + \frac{S^4}{8!} \cdots. \tag{14}$$

In practice keeping just the first 5 terms in Eq. (14) is sufficient. We note here the connection with the Raynal algorithm (Raynal #1) which is obtained by taking just the first 3 terms in Eq. (14). We must now evaluate a polynomial of a complex variable with real coefficients. There exists an algorithm [6] for doing this very quickly. Specifically, if

$$f(S) = c_n S^n + c_{n-1} S^{n-1} + \cdots + c_0 \tag{15}$$

let

$$\begin{aligned} r &= S + \bar{S}, & m &= S\bar{S} \\ a_1 &= c_n, & b_1 &= c_{n-1}; \end{aligned} \tag{16}$$

then define by recurrence

$$\begin{aligned} a_j &= b_{j-1} + r a_{j-1} \\ b_j &= c_{n-j} - m a_{j-1} \end{aligned} \tag{17}$$

and we get

$$f(S) = S a_n + b_n. \tag{18}$$

Equation (14) can be evaluated in 16 multiplications and 9 additions. If one is prepared to lose a little simplicity, then we note here that if $\cosh\sqrt{S(x)}$ is expanded in a Taylor series around $\cosh\sqrt{S(\infty)}$, only terms of order $\Delta S = S(\infty) - S(x)$ to the third power need be kept, resulting in a 10% further speed gain. However, for simplicity we ignore this and discuss (13). Each step now takes some 50% longer than that of the algorithm due to Raynal. Allowing for the integration being inside the turning point almost one-third of the time (where we use the simple Raynal algorithm), we find a gain in speed of more than a factor of 2.

We have recently become aware of a similar algorithm due to Raynal [7], whereby the real part of S is kept in the S^3 term in Eq. (14). If the potentials used are real this algorithm gives errors that are, typically, only about a factor of 2 larger than ENA. However, if the potentials are complex (as would happen for 500 MeV proton scattering from ^{90}Zr, for example) then keeping this imaginary part is very important. Shown in Fig. 2 is such a comparison for the $l = 9$ partial wave, using a potential $V_0 = 2.5 + 2.5i$, $k = 5$, $R = 5$, $a = 0.65$, and a step size $\Delta r = 0.125$ ($\Delta x = 0.725$). The curve labelled Raynal #1 is the algorithm as given in Eq. (14), Raynal #2 is with the (real part of the $S)^3$ term correction and the Raptis/Allison algorithm is also shown for comparison. ENA is the most accurate algorithm by about a factor of 10.

Error Estimation

Figure 1 has a rather eye-catching feature, namely that the two solid curves are parallel to each other. This is also true for the two dashed curves. Curves being parallel to each other on a logarithmic scale differ by an overall multiplicative constant which, in this case, is close to 81. Since the curves are computed with step

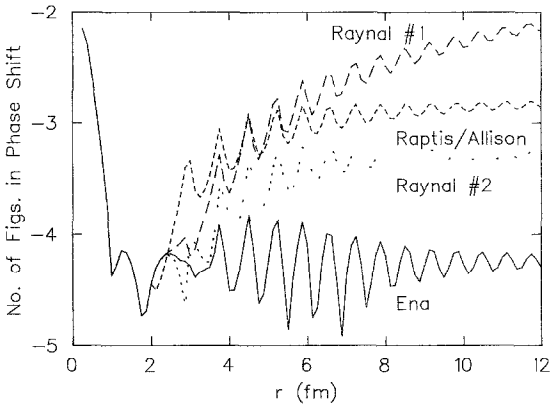

FIG. 2. The error accumated using the four algorithms explained in the text. The step size here is $\Delta r = 0.125$ ($\Delta x = 0.725$). The classical turning point is near $r = 1.8$.

sizes in the ratio of 1 : 3 this factor of 81 reflects the error at each point being proportional to h^4. For the Numerov algorithm this was pointed out, and proved, by Melkanoff *et al.* [3]. It turns out that the error at each point is actually given by $a_4h^4 + a_6h^6 + \cdots$ for both algorithms, and this is exactly the circumstance where Richardsonian extrapolation is expected to work. In practice we have found it possible to easily obtain machine-limited precision (32 figures on the TRIUMF VAX 11/780) using Richardsonian extrapolation on both the Raynal algorithm and the ENA. If one is interested in phase shifts which are accurate to 10 figures or more, then we highly recommend this procedure. However, we set ourselves the goal in this paper of obtaining phase shifts accurate to only 6 figures, and it turns out here that the amount that the Richardsonian extrapolation allows the step size to be increased is almost offset by the need to do the calculation several times. In light of the additional complexity involved with the extrapolation we do not recommend it here.

The local error in this method may be estimated as follows. There are two sources of local error and both should be calculated; the local error estimate being the larger of the two. The first source of error, and for the optical model problem discussed earlier the dominant one, is the error associated with $f(x)$ not being constant. This error may be estimated as follows.

$$\Delta w = \frac{3}{6!} h^6 [y^{(6)}(x) - (f(x))^3 y(x)] \tag{19}$$

$$\approx \frac{h^6}{60} f'(x) f(x) y'(x). \tag{20}$$

This is easily estimated by simple numerical differentiation. The second source of error is due to the truncation of the series in Eq. (14). This error is trivially estimated to be the first neglected term.

We do not have any estimates concerning the global error in the method (for fixed step size), however we point out that in Fig. 1 there is a rather convincing numerical demonstration that it is going as h^4. This we have confirmed numerically by the success of Richardsonian extrapolation to great accuracy.

Derivative Formula

Often a derivative of the function $y(x)$ will be needed. Following a very similar derivation to Eq. (10), we can obtain a derivative formula accurate to $o(h^4)$ everywhere and which is exact whenever $f(x)$ is locally constant. The formula is:

$$y'(r) = \frac{(1 - 2T(r+h))\, y(r+h) - (1 - 2T(r-h))\, y(r-h)}{(h/3)(6 - S)(\sinh \sqrt{S}/\sqrt{S})} \tag{21}$$

Again the hyperbolic sine may be expanded in powers for fast evaluation.

In summary, we have presented an algorithm which is straightforward to implement. It requires a uniform step size and results in a gain in speed of at least a factor of 2 over the simple Raynal algorithm.

We would like to thank J. Comfort and B. K. Jennings for useful comments.

REFERENCES

1. A. RAPTIS AND A. C ALLISON, *Comput. Phys. Commun.* **14**, 1 (1978).
2. J. RAYNAL, Optical Model and Coupled Channel Calculations in Nuclear Physics, Trieste, 1971 and IAEA, Vienna, 1972.
3. M. A. MELKANOFF, T. SAWADA, AND J. RAYNAL, *Meth. Comput. Phys.* **6**, 1 (1966).
4. P. H. COWELL AND A. C. D. CROMELIN, Appendix to Greenwhich Observatory for 1909, p. 62, Edingburgh, 1910.
5. B. V. NUMEROV, *Mont. Not. R. Astron. Soc.* **84**, 592 (1924).
6. *Nord. Tidskr. Informationsbehandl.* **5**, 142 (1965).
7. J. RAYNAL, private communication.