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Modification of the Variation-of-Parameters Method and Integration of the Schrödinger Equation*

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In the ordinary method of variation of parameters, a solution of a given linear differential equation is assumed to be a linear combination of independent solutions of an auxiliary solvable equation, and the coefficients in that linear combination are functions to be determined. A new version presented in this paper uses a linear combination including also *the first derivative* of the solution of an auxiliary equation. We have applied this method successfully to the stepwise numerical integration of the partial-wave Schrödinger equation in scattering theory. Since higher-order terms in a power-series solution can be included rather straightforwardly, the new method achieves high accuracy even when the step size is appreciably large. A numerical example is presented.

I. INTRODUCTION

It is the purpose of this paper to discuss a new version of the method of variation of parameters, with particular reference to numerical integration of the partial-wave Schrödinger equation in scattering theory. The key point of the new method is the form of a solution given by Eq. (10); we assume a linear combination of a solution of an auxiliary differential equation and its derivative, and subsequently solve for undetermined coefficients with the use of a power-series expansion around a given point. Those coefficients turn out to be slowly varying in a close neighborhood of the given point, a remakable result precisely stated in Lemma I, Eq. (17), and Lemma II, Eq. (22). Our proof of that result is elementary; it uses in effect

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only the existence and uniqueness theorem of solution of a differential equation in regular domain [1] [see statements that follow Eq. (12)].

Our new method is indeed applicable to a wide class of differential equations, but for the purpose of orientation we shall limit ourselves to its application to the partial-wave Schrödinger equation in atomic scattering theory.

For most collisions between atoms and ions at thermal energies, the potential is strong, supporting a substantial number of bound states, and it is of long range. Moreover, the de Broglie wavelength associated with the relative motion is short as compared to the range of the interatomic potential. Thus, the phase shift will take fairly large values in a wide range of angular momentum, and the need of selecting a suitable method of numerical integration is rather urgent. Actually it is in the course of our recent study on ion-atom collisions [2] that we have developed the new method described below.

The Runge–Kutta method has been adapted to atomic-scattering calculations by Bernstein [3]. The semiclassical or JWKB method is also widely adopted [4]. Also we must recall here such methods as Swan's multiple-step potential approximation [5, 6] and the method of variable phase [7, 8]. Recently, Gordon [9, 10] has discussed extensively the method of piecewise analytic solution. We have compared the multiple-step potential approximation, Calogero's method, and our own, in the above-mentioned study of ion–atom scattering [2]. We also have made some test calculations to compare the Runge–Kutta method with ours. The results of these investigations will be presented below.

2. General Formulation

Consider a solution ψ_E of the differential equation

$$d^2\psi_E/dr^2 + (E - U - V)\psi_E = 0 \tag{1}$$

in a domain D of r where both U and V are analytic functions of r, E being a given parameter. Suppose that the solution ψ_E specifically satisfies an initial condition that

$$\psi_E = a_0 \quad \text{and} \quad d\psi_E/dr = a_1 \quad \text{at} \quad r = r_0 \in D, \tag{2}$$

where a_0 and a_1 are given constants. The existence of the unique ψ_E for arbitrary a_0 and a_1 is guaranteed by the well-known Lipschitz condition, so long as the differential equation is regular at $r = r_0$ [1].

Suppose further that one knows the solution ϕ_λ of an auxiliary equation

$$d^2\phi_\lambda/dr^2 + (\lambda - U)\phi_\lambda = 0 \tag{3}$$

for arbitrary values of parameter λ under the same initial condition that

$$\phi_\lambda = a_0 \quad \text{and} \quad d\phi_\lambda/dr = a_1 \quad \text{at} \quad r = r_0 \in D. \tag{4}$$

It will be shown how efficiently one can use the knowledge of ϕ_λ for the determination of ψ_E.

In the scattering problem, which will be discussed in Section 4, U may represent the centrifugal potential [Eq. (41)] so that ϕ_λ is a free partial wave given by the Riccati–Bessel function. Then, ψ_E is the partial wave with energy E in a given central potential V. We defer further physical interpretation until Section 4 so that we may concentrate below on the mathematics. Note that the coefficients and the variables appearing in Eqs. (1) and (3) may be complex in general.

For brevity and transparency of presentation, one will hereafter use $x = r - r_0$ as the independent variable and denote by a prime the differentiation with respect to x. Also, one denotes by $\psi_E(x)$ the value of ψ_E at point x. Thus, $\psi_E(0)$ means the value of ψ_E at $x = 0$, i.e., $r = r_0$. This stipulation applies to all functions in this section.

One may rewrite Eqs. (1) and (2) as

$$\psi_E''(x) + [\epsilon - U(x) - v(x)]\,\psi_E(x) = 0 \tag{5}$$

and

$$\psi_E(0) = a_0 \quad \text{and} \quad \psi_E'(0) = a_1, \tag{6}$$

where ϵ and $v(x)$ are defined by

$$\epsilon = E - V(0), \tag{7}$$

and

$$v(x) = V(x) - V(0), \tag{8}$$

so that

$$v(0) = 0. \tag{9}$$

One now assumes the solution in the form

$$\psi_E(x) = e^{F(x)}[\phi_\epsilon(x) + G(x)\,\phi_\epsilon'(x)], \tag{10}$$

where $F(x)$ and $G(x)$ are unknown functions of x. In contrast, $\phi_\epsilon(x)$ is the known solution of Eqs. (3) and (4) for $\lambda = \epsilon$; in other words, $\phi_\epsilon(x)$ satisfies

$$\phi_\epsilon''(x) + [\epsilon - U(x)]\,\phi_\epsilon(x) = 0, \tag{11}$$

$$\phi_\epsilon(0) = a_0, \quad \text{and} \quad \phi_\epsilon'(0) = a_1. \tag{12}$$

Although each of the functions $\psi_E(x)$, $\phi_\epsilon(x)$, and $\phi_\epsilon'(x)$ is unique, a pair of functions $F(x)$ and $G(x)$ that expresses the same ψ_E according to Eq. (10) is nonunique. One may choose, however, a particular pair by assuming that $F(x)$ and $G(x)$ be independent of a_0 and a_1. We prove below that, as a consequence of the well-known existence theorem in a regular domain [1], this choice not only is legitimate, but also makes the resulting pair $F(x)$ and $G(x)$ unique.

The differentiation of Eq. (10) gives

$$\psi_E' = F'\psi_E + e^F(1 + G')\phi_\epsilon' + e^F(U - \epsilon)G\phi_\epsilon , \tag{13}$$

where Eq. (11) has been used and the argument x has been suppressed. Similarly, the differentiation of Eq. (13), again followed by the use of Eq. (11), leads to

$$\begin{aligned}\psi_E'' = {} & [F'' + (F')^2]\,\psi_E + e^F[2F'(1 + G') + G'' + (U - \epsilon)G]\,\phi_\epsilon' \\ & + e^F[(U - \epsilon)(2F'G + 2G' + 1) + U'G]\,\phi_\epsilon .\end{aligned} \tag{14}$$

The behavior of $F(x)$ and $G(x)$ near $x = 0$ may be readily studied. Setting $x = 0$ in Eq. (10) and using Eqs. (6) and (12), one may write

$$\begin{aligned}a_0 = \psi_E(0) &= e^{F(0)}[\phi_\epsilon(0) + G(0)\phi_\epsilon'(0)] \\ &= e^{F(0)}[a_0 + G(0)a_1].\end{aligned}$$

Because $F(0)$ and $G(0)$ are, by assumption, independent of a_0 and a_1, the above equation is satisfied only if $F(0) = G(0) = 0$. Similarly, one sets $x = 0$ in Eq. (13) and uses Eqs. (6) and (12) to obtain

$$\begin{aligned}a_1 &= F'(0)a_0 + e^{F(0)}[1 + G'(0)]\,a_1 + e^{F(0)}[U(0) - \epsilon]G(0)a_0 \\ &= F'(0)a_0 + [1 + G'(0)]a_1 .\end{aligned}$$

This relation requires that $F'(0) = G'(0) = 0$, so long as $F'(0)$ and $G'(0)$ are independent of a_0 and a_1. Finally, Eq. (14) leads to

$$\psi_E''(0) = F''(0)\,a_0 + G''(0)\,a_1 + [U(0) - \epsilon]\,a_0 , \tag{15}$$

while Eqs. (5), (6), and (9) give

$$\psi_E''(0) = [U(0) + v(0) - \epsilon]a_0 = [U(0) - \epsilon]a_0 . \tag{16}$$

The compatibility of Eqs. (15) and (16) requires that $F''(0) = G''(0) = 0$. In summary, one has obtained the following result:

LEMMA I. *The functions $F(x)$ and $G(x)$ as well as their first and second derivatives vanish at $x = 0$:*

$$F(0) = F'(0) = F''(0) = G(0) = G'(0) = G''(0) = 0. \tag{17}$$

At this point it is natural to derive differential equations for $F(x)$ and $G(x)$. The substitution of Eqs. (10) and (14) into Eq. (5) eliminates ψ_E. The result is

$$[F'' + (F')^2 - v]\, e^F(\phi_\epsilon + G\phi_\epsilon') + e^F[2F'(1 + G') + G'']\phi_\epsilon' + e^F[2(U - \epsilon)(F'G + G') + U'G]\phi_\epsilon = 0.$$

The particular pair of functions $F(x)$ and $G(x)$ that has been chosen earlier is independent of a_0 and a_1. Therefore, the $F(x)$ and $G(x)$ must satisfy equations that do not explicitly involve ϕ_ϵ or ϕ_ϵ'. Thus, equating the coefficients of ϕ_ϵ and ϕ_ϵ' to zero, one obtains a set of coupled equations for $F(x)$ and $G(x)$:

$$F'' + (F')^2 - v + 2(U - \epsilon)(F'G + G') + U'G = 0, \tag{18}$$

$$[F'' + (F')^2 - v]\, G + 2F'(1 + G') + G'' = 0. \tag{19}$$

Combining these two equations, one may obtain

$$G'' + 2F'(1 + G') - 2(U - \epsilon)(F'G + G')\, G - U'G^2 = 0. \tag{20}$$

This equation can be integrated once to give

$$G' = e^{-2F} - 1 + (U - \epsilon)G^2. \tag{21}$$

Any two of the three Eqs. (18), (19), and (21) will determine $F(x)$ and $G(x)$.

If one differentiates Eq. (20) at $x = 0$ and uses Lemma I, one readily obtains Lemma II.

LEMMA II. *The third derivative of $G(x)$ vanishes at $x = 0$:*

$$G'''(0) = 0. \tag{22}$$

A few remarks on the two lemmas are in order. First, notice that the dictation of the same initial conditions for ψ_E and ϕ_ϵ [Eqs. (6) and (12)] is crucial. The legitimacy of that dictation is ensured by the regularity of the differential equations (5) and (11). Second, Eq. (9) is essential to the proof for the vanishing of $F''(0)$, $G''(0)$, and $G'''(0)$. Finally, the lemmas indicate that $F(x)$ and $G(x)$ are nearly equal to zero in a sufficiently close neighborhood of $x = 0$.

3. Power-Series Solution for F and G

Since several lowest-order terms are missing from the Taylor series expansion around $x = 0$ of the functions F and G, we may expect that such series solutions are numerically efficient. We may use those series solutions to integrate numerically the differential equation (5) from $x = 0$ to another point, say, $x = h$ along with the formulas (10) and (13). If accurate values of $\phi_\epsilon(h)$ and its derivative $\phi_\epsilon'(h)$ are available, the proposed method is expected to be accurate for a sufficiently small value of h. If sufficiently large number of terms are included in the series, one may also try an appreciably large step size as long as it is within the convergence radii of the series for F and G.

One thus tries power-series solutions

$$F(x) = \sum_{n=3}^{\infty} f_n x^n, \tag{23}$$

$$G(x) = \sum_{n=4}^{\infty} g_n x^n, \tag{24}$$

as prescribed by Lemmas I and II. Suppose the coefficients of the expansions,

$$U(x) - \epsilon = \sum_{n=0}^{\infty} u_n x^n \tag{25}$$

and

$$v(x) = \sum_{n=1}^{\infty} v_n x^n, \tag{26}$$

are known. Then, substitution of Eqs. (23)–(26) into Eqs. (18) and (21) gives, after somewhat lengthy but straightforward calculations, the following result.

$$f_3 = v_1/6, \tag{27}$$

$$f_4 = v_2/12, \tag{28}$$

$$f_5 = v_3/20 + u_0 v_1/30, \tag{29}$$

$$f_6 = v_4/30 - v_1^2/120 + u_1 v_1/40 + u_0 v_2/90, \tag{30}$$

$$f_7 = v_5/42 - v_1 v_2/126 + u_0 v_3/210 + u_0^2 v_1/315 + 11 u_1 v_2/1260 + 5 u_2 v_1/252, \tag{31}$$

$$f_8 = v_6/56 - v_2^2/504 - v_1 v_3/224 + u_0 v_4/420 + 13 u_1 v_3/3360 + u_2 v_2/140 + 11 u_3 v_1/672 - 41 u_0 v_1^2/10080 + 11 u_0 u_1 v_1/2520 + u_0^2 v_2/1260, \tag{32}$$

$$g_4 = -v_1/12, \tag{33}$$

$$g_5 = -v_2/30 \tag{34}$$

$$g_6 = -v_3/60 - u_0v_1/90, \tag{35}$$

$$g_7 = -v_4/105 + 13v_1^2/1260 - u_1v_1/140 - u_0v_2/315, \tag{36}$$

$$g_8 = -v_5/168 - u_0v_3/840 - u_0^2v_1/1260 - 11u_1v_2/5040 - 5u_2v_1/1008 + v_1v_2/112. \tag{37}$$

The next coefficients f_9 and g_9 can be expressed most conveniently in terms of low-order coefficients as

$$f_9 = v_7/72 - f_3f_6/2 - 5f_4f_5/9 - 2u_0g_8/9 - u_0f_3g_5/12 - u_0f_4g_4/9, \tag{38}$$

$$g_9 = (-2f_8 + 2f_4^2 + 4f_3f_5 + u_0g_4^2)/9. \tag{39}$$

It may be added that the derivation of Eqs. (33)–(37) and (39) is facilitated by the relation

$$G(x) = \int_0^x [-2F(x') + 2F^2(x')]\,dx' + u_0g_4^2x^9/9 + O(x^{10}),$$

which follows from Eq. (21) and the lemmas.

4. Application to the Potential-Scattering Problem

The Schrödinger equation for the l-th partial wave ψ_E of energy E in a central potential V is

$$d^2\psi_E/dr^2 + [E - l(l+1)r^{-2} - V]\psi_E = 0, \tag{40}$$

where all the quantities are measured in a system of units in which $\hbar^2/(2m) = 1$, m being the particle mass. As a natural choice, one may let the function U of Section 2 be the centrifugal potential

$$U = l(l+1)r^{-2}. \tag{41}$$

Therefore, ϕ_ϵ is a linear combination of the Riccati–Bessel functions (defined in Appendix I of [7]):

$$\phi_\epsilon = \alpha\hat{j}_l(\kappa r) + \beta\hat{n}_l(\kappa r), \tag{42}$$

where

$$\kappa = \epsilon^{1/2}. \tag{43}$$

and the coefficients α and β are determined by means of Eq. (4). The coefficients of the expansion (25) are readily given by

$$u_0 = l(l+1)\, r_0^{-2} - \epsilon \tag{44}$$

and

$$u_n = l(l+1)(-1)^n(n+1)\, r_0^{-2-n} \qquad (\text{for} \quad n \geqslant 1). \tag{45}$$

Provided that the expansion coefficients for v [Eq. (26)] have been worked out, the results [Eqs. (27)–(39)] of Section 3 may readily apply to the numerical evaluation of the function ψ_E in a sufficiently close neighborhood of r_0. [Because the formalism of Section 2 fails at $r_0 = 0$, where U of Eq. (41) is singular unless $l = 0$, its application should start at a finite r_0; the solution ψ_E up to that point may be presumed as obtainable by another method, *e.g.*, the straightforward power-series expansion.]

It is appropriate to consider the physical meaning of the form [Eq. (10)] of the solution. The parameter ϵ, defined by Eq. (7), includes in effect the potential V averaged around the point $r = r_0$. In other words, the function ϕ_ϵ [Eq. (42)] takes into account an average effect of the potential V through the local wave number κ [Eq. (43)]. Additional effects due to the spatial variation of V are incorporated into the present formalism in terms of the functions F and G, both of which are slowly varying locally. One can evaluate these functions by Eqs. (27)–(39) and hence ψ_E up to a point r. The function G represents in effect the "local" phase shift that results from the spatial variation of the potential V in a small interval near $r = r_0$, while the function F describes a slow modulation of the amplitude of ψ_E in that interval. In this sense, the present formalism may be regarded as a modification of the method of variable phase [7].

When the potential contains a repulsive part, the ϵ of Eq. (7) may become negative in certain intervals of r. The general theory of Section 2 and 3 still applies formally in such a case. The only necessary modification then is to recognize the κ of Eq. (43) as pure imaginary and thus to use the modified Riccati–Bessel functios in Eq. (42).

Parenthetically it may be added that the division of the "effective potential" $U + V$ into U and V is arbitrary from the mathematical point of view, and that, depending upon alternative divisions, alternative applications of the general theory are possible. For instance, one may consider V as the centrifugal potential and U as a given potential for which the s-wave solution is readily obtained. An example of such a U may be of the form $-g \exp(-cr)$, where g and c are positive constants; the s-wave solution in this case may be expressed analytically [11]. In that application, the l-th partial wave ψ_E for energy E is related to the s wave ϕ_ϵ for a modified ϵ through Eq. (10). The expansion formulas (27)–(39) again determine F and G, at least locally, and their repeated applications over a number

of intervals will give F and G over the entire interval of r. In fact, this procedure may be regarded as an extension of Takayanagi's method of modified wave numbers [12]. Takayanagi points out that, when V is of sufficiently short range and l is not very large, it is reasonable to use the approximation $\psi_E \approx \phi_\epsilon$, and he applied it with considerable success to a great many calculations of distorted waves for molecular collisions. Considered from Takayanagi's point of view, the F and G of the general theory represent corrections to the modified-wave-number approximation.

5. A Numerical Example

To test the usefulness of our method, we have applied it to a simple example that permits exact analytical solution.

Consider the scattering of the s wave (for which $U = 0$) at $E = 0$ by an attractive exponential potential

$$V = -ge^{-r}, \tag{46}$$

where g is a positive constant. Then Eq. (40) becomes

$$d^2\psi/dr^2 + ge^{-r}\psi = 0 \tag{47}$$

with the boundary condition that

$$\psi = 0 \qquad \text{at} \qquad r = 0. \tag{48}$$

More specifically, one may choose the potential strength g such that there is a zero-energy resonance solution ψ. Then ψ satisfies the condition that

$$d\psi/dr \to 0 \qquad \text{as} \qquad r \to \infty. \tag{49}$$

As shown in [11], the solution that satisfies Eqs. (47)–(49) may be written, apart from an arbitrary normalization factor, as

$$\psi = J_0(2g^{1/2}e^{-r/2}), \tag{50}$$

where J_0 is the Bessel function of the first kind and of the zero order, and g is related to any zero j_{0s} of J_0 by

$$2g^{1/2} = j_{0s} \qquad (s = 1, 2, 3,...). \tag{51}$$

The application of our method to the particular problem in the neighborhood of any point $r = r_0$ proceeds as follows. The ϕ_ϵ of our general theory satisfies

$$d^2\phi_\epsilon/dx^2 + \epsilon\phi_\epsilon = 0, \tag{52}$$

where $x = r - r_0$ and

$$\epsilon = ge^{-r_0}. \tag{53}$$

The solution satisfying Eq. (5) is then

$$\phi_\epsilon = a_0 \cos \kappa x + (a_1/\kappa) \sin \kappa x, \tag{54}$$

where $\kappa = \epsilon^{1/2}$. The v of Eq. (8) is now given by

$$v = ge^{-r_0} - ge^{-r} \tag{55}$$

so that

$$v_n = (-1)^{n-1} ge^{-r_0}/n!. \tag{56}$$

Further, the u_n of Eq. (25) are given by

$$u_0 = -\epsilon = -ge^{-r_0} \tag{57}$$

and

$$u_n = 0 \qquad (\text{for} \quad n \geqslant 1). \tag{58}$$

Then, Eqs. (27)–(39) determine the F and G and thence ψ for sufficiently small intervals.

We wrote computer programs that integrate Eq. (47) both by our method and by the fourth-order Runge–Kutta method [13] and subsequently compare those results with the exact solution, Eq. (50). To demonstrate the performance of our method, we present some of the numerical results in Fig. 1. As a measure of the accuracy of an approximate solution $\psi^{(a)}$, we define the root-mean-square error

$$\Delta = \left\{N^{-1} \sum_{j=1}^{N} [\psi^{(a)}(r_j) - \psi^{(e)}(r_j)]^2\right\}^{1/2}, \tag{59}$$

where $\psi^{(e)}$ is the exact solution given by Eq. (50) and r_j are the points at which $\psi^{(a)}$ and $\psi^{(e)}$ are evaluated. For simplicity, we chose in all the programs equally spaced r_j in the interval $0 \leqslant r \leqslant 6$; in other words, $r_j = jh\,(j = 1, 2,..., N)$ and $Nh = 6$. The computation used 36-bits floating-point arithmetic (on a CDC-3600 computer), the precision of which corresponds to about 11 decimal digits.

We call the program that is based on our method the eighth-order program when it includes the ninth-order terms in the power series for F and G and thus

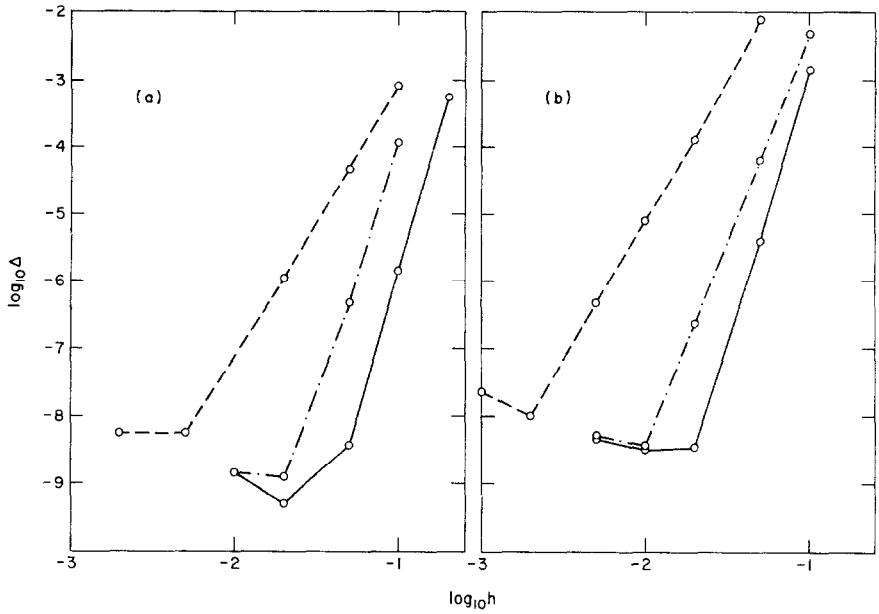

FIG. 1. The root-mean-square error Δ of an approximate solution as a function of the step size h. The precise definition of Δ is given by Eq. (59). The circles show data points which, for convenience, are connected by straight-line segments. The full lines represent the results of our eighth-order program, the dash–dot lines those of our sixth-order program, and the broken lines those of the fourth-order Runge–Kutta method. Case (a) corresponds to the zero-energy-resonance wavefunction with three nodes ($2g^{1/2} = j_{0,4} = 11.79...$), and case (b) to the zero-energy-resonance wavefunction with nine nodes ($2g^{1/2} = j_{0,10} = 30.63...$).

uses all coefficients listed in Eqs. (27)–(39). Note that the accuracy of the wavefunction derivative ψ_E' is of the eighth order, because on the right-hand side of Eq. (13) the derivative of F to be multiplied by ψ_E is of the eighth order. A program of smaller order will be defined similarly using a number which is less by one than the highest order that is included in the series for F and G. In Fig. 1, the results produced by our eighth-order program is shown by a full line; the results produced by the sixth-order program [using Eqs. (27)–(31) and (33)–(36)] are shown by a dot–dash curve; the results produced by the fourth-order Runge–Kutta method are shown by a dashed curve. Two different values of g have been chosen; in case (a) there are three nodes of ψ, i.e., $s = 4$ in Eq. (51), whereas in case (b) there are nine nodes, i.e., $s = 10$ in Eq. (51). As the step size is made smaller, the Δ decreases steadily until it levels off at some h. The leveling off results from the accumulation of round-off errors in the arithmetic. The Δ for our eighth-order method right before the leveling-off sets in is substantially smaller than that for the fourth-order Runge–Kutta method at the same h. The optimal step size that

gives the smallest Δ is considerably larger for our eighth-order method than for the fourth-order Runge–Kutta method. Further, the minimum value of Δ is somewhat smaller for our method. We have also run the seventh-, fifth-, and fourth-order programs. The results produced by the seventh-order program are virtually identical with the eighth-order results, except that the latter is slightly better near the minimum Δ. The curves for the fifth-order results lie just midway between the dot-dash curve and the dashed curve, but they are omitted from Fig. 1. Our fourth-order program is comparable with the fourth-order Runge–Kutta method. More specifically, our fourth-order program is slightly inferior in case (a) ($s = 4$, in Eq. (51)), while it is slightly superior in case (b) ($s = 10$, in Eq. (51)). We have also run another version of the Runge–Kutta method using the algorithm given in [14]. The Δ produced by this program is slightly better than the dashed curve of Fig. 1 (by a factor of $1.5 \sim 2.0$), except near the minimum of Δ in case (b). Since the difference is inappreciable, we have omitted this result from Fig. 1 for simplicity.

In summary, it is straightforward to include higher order terms in the power-series solutions for F and G using the results of Section 3. The curves in Fig. 1 demonstrate how the inclusion of a higher order term improves the accuracy for a fixed value of step size h. We have not tried the Runge–Kutta method of the sixth-order because of the complexity of the formula [15]. We have also examined the error of the first derivative $d\psi^{(a)}/dr$ simultaneously in all runs discussed above. The overall behavior of that error is slightly larger than the Δ discussed above, but the deviation remains always within the factor of 2.5. Thus, we conclude that no significantly new information is obtained from the study of the derivative $d\psi^{(a)}/dr$.

6. Concluding Remarks

The results of Section 5 clearly show that our method is suitable for numerical integration with appreciably large step sizes. Also, our method permits an arbitrary change of the step size from one interval to another, and therefore it is possible to adjust the step size in different regions according to the steepness of the potential, so that maximum efficiency may be achieved. In these respects, our method is similar to Gordon's method of piecewise analytic solution [9]. It is interesting to compare Gordon's method with ours and some work in this direction is underway.

In the course of a study on ion–atom scattering [2], we have also tried the multiple-step approximation [5, 6] and Calogero's method of variable phase [7]. As discussed in detail by Swan [5], the result derived from a multiple-step potential converges to the exact result from an originally smooth potential, in the limit of vanishing steps. Because of the simplicity of programming and of the speed of

calculation, the multiple-step approximation is especially convenient for a qualitative analysis—for instance, when one tries to analyze the characteristic differences between different potential shapes (such as those between a long-range potential and a short-range one). The multiple-step approximation, however, tends to enhance spuriously the scattering amplitude because a discontinuity in a potential in general is most efficient in producing a scattered wave [16]. Consequently, it fails to guarantee high accuracy of the result unless the step size is made extremely small. In fact, we devised our method in order to overcome those shortcomings.

The variable-phase method is theoretically attractive. When one follows the variation of the phase function from the origin to the asymptotic region, the phase shift, including integral multiples of π, is uniquely determined, whereas the asymptotic form of the wavefunction alone leaves an ambiguity in the phase shift by an integral multiple of π. Theoretically it is important to remove that ambiguity, as seen in Levinson's theorem on the number of bound states and the zero-energy phase shift. Further, the method of variable phase is powerful for analytical proofs of many other theorems [7]. Unfortunately, the method often requires integration with small steps and turns out time consuming. This is true even when one uses the version of the tangent–cotangent function that has been designed for speedier integration.

Turning back to our method, we may make a few additional remarks. When one uses the method with the choice of U given by Eq. (41), the "locally available" kinetic energy ϵ of Eq. (7) is independent of l. If the potential V is of short range (i.e., decreasing faster than r^{-2} at large r), one often encounters barrier penetration at low E and large l. In applying our method, a single algorithm is sufficient, regardless of the presence or absence of barrier penetration. That is clearly not the case with Swan's or any other similar method if the whole effective potential $U + V$ is replaced by a series of step functions. Actually, we have carefully examined the possibility of enhanced errors due to barrier penetration in ion–atom scattering [2]. However, no significant difference was found in the results produced by a program that treated barrier penetration separately.

In conclusion, our method enables one to integrate the partial-wave Schrödinger equation accurately. With an optimal choice of the step size, the required machine time can be made reasonably short. Although the paper has dealt exclusively with potential scattering, a generalization to coupled equations should be feasible upon replacing quantities U, V, F, and G with corresponding matrices.

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