PHYSICAL REVIEW A VOLUME 28, NUMBER 4 OCTOBER 1983

Method of continued fractions with application to atomic physics

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(Received 4 May 1983)

A new iterative method for solving scattering integral equations for local as well as nonlocal potentials is proposed. The scattering matrix is expressed in the form of a continued fraction. This method converges extremely fast for compact potentials with arbitrary strength. A high precision of the result is expected with a relatively small amount of numerical work. Starting from the second iteration, all functions which are to be computed in the course of iterations are regular at the origin and are of finite range in configuration space. The method is applied to the elastic scattering of electrons from hydrogen atoms in the static, exchange approximation. Its efficiency is compared with some recently proposed methods.

I. INTRODUCTION

The principal methods for solving the scattering equations used in atomic physics at the present time are as follows: (1) the linear-algebraic method,[1] (2) the R-matrix method,[2] (3) the method of noniterative integral equation (NIEM),[3] and (4) the variational method.[4] None of these methods is iterative. The iterative methods, although very simple and natural, are not in frequent use in atomic physics because they are usually slowly and nonmonotonically convergent, and in the range from low to middle energies they often diverge.[5] On the other hand, a renewed interest in iterative methods arose in few-body physics,[6] motivated by the fact that the equations of three-body scattering problems are so complicated that the direct noniterative solution for the physically realistic problem can not be obtained on present-day computers. To overcome this difficulty we have proposed a method[7] in which the three-body equation is split into two parts: one part containing contributions from all physically important poles and another part which yields less important contributions compared with the first one. The first part is relatively easily solved, while the second part may be treated iteratively. Therefore, having an efficient iterative algorithm is crucial, and some progress in this subject has already been made.[8] Also, we mention that in the theory of electron-molecule scattering, several very interesting methods using projections of the interaction potential onto a finite set of square-integrable functions have been developed.[9] In this paper we propose a new method of iteration for the scattering equations which surpasses previously proposed methods in many respects. The main features of our method are simplicity, extremely high efficiency, and high accuracy.

Recently, Rescigno and Orel[10] have proposed a method in which the interaction potential is projected on a finite set of functions and it is represented as a sum of separable potentials. In our method, the interaction potential is also projected on a finite set of functions. However, contrary to Ref. 10, these functions are not given in advance, but are generated at each step and, as a result, the matrix inversion is not necessary. Starting from the second iteration, all functions are square-integrable and are regular at the origin. The scattering matrix computed in this way is represented in the form of a continued fraction. In order to study the efficiency of this method for simple problems, we apply the method to the elastic $e+\mathrm{H}$ scattering in the static, exchange approximation. It turns out that the method is so rapidly convergent that just two or three iterations yield results which are correct up to several significant figures.

The theory for one-channel scattering is presented in Sec. II, and its generalization to multichannels in Sec. III. Some important properties of our method are briefly sketched in Sec. IV. We generalize our method to distorted waves in Sec. V. We apply our method to local and nonlocal interactions in the e-H elastic scattering in Sec. VI. Some concluding discussions are given in Sec. VII.

II. THEORY FOR ONE-CHANNEL SCATTERING

For a local or nonlocal potential U that is supposed to be Hermitian, let us consider the scattering equation

$$\phi=u+G_0U\phi \ . \tag{1}$$

Here G_0 denotes the standing-wave Green function, which is given in terms of the Ricatti-Bessel (Riccatti-Neumann) function $u_l(kr)$ $[v_l(kr)]$ by

$$G_0=-\frac{1}{k}\times\begin{cases}u_l(kr)v_l(kr'), & r'>r\\ u_l(kr')v_l(kr), & r>r' \ .\end{cases} \tag{2}$$

Our purpose is to calculate the scattering matrix K defined by

$$K=\langle u \mid U \mid \phi\rangle \ , \tag{3}$$

which is related to the phase shift δ by

$$K=-\frac{1}{k}\tan\delta\ . \tag{4}$$

Let us suppose that the first Born approximation to K is not equal to zero, namely, $\langle u \mid U \mid u\rangle \neq 0$. We define a potential $U^{(1)}$ by

$$U^{(1)}=U-\frac{U\mid u\rangle\langle u\mid U}{\langle u\mid U\mid u\rangle}\ . \tag{5}$$

Putting this expression into Eq. (1), one obtains

$$\phi=u+G_0U\mid u\rangle\frac{\langle u\mid U\mid \phi\rangle}{\langle u\mid U\mid u\rangle}+G_0U^{(1)}\mid\phi\rangle\ . \tag{6}$$

The solution ϕ of this equation is expressed formally as

$$\phi=u+(1-G_0U^{(1)})^{-1}G_0U\mid u\rangle\frac{\langle u\mid U\mid \phi\rangle}{\langle u\mid U\mid u\rangle}\ , \tag{7}$$

where we have made use of the property that $U^{(1)}$ is orthogonal to u,

$$U^{(1)}\mid u\rangle=0,\quad \langle u\mid U^{(1)}=0\ . \tag{8}$$

We define two functions u_1 and ϕ_1 by

$$u_1=G_0Uu\ , \tag{9}$$

$$\phi_1=(1-G_0U^{(1)})^{-1}u_1\ . \tag{10}$$

In terms of these functions, Eq. (7) reads

$$\phi=u+\phi_1\frac{\langle u\mid U\mid \phi\rangle}{\langle u\mid U\mid u\rangle}\ . \tag{11}$$

Multiplying $\langle u\mid U$ from the left on both sides of Eq. (11), we obtain, after some calculations

$$\phi=u+\phi_1\frac{\langle u\mid U\mid u\rangle}{\langle u\mid U\mid u\rangle-\langle u\mid U\mid \phi_1\rangle}\ . \tag{12}$$

Further, if we put this expression in Eq. (3) we get

$$K=\frac{\langle u\mid U\mid u\rangle^2}{\langle u\mid U\mid u\rangle-\langle u\mid U\mid \phi_1\rangle}\ . \tag{13}$$

With these equations, we terminate the first step.

In the next step, we follow a similar procedure. From Eq. (10), we see that the function ϕ_1 satisfies the Lippmann-Schwinger equation

$$\phi_1=u_1+G_0U^{(1)}\phi_1\ , \tag{14}$$

which is of the same type as the starting equation at the first step, namely, Eq. (1). Therefore, we can follow the same procedure as in the first step. Analogously to Eqs. (5), (9), and (10), we define $U^{(2)}$, u_2, and ϕ_2 by

$$U^{(2)}=U^{(1)}-\frac{U^{(1)}\mid u_1\rangle\langle u_1\mid U^{(1)}}{\langle u_1\mid U^{(1)}\mid u_1\rangle}\ , \tag{15}$$

$$u_2=G_0U^{(1)}u_1\ , \tag{16}$$

and

$$\phi_2=(1-G_0U^{(2)})^{-1}u_1\ . \tag{17}$$

The potential $U^{(2)}$ is orthogonal to both u and u_1,

$$\begin{gathered}U^{(2)}\mid u\rangle=U^{(2)}\mid u_1\rangle=0\ ,\\ \langle u\mid U^{(2)}=\langle u_1\mid U^{(2)}=0\ .\end{gathered} \tag{18}$$

Proceeding similarly to the previous steps, we obtain the following equations for ϕ_1 and ϕ_2:

$$\phi_1=u_1+\phi_2\frac{\langle u_1\mid U^{(1)}\mid u_1\rangle}{\langle u_1\mid U^{(1)}\mid u_1\rangle-\langle u_1\mid U^{(1)}\mid \phi_2\rangle}\ , \tag{19}$$

$$\phi_2=u_2+G_0U^{(2)}\phi_2\ . \tag{20}$$

This procedure is repeated. After some N steps, we have

$$\phi_N=u_N+\phi_{N+1}\frac{\langle u_N\mid U^{(N)}\mid u_N\rangle}{\langle u_N\mid U^{(N)}\mid u_N\rangle-\langle u_N\mid U^{(N)}\mid \phi_{N+1}\rangle}\ , \tag{21a}$$

$$u_{N+1}=G_0U^{(N)}u_N\ , \tag{21b}$$

$$\phi_{N+1}=u_{N+1}+G_0U^{(N+1)}\phi_{N+1}\ . \tag{21c}$$

The operator $U^{(N)}$ is orthogonal to $u,u_1,\ldots,u_{N-1}$,

$$U^{(N)}\mid u_i\rangle=0,\quad \langle u_i\mid U^{(N)}=0\ ,\qquad \text{for } i=0,1,\ldots,N-1\ . \tag{22}$$

Therefore, we expect the operator $U^{(N)}$ to become weaker and weaker with increasing N. As a result, we will be able to stop the procedure after some number of steps M. Neglecting the term $G_0U^{(M)}\phi_M$, we can set

$$\phi_M\simeq u_M\ , \tag{23}$$

and using Eqs. (21) backwards, we construct the wave function ϕ.

In practice, the calculation of the scattering amplitude is simpler than the wave function. By virtue of Eqs. (21b) and (22), we get the following relations:

$$\begin{gathered}\langle u_N\mid U^{(N)}\mid u_{N+2}\rangle=\langle u_{N+1}\mid U^{(N+1)}\mid u_{N+1}\rangle\ ,\\ \langle u_N\mid U^{(N)}\mid u_{N+M}\rangle=0,\quad \text{for } M=3,4,\ldots\ .\end{gathered} \tag{24}$$

Here,

$$u_0=u,\quad U^{(0)}=U\ .$$

Let us define the partial amplitude K_i $(i=1,2,\ldots)$ by

$$K_i=\langle u_{i-1}\mid U^{(i-1)}\mid \phi_i\rangle\ . \tag{25}$$

If we use Eqs. (21) and (24), we can express K_i in the form of a continued fraction:

$$K_i=\langle u_{i-1}\mid U^{(i-1)}\mid u_i\rangle+\frac{\langle u_i\mid U^{(i)}\mid u_i\rangle^2}{\langle u_i\mid U^{(i)}\mid u_i\rangle-K_{i+1}}\ . \tag{26}$$

The amplitude K_1 is given by Eq. (26), while it is related to the scattering amplitude K by

$$K=K_B+K_1\frac{K_B}{K_B-K_1},\quad K_B=\langle u\mid U\mid u\rangle\ . \tag{27}$$

Since the core of the proposed method is Eq. (26), we would call this method the method of continued fraction (MCF). Once K_1 is obtained, the wave function ϕ is calculated with the aid of ϕ_1 by Eq. (12),

$$\phi=u+\phi_1\frac{K_B}{K_B-K_1}\ . \tag{28}$$

We conclude this section by summarizing the iteration scheme. We begin with $i=1$. The partial amplitude K_1 is calculated by putting $K_2=0$ in Eq. (26),

$$K_1=\langle u \mid U \mid u_1\rangle+\langle u_1 \mid U^{(1)} \mid u_1\rangle \ .$$

We store two integrals $\langle u \mid U \mid u_1\rangle$ and $\langle u_1 \mid U^{(1)} \mid u_1\rangle$ and the function u_1 in the memory. For $i=N$ (≥ 2), we calculate the function u_N, two integrals $\langle u_{N-1} \mid U^{(N-1)} \mid u_N\rangle$ and $\langle u_N \mid U^{(N)} \mid u_N\rangle$. We store these in the memory and erase u_{N-1}. Putting $K_{N+1}=0$, we calculate $K_N, K_{N-1}, \dots, K_1$ using the stored $\langle u_{i-1} \mid U^{(i-1)} \mid u_i\rangle$ and $\langle u_i \mid U^{(i)} \mid u_i\rangle$ for $i=1,2,\dots,N$. We follow this procedure in the calculation of K_{N+1}. We calculate $\langle u_N \mid U^{(N)} \mid u_{N+1}\rangle$, $\langle u_{N+1} \mid U^{(N+1)} \mid u_{N+1}\rangle$, and the function u_{N+1}. We store these in the memory and erase u_N. We calculate K_{N+1}, putting $K_{N+2}=0$. The improved values of $K_N, \dots, K_1$ are obtained by the use of the value of K_{N+1} and the stored integrals $\langle u_{i-1} \mid U^{(i-1)} \mid u_i\rangle$ and $\langle u_i \mid U^{(i)} \mid u_i\rangle$ for $i=1,\dots,N$. We repeat this procedure until the value of K_1 does not change any more. Then we stop the iteration procedure. We take this value of K_1 in Eq. (27) to obtain the scattering amplitude. Having the convergent values of $K_N, \dots, K_1$, and making use of Eq. (25) in Eqs. (19), (21a), and (28), we can calculate the wave function.

III. THEORY FOR MULTICHANNEL SCATTERING

In this section we generalize the MCF proposed in the previous section to the coupled integral equations. The multichannel scattering equations have, in general, the same form as Eq. (1), but now have the channel indices. Let us write the multichannel integral equation explicitly as

$$F_{ii_0}(E,r)=\phi_i(E,r)\delta_{ii_0}+\sum_{j=1}^{N} G_i^{(0)}(k_i)U_{ij}F_{ji_0}(E,r) \ , \tag{29}$$

where $G_i^{(0)}(k_i)$ denotes the free-particle Green function in the ith channel and k_i is the corresponding wave vector given by

$$E=\frac{\hbar^2k^2}{2\mu}+\epsilon_0=\frac{\hbar^2k_i^2}{2\mu}+\epsilon_i \ , \tag{30}$$

where ϵ_0 (ϵ_i) and μ are the energy of the ground (excited) state and the reduced mass, respectively. The function ϕ_{i_0} denotes the wave function of the incident channel. The first step in our method is to construct the subtracted potential $U^{(1)}$. There exist several ways of defining this potential in the multichannel case. Here we set out just the simplest form. We define

$$U_{ij}^{(1)}=U_{ij}-\frac{\sum_{m=1}^{N} U_{im} \mid \phi_m\rangle \sum_{n=1}^{N} \langle \phi_n \mid U_{nj}}{D} \ , \tag{31}$$

where

$$D=\sum_{i=1}^{N}\sum_{j=1}^{N} \langle \phi_i \mid U_{ij} \mid \phi_j\rangle \ . \tag{32}$$

Among the functions ϕ_i which appeared in Eqs. (31) and (32), only the function ϕ_{i_0} is given in advance and other functions are rather arbitrary. The discussions about the optimum choice of these functions is set aside in the present paper. In any case, with Eq. (31), the potential $U_{ij}^{(1)}$ is orthogonal to all functions ϕ_i,

$$\sum_{j=1}^{N} U_{ij}^{(1)} \mid \phi_j\rangle=0, \quad \sum_{j=1}^{N} \langle \phi_j \mid U_{ji}^{(1)}=0 \ . \tag{33}$$

Making use of Eq. (31), we write Eq. (29) as

$$F_i=\phi_i\delta_{ii_0}+\sum_{m=1}^{N} G_i^{(0)}U_{im} \mid \phi_m\rangle \frac{1}{D}\sum_{n=1}^{N}\sum_{j=1}^{N} \langle \phi_n \mid U_{nj} \mid F_j\rangle + \sum_{j=1}^{N} G_i^{(0)}U_{ij}^{(1)}F_j \ . \tag{34}$$

After some calculations, Eq. (34) may be expressed as

$$F_i=\phi_i\delta_{ii_0}+\sum_{j=1}^{N} [(1-G^{(0)}U^{(1)})^{-1}]_{ij}\phi_j^{(1)} \times\frac{\sum_l\sum_m \langle \phi_l \mid U_{lm} \mid F_m\rangle}{D} \ , \tag{35}$$

where

$$\phi_j^{(1)}=\sum_{l=1}^{N} G_j^{(0)}U_{jl} \mid \phi_l\rangle \ , \tag{36}$$

and

$$F_i=\phi_i\delta_{ii_0}+F_i^{(1)}\frac{\sum_l\sum_m \langle \phi_l \mid U_{lm} \mid F_m\rangle}{D} \ . \tag{37}$$

Here the new functions $F_i^{(1)}$ are the solution of the integral equation

$$F_i^{(1)}=\phi_i^{(1)}\delta_{ii_0}+\sum_{j=1}^{N} G_i^{(0)}U_{ij}^{(1)}F_j^{(1)} \ . \tag{38}$$

As in Sec. II, we can reduce Eq. (37) to the form

$$F_i=\phi_i\delta_{ii_0} +F_1^{(1)}\frac{\sum_l\sum_m \langle \phi_l \mid U_{lm} \mid \phi_m\rangle}{\sum_l\sum_m \langle \phi_l \mid U_{lm} \mid \phi_m\rangle-\sum_l\sum_m \langle \phi_l \mid U_{lm} \mid F_m^{(1)}\rangle} \ , \tag{39}$$

analogously to Eq. (12). Equations (38) and (39) together with the definitions (31), (32), and (36) are the generalization of MCF to coupled-channel scattering.

IV. PROPERTIES OF MCF

The MCF has several remarkable properties which will be briefly reviewed in this section.

(1) We can show that for an N-term separable potential

$$U=\sum_{i=1}^{N} \mid g_i\rangle\langle g_i \mid \ , \tag{40}$$

the potential $U^{(N)}$ vanishes. As a result, we obtain the exact result after N iterations.

Let us briefly demonstrate the above statement taking the two-term separable potential as an example,

$$U=|g_1\rangle\langle g_1|+|g_2\rangle\langle g_2| \; . \tag{41}$$

We can show that $U^{(2)}=0$ in the following manner. Let us express $U^{(1)}$ as

$$\begin{aligned} U^{(1)}=&\alpha_{11}|g_1\rangle\langle g_1|+\alpha_{12}|g_1\rangle\langle g_2| \\ &+\alpha_{21}|g_2\rangle\langle g_1|+\alpha_{22}|g_2\rangle\langle g_2| \; . \end{aligned} \tag{42}$$

Here,

$$\begin{aligned} \alpha_{11}&=1-\frac{\langle g_1|u\rangle\langle u|g_1\rangle}{\langle u\,|\,U\,|\,u\rangle} \; , \\ \alpha_{12}=\alpha_{21}&=\frac{\langle g_1|u\rangle\langle u|g_2\rangle}{\langle u\,|\,U\,|\,u\rangle} \; , \\ \alpha_{22}&=1-\frac{\langle g_2|u\rangle\langle u|g_2\rangle}{\langle u\,|\,U\,|\,u\rangle} \; . \end{aligned} \tag{43}$$

For the potential (41), the following relation is satisfied:

$$\alpha_{11}\alpha_{22}=\alpha_{12}\alpha_{21} \; . \tag{44}$$

Then we can easily show that all the coefficients β_{ij} $(i,j=1,2)$ of the expression

$$\begin{aligned} U^{(2)}=&\beta_{11}|g_1\rangle\langle g_1|+\beta_{12}|g_1\rangle\langle g_2| \\ &+\beta_{21}|g_2\rangle\langle g_1|+\beta_{22}|g_2\rangle\langle g_2| \end{aligned} \tag{45}$$

vanish.

Since the nonlocal potential is supposed to be a compact operator, and every compact operator can be approximated by a sum of separable terms with an arbitrary accuracy, we conclude that the scattering matrix of a nonlocal potential can be calculated by the MCF with any desired accuracy.

(2) Starting from the second iteration, all functions that must be computed in the MCF are of finite range. This follows from the orthogonality relations (22), of which the relevant one is

$$\langle u\,|\,U^{(n)}=0, \quad n=1,2,\ldots \tag{46}$$

and from the fact that the free-particle Green function G_0 behaves asymptotically as

$$G_0\sim-\frac{1}{k}\,|v\rangle\langle u| \; . \tag{47}$$

Therefore, for any function ξ for which $U^{(n)}|\xi\rangle$ exists, we have the following asymptotic behavior:

$$\lim_{r\to\infty} G_0U^{(n)}|\xi\rangle=-\frac{1}{k}\,|v\rangle\langle u\,|\,U^{(n)}|\xi\rangle=0 \; . \tag{48}$$

As a result, all functions u_i $(i=2,3,\ldots)$, which were defined by Eq. (21b), are of finite range. Moreover, by the definition, these functions are regular at the origin. These properties are of practical importance, especially in the case of coupled channels where one should calculate the matrix elements $\langle u_l\,|\,U\,|\,u_{l'}\rangle$ between different angular momenta. (It has been known that in the case of the Jost method, special care must be given to the calculations of the matrix elements between different angular momenta for some kind of potentials.[11,12])

(3) As illustrated in Sec. VI, the MCF shows extremely fast convergence. This can be explained by the following. Let us multiply the interaction potential in Eq. (1) by a parameter λ. Then, for small λ, the scattering amplitude K may be expressed in the ascending power of λ (the Neumann series) as

$$\begin{aligned} K&=\lambda\langle u\,|\,U\,|\,\phi\rangle \\ &=\lambda\langle u\,|\,U\,|\,u\rangle+\lambda^2\langle u\,|\,UG_0U\,|\,u\rangle+\cdots \; . \end{aligned} \tag{49}$$

If we define λ_n by

$$\lambda_n\equiv\lambda^n\langle u\,|\,U(G_0U)^{n-1}|\,u\rangle \; , \tag{50}$$

Eq. (44) takes the form

$$K=\lambda_1+\lambda_2+\lambda_3+\cdots \; . \tag{51}$$

Now, suppose that we calculate K_1 by Eq. (26),

$$K_1=\langle u\,|\,V\,|\,u_1\rangle+\frac{\langle u_1\,|\,U^{(1)}|\,u_1\rangle^2}{\langle u_1\,|\,U^{(1)}|\,u_1\rangle-K_2} \; . \tag{52}$$

The value of K_1 depends on the value of K_2 which is determined by how far we calculate the continued fractions given by (26). For instance, if we approximate K_2 by the lowest-order term,

$$K_2=\langle u_1\,|\,U^{(1)}|\,u_2\rangle=\lambda_4+\cdots \; , \tag{53}$$

and use this value in Eq. (52), we get

$$K_1=\lambda_2+\lambda_3+\lambda_4+\cdots \; , \tag{54}$$

which is correct up to λ^4. Further, if we approximate K_2 by

$$\begin{aligned} K_2&=\langle u_1\,|\,U^{(1)}|\,u_2\rangle+\frac{\langle u_2\,|\,U^{(2)}|\,u_2\rangle^2}{\langle u_2\,|\,U^{(2)}|\,u_2\rangle-\langle u_2\,|\,U^{(2)}|\,u_3\rangle} \\ &=\lambda_4+\lambda_5+\lambda_6+\cdots \; , \end{aligned} \tag{55}$$

we get the value of K_1 which may be expressed as

$$K_1=\lambda_2+\lambda_3+\lambda_4+\lambda_5+\lambda_6+\cdots \; , \tag{56}$$

which is correct up to λ^6. In general, we can show that the nth step of MCF yields a result which is correct up to λ^{2n}.

V. DISTORTED WAVES

In atomic physics, the interaction potential U usually consists of two parts: one is the static local interaction, and the other is the exchange nonlocal interaction. Generally, it is much easier to solve the scattering problem when only local interaction is effective than to solve the scattering equation with full nonlocal interaction. Therefore, it is natural to apply the MCF to the nonlocal part of the interaction and to treat the local part in the usual manner. This method corresponds to the modified approach of Rescigno and Orel.[10]

Let interaction U be split into two parts V and W

$$U=V+W\ , \tag{57}$$

where V (W) denotes a local (nonlocal) potential. The Lippmann-Schwinger equation (1) may formally be represented as

$$\phi=\bar{u}+GW\phi\ , \tag{58}$$

where $\bar{u}$ denotes the distorted wave

$$\bar{u}=(1-G_0V)^{-1}u \tag{59}$$

and G the Green function of the distorted wave

$$G=(1-G_0V)^{-1}G_0\ . \tag{60}$$

Equation (58) takes the same form as Eq. (1) with the replacements $u \rightarrow \bar{u}$ and $G_0 \rightarrow G$. Now, the full scattering matrix K is given by

$$K=K_v+K_w\ , \tag{61}$$

where

$$K_v=\langle u \mid V \mid \bar{u}\rangle,\quad K_w=\langle \bar{u} \mid W \mid \phi\rangle\ . \tag{62}$$

We calculate K_w in the same manner as in Sec. II. For instance, $W^{(1)}$ is defined by

$$W^{(1)}=W-\frac{W \mid \bar{u}\rangle\langle \bar{u} \mid W}{\langle \bar{u} \mid W \mid \bar{u}\rangle}\ . \tag{63}$$

The Green function G need not be computed explicitly. What is needed is to solve, at every iteration step, an equation for a local potential

$$\xi=\eta+G_0V\xi\ , \tag{64}$$

which can be solved in the usual manner.

VI. NUMERICAL RESULTS

We have applied the MCF to the elastic scattering of electrons from hydrogen atom in the static, exchange approximation. In this case, the static local interaction V and the exchange interaction W are given, respectively, by

$$V=-2\left[1+\frac{1}{r}\right]e^{-2r} \tag{65}$$

and

$$W=-2\phi_{1s}(r)\phi_{1s}(r')/r_>-(1+k^2)\phi_{1s}(r)\phi_{1s}(r')\ . \tag{66}$$

Here $r_>$ is the larger one of r and r', and ϕ_{1s} denotes the normalized wave function of the hydrogen ground state. The second part of the interaction (66) is omitted in the case of the triplet scattering due to the orthogonality relations. Although the MCF has been intended primarily for the treatment of nonlocal interactions, we study first its efficiency in the case of the local interaction (65). The results of the computations of the static phase shifts for the same energies as in Ref. 10 are given in Table I. From this table, we see that the MCF is also effective for the local potential and, in fact, the third iteration already yields the phase shifts which are correct up to four significant figures. The convergence is very fast and the subsequent iterations approach the limiting value monotonically. The rate of convergence does not seem to depend on energy. As a second test, we take the full interaction $V+W$ into account again for the same energies. The calculated phase shifts are given in Tables II (III) for the triplet (singlet) scattering and are denoted as δ_{unmod} (for unmodified). The phase shifts denoted as δ_{mod} (for modified) are due to the distorted-wave method of Sec. V. These results should be compared with Table I of Ref. 10. Then the efficiency of the MCF and especially of the distorted-wave MCF may be clear. The modified results should also be compared with the method of John,[5] where eight iterations were necessary to obtain the results with similar accuracy. Finally, we have applied the MCF to the model proposed by Rescigno and Orel.[10] In this model, a long-range term is added to the triplet e + H static local potential

$$V=-2\left[1+\frac{1}{r}\right]e^{-2r}-\frac{2}{1+r^3}\ . \tag{67}$$

TABLE I. The s-wave phase shift for the static potential (65) calculated by MCF.

N	δ_N $k=0.2$	δ_N $k=1.0$
1	0.868 5	0.792 6
2	0.971 8	0.903 8
3	0.972 5	0.905 5
Exact	0.972 521	0.905 523

TABLE II. The s-wave triplet phase shift for the full nonlocal interaction $V+W$, where Eq. (65) is used for V and Eq. (66) for W. Phase shift δ_{unmod} is obtained by applying the MCF to the full static interaction (57), while δ_{mod} is obtained by the distorted-wave MCF described in Sec. V.

N	δ_{unmod}	δ_{mod}	Exact
		$k=0.2$	
1	2.603	2.667	
2	2.677	2.679	2.679 148
3	2.679		
		$k=1.0$	
1	1.303	1.405	
2	1.387	1.391	1.390 52
3	1.391		

TABLE III. Same as in Table II, but for the singlet scattering.

N	δ_{unmod}	δ_{mod}	Exact
		$k=0.2$	
1	1.856	1.870	
2	1.866		1.870 16
3	1.870		
		$k=1.0$	
1	0.5101	0.5428	
2	0.5412	0.5429	0.542 894
3	0.5429		

The modified and nonmodified results are summarized in Table IV. Again, the MCF is found to converge very rapidly.

VII. DISCUSSION

In this paper we have proposed a new iterative method for solving the scattering integral equation and studied its efficiency in the case of the electron-hydrogen scattering in the static, exchange approximation. The proposed method is extremely rapidly convergent for all potentials that we have studied. The method is easily adaptable to the multichannel scattering problems. Usual noniterative methods for solving the scattering integral equation require the calculation of the inverses or determinants of matrices which usually are of large dimension. This often causes instability in the course of calculations. In our approach, no inversion nor computation of determinants is necessary. In fact, at each iteration step, with the computation of the function $G_0 U^{(i)} \mid u_i \rangle$, just two integrals need be computed. Therefore, with a relatively small amount of numerical work, a high precision is expected to result from our approach.

TABLE IV. The *s*-wave triplet phase shifts for the model long-range interaction (67) in place of (65). Other labels are the same as in Table II.

N	δ_{unmod}	δ_{mod}
	$k=0.2$	
1	2.7258	3.5360
2	3.0676	3.1483
3	3.1461	
4	3.1483	
	$k=1.0$	
1	1.7375	2.0311
2	1.9851	2.0175
3	2.0168	
4	2.0175	

The applicability of our method is not limited to the case of the Lippmann-Schwinger-type equations. We expect that this method will find application in few-body physics as well as in other fields where a description by Fredholm-type equations is feasible.

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[1] W. Eissner and M. J. Seaton, J. Phys. B 5, 2187 (1972); M. J. Seaton, Comput. Phys. Commun. 6, 247 (1973); J. Phys. B 7, 1817 (1975); L. A. Collins and B. I. Schneider, Phys. Rev. A 24, 2387 (1981).

[2] P. G. Burke, Comput. Phys. Commun. 6, 288 (1973); P. G. Burke and W. D. Robb, in *Advances in Atomic and Molecular Physics*, edited by D. R. Bates and B. Bederson (Academic, New York, 1975), pp. 143—214.

[3] E. R. Smith and R. J. W. Henry, Phys. Rev. A 7, 1585 (1973).

[4] F. E. Harris and H. H. Michels, Methods Comput. Phys. 10, 143 (1971); D. G. Truhlar, J. Abdallah, and B. I. Smith, Adv. Chem. Phys. 25, 211 (1974); R. K. Nesbet, Adv. Quantum Chem. 9, 215 (1975); J. Callaway, Phys. Rep. 45, 89 (1978); Y. Hahn and R. Luddy, Phys. Rev. C 24, 1 (1981).

[5] T. L. John, Proc. Phys. Soc. London 76, 532 (1960); A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, Phys. Rev. A 3, 1328 (1971); B. Ritchie, M. S. Pindzola, and W. R. Garrett, *ibid*. 23, 2905 (1981).

[6] An extensive list of the iterative method intended for applications to few-body physics is found in J. Horáček and T. Sasakawa (unpublished).

[7] T. Sasakawa, H. Okuno, S. Ishikawa, and T. Sawada, Phys. Rev. C 26, 42 (1982); T. Sasakawa, J. Hoŕček, and T. Sawada, *ibid*. 27, 18 (1983).

[8] J. Hoŕaček and T. Sasakawa in Ref. 6.

[9] B. I. Schneider, Chem. Phys. Lett. 31, 237 (1975); Phys. Rev. A 11, 1957 (1975); T. N. Rescigno, C. W. McCurdy, and V. McKoy, Chem. Phys. Lett. 27, 401 (1979); Phys. Rev. A 10, 2240 (1974); 11, 825 (1975); A. W. Fliflet and V. McKoy *ibid*. 18, 1048 (1978); D. K. Watson and V. McKoy *ibid*. 20, 1474 (1979); R. R. Lucchese and V. McKoy, J. Phys. B 12, L421 (1979); D. K. Watson, R. R. Lucchese, V. McKoy, and T. N. Rescigno, Phys. Rev. A 21, 738 (1980).

[10] T. N. Rescigno and A. E. Orel, Phys. Rev. A 23, 1134 (1981); 24, 1267 (1981).

[11] R. G. Newton, in *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), p. 464; Phys. Rev. 100, 412 (1955).

[12] T. Sasakawa and T. Sawada, Phys. Rev. C 11, 87 (1975).