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Method of continued fractions with application to atomic physics. II

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This paper presents an alternative form of the method of continued fractions proposed by the authors recently. The present form is based on a subtraction of a separable operator from an appropriate Green function and shows faster convergence than the original method. The method is again applied to the elastic scattering of the electron from the hydrogen atom. The relation to certain variational principles with functionals of a fractional form is discussed.

I. INTRODUCTION

In a previous paper,[1] hereafter referred to as I, we have proposed the method of continued fraction (MCF) for solving the Lippmann-Schwinger scattering equation for a local or a nonlocal potential. In this method, with the increase in the number of iterations, a series of potentials are successively defined by subtracting a separable term from the previously given potential. These potentials become weaker and weaker. We have demonstrated that the method is very efficient, yielding a very accurate result after a few iterations. This method works surprisingly well not only for atomic scattering problems, but also for the nuclear scattering where the interaction potential is very strong at short distances.[2] In the present paper we propose an alternative form of the MCF which is based on a subtraction of a separable term from the Green function and which is, to some extent, superior to the method proposed in I. In order to distinguish between these two methods, we call the method based on a subtraction from the potential MCFV and the newly proposed method MCFG.

We describe the new method in Sec. II. A comparison between MCFV and MCFG in application to the elastic scattering of the electron from the hydrogen atom in the static-exchange approximation is made in Sec. III. A relation between MCF and some variational principles is discussed in Sec. IV. Concluding remarks are given in Sec. V. A practical method for calculating the wave function and amplitude by MCF is written in the Appendix.

II. METHOD OF CONTINUED FRACTIONS—MCFG

For any local, nonlocal, energy dependent, etc., interaction V, we want to solve the Lippmann-Schwinger equation

$$\phi = u + G_0 V \phi \ . \tag{1}$$

As in I, but with the introduction of G_1 in place of V_1 in MCFV, the MCFG is based on the following set of four equations:

$$\phi = u + \phi_1 \frac{\langle u \mid V \mid u_1 \rangle}{\langle u \mid V \mid u_1 \rangle - \langle u_1 \mid V \mid \phi_1 \rangle} \ , \tag{2}$$

$$\phi_1 = u_1 + G_1 V \phi_1 \ , \tag{3}$$

$$u_1 = G_0 V u \ , \tag{4}$$

$$G_1 = G_0 - \frac{\mid u_1 \rangle \langle u_1 \mid}{\langle u \mid V \mid u_1 \rangle} \ . \tag{5}$$

Equation (3), which is the same type as the original equation (1), is solved similarly. Thus, we continue with a set of equations for $i = 1, 2, \ldots,$

$$\phi_i = u_i + \phi_{i+1} \frac{\langle u_i \mid V \mid u_{i+1} \rangle}{\langle u_i \mid V \mid u_{i+1} \rangle - \langle u_{i+1} \mid V \mid \phi_{i+1} \rangle} \ , \tag{6}$$

$$\phi_{i+1} = u_{i+1} + G_{i+1} V \phi_{i+1} \ , \tag{7}$$

$$u_{i+1} = G_i V u_i \ , \tag{8}$$

$$G_{i+1} = G_i - \frac{\mid u_{i+1} \rangle \langle u_{i+1} \mid}{\langle u_i \mid V \mid u_{i+1} \rangle} \ . \tag{9}$$

Owing to the definition of G_i, the operator $G_i V$ is orthogonal to the function u_i, namely,

$$\langle u_j \mid V G_i = G_i V \mid u_j \rangle = 0 \quad \text{for } j = 0, 1, \ldots, i-1 \ , \tag{10}$$

where

$$u_0 = u \ .$$

Thus, the operator $G_i V$ becomes weaker and weaker as the number of iterations increases.

The function $\langle u_i \mid V \mid \phi_i \rangle$ $(i = 1, 2, \ldots)$ that appears in Eq. (6) is calculated as continued fractions. We define the matrix elements t_i for $i = 0, 1, 2, \ldots$ by

$$t_i = \langle u_i \mid V \mid \phi_i \rangle \ . \tag{11}$$

The quantity t_0 is the usual t-matrix element. If we put Eq. (6) in Eq. (11) and make use of Eq. (10), we obtain continued fractions

$$t_i = q_{2i+1} + \frac{q_{2i+2}^2}{q_{2i+2} - t_{i+1}} \ , \tag{12}$$

with

$$q_{2i}=\langle u_{i-1}\,|\,V\,|\,u_i\rangle,\quad i=1,2,\ldots,$$

$$q_{2i+1}=\langle u_i\,|\,V\,|\,u_i\rangle,\quad i=0,1,2,\ldots .$$

In calculating the continued fractions, we stop them if $G_{N+1}V$ and, consequently, t_{N+1} are sufficiently small.

The MCFG has the following important properties.

(1) It is convergent for all interactions, independently of their strength, provided that G_0V is a compact operator.

(2) For an N-term separable interaction V,

$$V=\sum_{i=1}^{N}|g_i\rangle\langle h_i|\;,$$

the Nth step of the MCFG yields the exact result.

(3) All functions u_i are regular at the origin.

(4) If the interaction is written as λV, where λ denotes a complex parameter, then the Nth term of the MCFG is correct at least to the $(2N+1)$th order. For instance, the first approximation of t $(=t_0)$ in the MCFG is

$$t^{(1)}=q_1+\frac{\lambda^2 q_2^2}{q_2-q_3}\;. \tag{13}$$

If we expand Eq. (13) in the ascending power of λ, we get

$$\begin{aligned}t^{(1)}&=\lambda q_1+\lambda^2q_2+\lambda^3q_3+\cdots\\&=\lambda\langle u\,|\,V\,|\,u\rangle+\lambda^2\langle u\,|\,VG_0V\,|\,u\rangle\\&\quad+\lambda^3\langle u\,|\,VG_0VG_0V\,|\,u\rangle+\cdots .\end{aligned}$$

Thus the first approximation of MCFG is correct up to the third-order term in λ.

Let us compare this result with that of MCFV. With the definitions

$$t=\tau_0=\langle u\,|\,V\,|\,\phi\rangle,\quad \tau_i=\langle u_i\,|\,V_i\,|\,\phi_i\rangle\;,$$

$$p_{2i}=\langle u_{i-1}\,|\,V_{i-1}\,|\,u_i\rangle,\quad i=1,2,\ldots,$$

$$p_{2i+1}=\langle u_i\,|\,V_i\,|\,u_i\rangle,\quad i=0,1,\ldots,$$

the iteration scheme of MCFV is given by[1]

$$\tau_i=\frac{p_{2i+1}^2}{p_{2i+1}-p_{2i+2}-\tau_{i+1}}\;. \tag{14}$$

(The definition of u_i for MCFV is given by

$$u_{i+1}=G_0V_iu_i\;. \tag{15}$$

This is different from the definition of u_i in MCFG.) As we have stated in I, the Nth term of MCFV is correct at least up to the $(2N)$th-order term in the Neumann series. For instance, the first approximation is now

$$t^{(1)}=\frac{\lambda p_1^2}{p_1-p_2}=\lambda p_1+\lambda^2p_2+\lambda^3\frac{p_2^2}{p_1}+\cdots\;,$$

which is correct up to the second-order term.

III. APPLICATION

In the previous paper[1] we have applied the MCFV to the elastic scattering of the electron from the hydrogen atom in the static-exchange approximation. In order to compare these two methods we apply the method MCFG to the same problem. The interaction of the static-exchange approximation consists of two terms, the static local interaction[3]

$$V_L=-2\left[1+\frac{1}{r}\right]e^{-2r} \tag{16}$$

and the nonlocal exchange interaction

$$V_N=-2\phi_{1s}(r)\phi_{1s}(r')/r_>-(1+k^2)\phi_{1s}(r)\phi_{1s}(r')\;. \tag{17}$$

Here $r_>$ is the larger one of r and r', and ϕ_{1s} denotes the normalized wave function of the hydrogen ground state. For the numerical example in the present section we have used the real standing-wave Green function instead of the complex propagating Green function for G_0. As a result, the quantity t stands for the on-shell K-matrix elements. The results of the computation of the static-exchange phase shift are given in Table I (Table II) for the triplet (singlet) scattering.

From these tables we see that for all energies the convergence is so fast that already the fourth approximation leads to the results which are correct at least to six significant digits. Both forms work equally well in this case. This is because the interaction between electrons and atoms is not very strong.

TABLE I. The phase shift for the triplet static-exchange e-H scattering computed by MCFG (MCFV) is shown in the left (right) column.

N	δ_{MCFG}		δ_{MCFV}
		$k=0.2$	
1	2.618 46		2.602 73
2	2.677 73		2.676 83
3	2.679 14		2.679 14
4	2.679 15		2.679 15
		$k=1.0$	
1	1.107 01		1.302 86
2	1.387 29		1.387 11
3	1.390 51		1.390 50
4	1.390 52		1.390 52

TABLE II. The same as in Table I, but for the singlet scattering.

N	δ_{MCFG}		δ_{MCFV}
		$k=0.2$	
1	1.856 659		1.856 000
2	1.869 583		1.866 280
3	1.870 158		1.870 158
		$k=1.0$	
1	0.503 366 3		0.510 141 3
2	0.542 726 3		0.541 182 2
3	0.542 893 9		0.542 893 3
4	0.542 894 6		0.542 894 6

IV. RELATION TO VARIATIONAL PRINCIPLES

We have demonstrated that both forms of MCF work surprisingly well for atomic collisions. This is partly because there exists a close relationship between the MCF and a certain class of variational principles using functionals of fractional form. We show this relation for the MCFV. According to I, the K matrix is given by

$$K=\frac{\langle u \mid V \mid u \rangle^2}{\langle u \mid V \mid u \rangle - \langle u \mid V \mid \phi_1 \rangle} , \tag{18}$$

where

$$\phi_1 = u_1 + G_0 V_1 \phi_1 . \tag{19}$$

Here V_1 and all other quantities were defined in I. The Schwinger variational principle[4] states that the functional F

$$[F]=\frac{\langle \Psi_T \mid V \mid u \rangle \langle u \mid V \mid \Psi_T \rangle}{\langle \Psi_T \mid (V - VG_0V) \mid \Psi_T \rangle} \tag{20}$$

is stationary under variation of Ψ_T about its exact value ψ. Here ψ is a solution of the Lippmann-Schwinger equation

$$\psi = u + G_0 V \psi .$$

The first iteration of the MCFV is

$$K_1=\frac{\langle u \mid V \mid u \rangle^2}{\langle u \mid V \mid u \rangle - \langle u \mid VG_0V \mid u \rangle} \tag{21}$$

which coincides with the Schwinger variational principle, if one sets

$$\Psi_T = u . \tag{22}$$

The second iteration of the MCFV is

$$K_2=\frac{\langle u \mid V \mid u \rangle^2}{\langle u \mid V \mid u \rangle - \langle u \mid VG_0V \mid u \rangle - F_2} , \tag{23}$$

where

$$F_2=\frac{\langle u_1 \mid V_1 \mid u_1 \rangle^2}{\langle u_1 \mid V_1 \mid u_1 \rangle - \langle u_1 \mid V_1 G_0 V_1 \mid u_1 \rangle} \tag{24}$$

which coincides with the Schwinger variational principle for Eq. (19), u_1 being taken as the trial function. Similarly at the Nth step of the MCFV we calculate the quantity F_N given by

$$F_N=\frac{\langle u_N \mid V_N \mid u_N \rangle^2}{\langle u_N \mid V_N \mid u_N \rangle - \langle u_N \mid V_N G_0 V_N \mid u_N \rangle} , \tag{25}$$

which is the value of the Schwinger variational functional applied to the Lippmann-Schwinger-type equation

$$\phi_N = u_N + G_0 V_N \phi_N \tag{26}$$

when the function u_N is taken as the trial function. At the last iteration, we can practically take $\phi_N = u_N$ or $G_0 V_N \phi_N = 0$. Here the function ϕ_N satisfies the Schwinger variational principle.

The situation is similar in the case of the MCFG. The only difference is that instead of the Schwinger variational principle, we have to use the variational principle discussed recently by Gross and Runge.[5] The required functional is

$$[F]=\frac{\langle u \mid VG_0V \mid \Psi_T \rangle \langle \Psi_T \mid VG_0V \mid u \rangle}{\langle \Psi_T \mid (VG_0V - VG_0VG_0V) \mid \Psi_T \rangle} + \langle u \mid V \mid u \rangle . \tag{27}$$

In conclusion, at each step the MCF generates one equation of the Lippmann-Schwinger type and computes the value of the corresponding variational functional using the leading term of the equation as the trial function. Such repeated use of the variational principle results in the high effectivity of the MCF. As discussed in the Appendix, the MCF is simply related to the $[N,N]$ Padé approximant.

Here we note the difference between the MCF and the iterative Schwinger method,[6] which is also related to the Padé approximant.[7] In the MCFV, we successively introduce partially separable potentials $V_1, V_2, \dots$ [which are equal to $U^{(1)}, U^{(2)}, \dots$ of Eqs. (5) and (15) of Ref. 1]. The potential V_i operates to a function u_i. Since V_N is orthogonal to u_i ($i=0,1,\dots,N-1$) as shown by Eq. (22) of Ref. 1, V_N becomes weaker and weaker as N increases and at last the equality $\phi_N = u_N$ practically holds. In the iterative Schwinger method, using a set of Cartesian-Gaussian functions we first construct a separable approximation to the original potential. The exact solution to the approximate potential is used in the Schwinger variational expression of the t matrix. This process is repeated until we get a convergent value of t. Technically, in this method, we have to deal with n-scattering equations at each step, if we choose n-trial functions in the beginning, and also we should perform a matrix inversion at each step. In the MCF, for instance in the MCFV, we have only one equation to handle, $u_i = G_0 V_{i-1} u_{i-1}$, at each step and we do not need any matrix inversion.

V. CONCLUDING REMARKS

So far we have confined our demonstrations to the on-energy-shell quantities. The treatment is extended to an off-shell quantity. For instance, the off-shell t matrix $\langle p \mid t(E) \mid p' \rangle$, where $(\hbar^2/2M)p^2 \neq E \neq (\hbar^2/2M)p'^2$, is calculated in the following manner. We take $u(p',r)$ for u and $G_0(r,r';E)$ for G_0 in Eq. (1). Then we calculate the off-shell function $\phi(p',E;r)$ by the MCFG. This is related to the wave matrix $\Omega(E)$ by

$$\langle r \mid \Omega(E) \mid p' \rangle = \phi(p',E;r) . \tag{28}$$

The off-shell t matrix is then given by

$$\langle p \mid t(E) \mid p' \rangle = \langle p \mid V\Omega(E) \mid p' \rangle . \tag{29}$$

Having calculated the off-shell t matrix, we may find applications in various many-body problems.

To summarize, we have proposed a method for treating the scattering integral equations. This method, MCFG, is a better alternative to the MCFV proposed in I. The method is iterative, very efficient, simple, and accurate, and is especially suitable to the treatment of complicated nonlocal interactions. In the present paper we have applied the MCFG to the same physical problem as in I, i.e., to the elastic scattering of the electron from the hydrogen atom in the static-exchange approximation. It turned out that the MCFG yields excellent results in all cases that we have studied. We have also discussed the relationship between the MCF and the variational principles with functionals of fractional forms. This explains why the MCF is so efficient.

APPENDIX

In this appendix we first discuss the relation between MCF and the Padé approximant and then demonstrate the procedure for calculating the amplitude and the wave function. We define f_i and α_i $(i=1,2,3,\ldots)$ for MCFG by

$$f_i=\frac{q_{2i}-t_i}{q_{2i}-q_{2i+1}}\,,\qquad \alpha_i=-\frac{q_{2i+2}^2}{(q_{2i}-q_{2i+1})(q_{2i+2}-q_{2i+3})}\,, \tag{A1}$$

and for MCFV,

$$f_i=1-\frac{\tau_i}{p_{2i-1}-p_{2i}}\,,\qquad \alpha_i=-\frac{p_{2i+1}^2}{(p_{2i-1}-p_{2i})(p_{2i+1}-p_{2i+2})}\,. \tag{A2}$$

Then both Eqs. (12) and (14) for $i=1,2,\ldots$ take a form

$$f_i=1+\alpha_i/f_{i+1}\,, \tag{A3}$$

where α_i is supposed to become negligibly small at $i=N$. Equation (A3) is simply related to the Padé approximant.[8] If we put $f_n^{\text{Padé}}=P_n/Q_n$, $n=1,2,\ldots$ the reduction formula is given by $P_{n+1}=P_n+\alpha_n P_{n-1}$, $Q_{n+1}=Q_n+\alpha_n Q_{n-1}$ with $P_0=1$, $Q_0=0$, $P_1=Q_1=1$.

However, since α_i are simple numbers, we need not resort to the Padé approximant. Here we demonstrate the procedure of calculating the amplitude and the wave function for MCFG. The procedure for MCFV is then clear.

(1) We calculate u_1 and u_2 by Eq. (8). We store u_1 and u_2 in the memory space. Using u_1 and u_2, we calculate q_2, q_3, q_4, and q_5, according to the equations below Eq. (12). Then we calculate α_1 by Eq. (A1).

(2) We calculate u_3 and store it. Using u_2 and u_3, we calculate q_6 and q_7. Then we calculate α_2.

(3) This process is repeated until α_i becomes negligibly small at $i=N$.

(4) By Eq. (A3) we obtain $f_N=1$, $f_{N-1}=1+\alpha_{N-1}$, $f_{N-2}=1+\alpha_{N-2}/f_{N-1}$, $\ldots$, $f_1=1+\alpha_1/f_2$. Now, we express Eq. (6) for $i=1,2,\ldots$ in the form

$$\phi_i=u_i+\phi_{i+1}\eta_{i+1}\,, \tag{A4}$$

where

$$\eta_{i+1}=\frac{q_{2i+2}}{q_{2i+2}-t_{i+1}}=\frac{q_{2i+1}-q_{2i}}{q_{2i+2}}\frac{\alpha_i}{f_{i+1}}\,. \tag{A5}$$

The amplitude η_1 is given by

$$\eta_1=\frac{q_2}{q_2-t_1}=\frac{q_2}{(q_2-q_3)f_1}\,. \tag{A6}$$

The full wave function is given in terms of η_1 by

$$\phi=u+\phi_1\eta_1\,. \tag{A7}$$

(5) We calculate η_i $(i=N,N-1,\ldots,2)$ and η_1 by using Eqs. (A5) and (A6).

(6) The wave function is then calculated as

$$\begin{aligned}&\phi_N=u_N\,,\\&\phi_{N-1}=u_{N-1}+\phi_N\eta_N\,,\\&\ldots,\\&\phi=u+\phi_1\eta_1\,.\end{aligned} \tag{A8}$$

(7) Finally, the amplitude t is calculated by Eq. (11) for $i=0$.

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