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Complex Kohn Variational Principle for the Solution of Lippmann–Schwinger Equations

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A recently proposed version of the Kohn variational principle for the t matrix incorporating the correct boundary condition is applied for the first time to the study of nucleon–nucleon scattering. Analytic expressions can be obtained for all the integrals in the method for a wide class of potentials and for a suitable choice of trial functions. Closed-form analytic expressions for these integrals are given for Yakawa and exponential potentials. Calculations with two commonly used S-wave nucleon–nucleon potentials show that the method may converge faster than other solution schemes not only for the phase-shifts but also for the off-shell t matrix elements if the freedom in the choice of the trial function is exploited.

1. INTRODUCTION

Variational principles (v.p.'s) have proved [1–7] to be very useful for solving scattering equations which usually have the Lippmann–Schwinger (LS) form [8]

$$t(E) = V + VG_0^{(+)}(E)\, t(E), \tag{1}$$

where t is the transition (t) matrix, V the potential, and $G_0^{(+)}(E)$ is the free Green function at energy E. There are different types of v.p.'s. We follow the classification of Ref. [5]. A Kohn-type [2] v.p. is essentially a v.p. for the operator $(t(E) - V)$. The simplest v.p. of this class is the usual Kohn v.p. for the phase shift or for the real reactance (K) matrix elements. A Schwinger [1] v.p., on the other hand, is a v.p. for the transition matrix $t(E)$.

The usual Kohn v.p. does not require the calculation of integrals involving the free Green function and is the simplest of all the available v.p.'s. This v.p. for the K matrix elements requires trial functions satisfying scattering boundary conditions. It was noted by Schwartz [9] that the K matrix calculated by the Kohn v.p. exhibit's anomalous singularities. This has limited significantly the use of Kohn v.p.'s in scattering calculations. In the Kohn method one has to invert the operator $(E - H)$, where H is the full Hamiltonian in the space of the real trial functions. As H has a continuum spectrum at positive energies this process of inversion leads to spurious singularities. The advantage of the Kohn v.p. over the Schwinger v.p. in having simple integrals to deal with is more than offset by the presence of these anomalous singularities.

It has recently been suggested [10] that by choosing complex boundary conditions for the full Green function the Kohn v.p. readily yields the complex t matrix elements. In the space spanned by the complex trial function the operator $(E - H)^{-1}$ does not present anomalous singularities. So the difficulties associated with the appearance of anomalous singularities in the usual Kohn method for the K matrix are circumvented in the complex Kohn method for the t matrix. A variant of the complex Kohn method for directly calculating the scattering (S) matrix elements has also been suggested and used [10]. The complex Kohn method for the t and S matrix elements are closely related to each other, and the S matrix version of the complex Kohn v.p. is also claimed to be free of anomalous singularities.

The complex Kohn v.p. has only been suggested recently and has seen only limited application for a very special class of scattering problems in atomic physics. In the single channel case only an exponential potential has been considered. In the present work we apply the complex Kohn v.p. for the t matrix in solving the nucleon–nucleon (NN) scattering problem with two phenomenological potentials with soft core [11], where precision calculations have been performed using other methods [4, 5]. This will allow us to compare the results obtained with the complex Kohn v.p. with those obtain with other methods. Because of the presence of a soft core these phenomenological NN potentials are difficult to deal with both in configuration and momentum space calculations. There are difficulties with configuration space integration at small r. In a momentum space treatment the momentum space infinite integrals are discretized by employing a momentum space mesh which extends to a very large value of momentum. Hence the study of NN scattering employing phenomenological potentials with soft core should be considered to be a welcome test for

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the usefulness of any numerical method for solving LS equations.

It has been shown that the Schwinger v.p. may possess spurious singularities [12]. But it has been pointed out [13] that they should be rare in practice and are expected to have little relevance to the usefulness of Schwinger v.p. Anomalous singularities have been recently observed [14] in the complex Kohn v.p. In view of this it is interesting to see if this has any relevance to the application of this v.p. to other problems in scattering, for example, NN scattering with phenomenological potentials with soft core.

We find that for the problem studied, the complex Kohn v.p. produces very good convergence and the accidental appearance of spurious singularities seems to have no relevance to the usefulness of this method. The final convergence obtained with the complex Kohn v.p. is better than the best convergence obtained so far for these potentials with the Schwinger v.p.

We not only calculated the phase-shifts but also the off-shell t matrix elements using the present method and find that both the phase shifts and the off-shell t matrix elements converge equally rapidly. This was tested by calculating the Kowalski–Noyes [14] universal half-shell functions. A knowledge of the on-shell t matrix and the Kowalski–Noyes half-shell function at all energies is enough to calculate the fully off-shell t matrix elements, [5] which in standard numerical algorithms is directly determined from the Lippmann–Schwinger equation.

The plan of the paper is as follows. In Section 2 we present a degenerate kernel derivation of the complex Kohn v.p. of Ref. [10]. Explicit analytic expressions for all matrix elements involved in this method are given in Section 3 for two choices ((11)–(13)) of expansion functions for the exponential and the Yukawa potentials. The exponential potential is of interest in atomic scattering problems [10] and the Yukawa potential in nuclear scattering problems [11]. In Section 4 we present numerical results for two phenomenological NN potentials for both choices of expansion functions and compare the results with those obtained by the use of Schwinger v.p. and other methods. Finally, we present a brief summary of our study in Section 5.

2. COMPLEX KOHN VARIATIONAL PRINCIPLE

In this section we present an alternate derivation of the complex Kohn v.p. Formally, this v.p. can be considered as the degenerate kernel solution of Eq. (1) with the following degenerate approximation to $G_0^{(+)}(E) \equiv (E - H_0 + i0)^{-1}$ (with H_0 the free Hamiltonian);

$$[G_0^{(+)}(E)]_N = \sum_{n,j=1}^{N} |u_n\rangle D_{nj} \langle u_j|, \tag{2}$$

where

$$(D^{-1})_{jn} = \langle u_j | (E - H_0 + i0) | u_n \rangle, \tag{3}$$

where u_j, $j = 1, 2, ..., N$, is a set of suitably chosen functions so as to satisfy certain boundary conditions of $G_0^{(+)}(E)$. For calculational sake, we consider all the equations in this work to be in partial wave form. The configuration space matrix element of Eq. (2) should satisfy certain desired properties of the partial wave outgoing Green function

$$\langle r | G_0^{(+)}(E) | r' \rangle_l = ikj_l(kr_<) h_l^{(1)}(kr_>), \tag{4}$$

where j and $h_l^{(1)}$ are the usual spherical Bessel and Hankel functions, and $r_<$ ($r_>$) is the smaller (larger) of r and r'. Expression (4) is symmetric in r and r' and satisfies the following boundary conditions for small and large r for a fixed r' and $l = 0$:

$$\lim_{r \to \infty} \langle r | G_0^{(+)}(E) | r' \rangle = \frac{e^{ikr}}{r} \times \text{function}(r'), \tag{5}$$

$$\lim_{r \to 0} \langle r | G_0^{(+)}(E) | r' \rangle = \text{constant} \times \text{function}(r'). \tag{6}$$

A similar set of equations hold for limits $r' \to 0$ and $r' \to \infty$. The expansion functions u_j of Eqs. (2)–(3) can be easily chosen so as to satisfy the correct outgoing wave boundary conditions (5)–(6) for the Green function consistent with the $+i0$ prescription.

The exact expression (4) for the Green function $G_0^{(+)}(E)$ has a complex analytic structure as functions of r and r'; e.g., it has a discontinuity in the first derivative at $r = r'$. The approximation (2) does not have this behavior. Nevertheless, the t matrix constructed with the use of this approximate Green function is numerically very accurate as we see in the following. In the t matrix the Green function is sandwiched between the potential operators and a good pointwise representation of the Green function is not needed for an accurate representation of the t matrix.

The approximate degenerate Green function of Eqs. (2)–(3) can be easily made to satisfy boundary conditions (5)–(6) if $|u_1\rangle$ is taken to satisfy

$$\lim_{r \to \infty} u_1(r) \equiv \langle r | u_1 \rangle \equiv \langle u_1 | r \rangle = \frac{e^{ikr}}{r}, \tag{7}$$

$$\lim_{r \to 0} u_1(r) = \text{constant}, \tag{8}$$

and the remaining functions $|u_j\rangle$, $j \neq 1$, are taken to satisfy

$$\lim_{r \to \infty} u_j(r) = 0, \tag{9}$$

$$\lim_{r \to 0} u_j(r) = \text{constant}. \tag{10}$$

The simplest choices satisfying these conditions are

$$u_1(r) \equiv \langle r | u_1 \rangle \equiv \langle u_1 | r \rangle = (1 - e^{-\alpha r}) \frac{e^{ikr}}{r} \tag{11}$$

and

Choice A

$$u_j(r) = r^{j-2} e^{-\alpha r}, \qquad j = 2, 3, ..., N, \tag{12}$$

or

Choice B

$$u_j(r) = e^{-(j-1)\alpha r}, \qquad j = 2, 3, ..., N, \tag{13}$$

where α in Eqs. (11)–(13) is supposed to be a variational parameter which should be varied so as to obtain the best convergence. It is obvious that these are not the only possible choices for u_j. There could be many other possible choices. The objective of this work is not to exhaust all these possibilities but to see if these two simple choices produce good convergence in NN scattering involving soft core potentials. Of these choices only choice A has been applied in other numerical applications [10].

When approximation (2) is used in the kernel of the LS equation (1), it yields the following solution,

$$t_N(E) = V + \sum_{n,j=1}^{N} V |u_n\rangle J_{nj} \langle u_j| V, \tag{14}$$

where

$$(J^{-1})_{jn} = \langle u_j | (E - H + i0) | u_n \rangle, \tag{15}$$

with $H = H_0 + V$. Equation (14) is the desired complex Kohn v.p. for the t matrix [10]. The variational property of expression (14), and its equivalence with the Kohn v.p. are established in Ref. [5].

In this method the outgoing wave nature of the t matrix is taken care of via the choice of expansion functions (11)–(13). The function u_1 is complex and the functions u_j, $j = 2, ..., N$, are real. The correct boundary condition is imposed by taking $\langle u_1 | r \rangle$ and $\langle r | u_1 \rangle$ to be equal and not complex conjugate of each other as in the case of complex functions in quantum mechanics [10]. As in the usual Kohn method, in expansion (14)–(15) one does not require integrals involving the Green function.

In previous calculations using the Kohn v.p. only the partial wave phase shifts or the on-shell K-matrix elements were calculated. However, if one is interest in solving few-body scattering problems using the two-body t matrix elements one needs the off-shell t matrix elements. The universal Kowalski–Noyes half-shell functions at all energies define the off-shell t matrix elements at an energy and we study the convergence of these functions also in our numerical study [5].

3. EXPLICIT MATRIX ELEMENTS

One reason for choosing the functions (11)–(13) in the present method is that for the commonly used exponential and Yukawa potentials all the matrix elements needed in the numerical evaluation of the t matrix elements using Eqs. (14)–(15) can be evaluated analytically. Consequently, the only numerical task is the inversion of an analytically known matrix and simple matrix-vector multiplication, which can be executed on a personal computer.

The on-shell S wave ($l = 0$) t matrix elements are parametrized by means of the phase-shift δ via

$$\langle k | t(E) | k \rangle = -\frac{e^{i\delta} \sin \delta}{k}, \tag{16}$$

where $k^2 = 2mE/\hbar^2$, with m the reduced mass.

The explicit S wave matrix elements of the t matrix (14) is given by

$$\langle p | t_N(E) | q \rangle = \langle p | v | q \rangle + \sum_{n,j=1}^{N} \langle p | v | u_n \rangle J_{nj} \langle u_j | v | q \rangle, \tag{17}$$

$$(J^{-1})_{jn} = \langle u_j | (k^2 - \mathscr{H}) | u_n \rangle. \tag{18}$$

In Eqs. (17)–(18) $v \equiv 2mV/\hbar^2$ and

$$\mathscr{H} \equiv 2mH/\hbar^2 = -\frac{d^2}{dr^2} + v(r). \tag{19}$$

The matrix elements of Eqs. (17)–(18) are explicitly written as

$$\langle u_j | (k^2 - \mathscr{H}) | u_i \rangle = \int_0^\infty (ru_j(r)) \left[k^2 + \frac{d^2}{dr^2} - v(r) \right] \times (ru_i(r))\, dr, \tag{20}$$

$$\langle u_j | v | q \rangle \equiv \langle q | v | u_j \rangle = \int_0^\infty u_j(r)\, v(r) \frac{\sin qr}{qr} r^2\, dr. \tag{21}$$

We consider the matrix elements of the following potential with the parameter $P(=0, 1)$,

$$V(r) = V_0 r^{-P} e^{-\mu r}, \tag{22}$$

where $P=0$ (1) corresponds to the exponential (Yukawa) potential. In this case

$$\begin{aligned}\langle p|\, v\,|q\rangle &= \{v_0/(4pq)\}\ln[\{\mu^2+(p+q)^2\}\\ &\quad\times\{\mu^2+(p-q)^2\}^{-1}], \qquad P=1, \qquad (23)\\ &= 2\mu v_0\{\mu^2+(p-q)^2\}^{-1}\\ &\quad\times\{\mu^2+(p+q)^2\}^{-1}, \qquad P=0, \qquad (24)\end{aligned}$$

where $v_0 = 2mV_0/\hbar^2$.

For the choice A expansion functions (11)–(12) the necessary matrix elements are given by

$$\begin{aligned}\langle u_1|\,(k^2-\mathscr{H})\,|u_1\rangle &= v_0[\ln(\mu-2ik)+\ln(\mu+2\alpha-2ik)\\ &\quad-2\ln(\mu+\alpha-2ik)]\\ &\quad-\alpha-\alpha(2ik-\alpha)(2\alpha-2ik)^{-1}, \qquad P=1, \qquad (25)\\ &= -v_0\{(\mu-2ik)^{-1}+(\mu+2\alpha-2ik)^{-1}\\ &\quad-2(\mu+\alpha-2ik)^{-1}\}\\ &\quad-\alpha-\alpha(2ik-\alpha)(2\alpha-2ik)^{-1}, \qquad P=0, \qquad (26)\end{aligned}$$

$$\begin{aligned}\langle u_1|\, v\,|p\rangle &= \{v_0/(2p)\}[\tan^{-1}\{(p+k)/\mu\}+\tan^{-1}\{(p-k)/\mu\}\\ &\quad-\tan^{-1}\{(p+k)/(\alpha+\mu)\}\\ &\quad-\tan^{-1}\{(p-k)/(\alpha+\mu)\}]\\ &\quad+i\{v_0/(4p)\}\ln[\{\mu^2+(p+k)^2\}\\ &\quad\times\{(\mu+\alpha)^2+(p-k)^2\}\\ &\quad\times\{\mu^2+(p-k)^2\}^{-1}\{(\mu+\alpha)^2\\ &\quad+(p+k)^2\}^{-1}], \qquad P=1, \qquad (27)\\ &= v_0(\mu^2+p^2-k^2+2i\mu k)\\ &\quad\times\{\mu^2+(p-k)^2\}^{-1}\{\mu^2+(p+k)^2\}^{-1}\\ &\quad-v_0\{(\alpha+\mu)^2+p^2-k^2+2i(\alpha+\mu)k\}\\ &\quad\times\{(\alpha+\mu)^2+(p-k)^2\}^{-1}\\ &\quad\times\{(\alpha+\mu)^2+(p+k)^2\}^{-1}, \qquad P=0 \qquad (28)\end{aligned}$$

$$\begin{aligned}\langle u_j|\,(k^2-\mathscr{H})\,|u_1\rangle &= -v_0(j-P-1)!\,[(\alpha+\mu-ik)^{P-j}\\ &\quad-(2\alpha+\mu-ik)^{P-j}]\\ &\quad+(j-1)!\,\alpha(2ik-\alpha)(2\alpha-ik)^{-j},\\ &\qquad j>1,\ P=0,\ 1, \qquad (29)\end{aligned}$$

$$\begin{aligned}\langle u_j|\, v\,|p\rangle &= (v_0/p)(j-P-1)!\,\{(\alpha+\mu)^2+p^2\}^{(P-j)/2}\\ &\quad\times\sin[(j-P)\tan^{-1}\{p/(\alpha+\mu)\}],\\ &\qquad j>1,\ P=0,\ 1, \qquad (30)\end{aligned}$$

$$\begin{aligned}\langle u_j|\,(k^2-\mathscr{H})\,|u_n\rangle &= k^2(j+n-2)!\,(2\alpha)^{1-j-n}+(j+n-4)!\,(2\alpha)^{3-j-n}\\ &\quad\times(j^2+n^2-2nj-j-n+2)/4\\ &\quad-v_0(j+n-P-2)!\,(2\alpha+\mu)^{1+P-j-n},\\ &\qquad j,n>1,\ P=0,\ 1, \qquad (31)\end{aligned}$$

where j and n are used to label the expansion functions and $i=(-1)^{1/2}$.

For the choice B expansion function given by Eqs. (11) and (13) we need the following integrals in addition to those given by Eqs. (23)–(28):

$$\begin{aligned}\langle u_j|\,(k^2-\mathscr{H})\,|u_1\rangle &= -v_0[\{\mu+(j-1)\alpha-ik\}^{P-2}-(j\alpha+\mu-ik)^{P-2}]\\ &\quad+\alpha(2ik-\alpha)(j\alpha-ik)^{-2}, \quad P=0,\ 1;\ j>1 \qquad (32)\\ \langle u_j|\, v\,|p\rangle &= v_0[2\{\mu+(j-1)\alpha\}]^{1-P}\\ &\quad\times[\{\mu+(j-1)\alpha\}^2+p^2]^{P-2}, \quad P=0,\ 1;\ j>1, \qquad (33)\\ \langle u_j|\,(k^2-\mathscr{H})\,|u_n\rangle &= -v_0 2^{1-P}\{\mu+(j-1)\alpha+(n-1)\alpha\}^{P-3}\\ &\quad+2\alpha^{-3}(j+n-2)^{-3}\\ &\quad\times\{k^2-\alpha^2(j-1)(n-1)\}, \quad P=0,\ 1;\ j,n>1. \qquad (34)\end{aligned}$$

4. NUMERICAL RESULTS

To see how the complex Kohn v.p. works in practice, we have carried out additional numerical calculations with two of the semiphenomenological NN potentials [11] which have been frequently used in few-nucleon calculations. These potentials possess soft cores and present difficulties in convergence in numerical treatment. So, if we can demonstrate good convergence with these potentials, it is expected that the method will converge well for other methods. These potentials are superposition of Yukawa potentials. Explicitly, these potentials have the form

$$V(r) = \sum_{j=1}^{M} V_j r^{-1} e^{-\mu_j r}, \tag{35}$$

where for the $^1S_0$ Reid soft core potential $M=3$ and $V_1 = -10.463/0.7$ MeV fm, $V_2 = -1650.6/0.7$ MeV fm, $V_3 =$

TABLE I

Phase-Shifts for the Reid Potential for Different N calculated by the Complex Kohn Method with Choices A and B of Expansion Functions given by Eqs. (11)–(13)

$E_{c.m.}$ (MeV)	Choice	Results for $N=$ 4	6	8	10	14	16
	A	-0.85749	0.85986	0.86058	0.86062	0.86063	0.86063
12	B	0.83131	0.86002	0.86062	0.86063		
	S	0.8500	0.8554	0.8604	0.8604	0.8605	0.8606
	A	0.42694	0.43974	0.44015	0.44018	0.44019	0.44019
48	B	0.40785	0.43974	0.44023	0.44020		
	S	0.4535	0.4363	0.4398	0.4398	0.4401	0.4402
	A	0.23146	0.26253	0.26302	0.26303	0.26303	0.26303
72	B	0.21178	0.26249	0.26306	0.26303		
	S	0.2783	0.2577	0.2620	0.2624	0.2627	0.2630
	A	-0.16714	-0.21652	-0.21608	-0.21638	-0.21638	-0.21638
176	B	-0.11473	-0.21709	-0.21631	-0.21631		
	S	-0.2499	-0.2217	-0.2167	-0.2180	-0.2167	-0.2164

Note. The choice S represents the Schwinger variational phase shifts taken from Table II of Ref. [4] denoted choice A there.

6484.2/0.7 MeV fm, $\mu_1 = 0.7\ \text{fm}^{-1}$, $\mu_2 = 4\mu_1$, $\mu_3 = 7\mu_1$, and for the alternate potential $M=2$ and $V_1 = -570.3316$ MeV fm, $V_2 = 1438.4812$ MeV fm, $\mu_1 = 1.55\ \text{fm}^{-1}$, $\mu_2 = 3.11\ \text{fm}^{-1}$. The latter has a single bound state at $E = -0.35$ MeV. It is interesting to recall that previous numerical study of the complex Kohn method used a simple exponential potential and confirmed rapid convergence when compared [10] to other methods such as the one based on the usual Schwinger v.p.

We present results for both choices of expansion functions, for both these potentials. The parameter α in the expansion functions is supposed to be varied to improve the convergence rate. The values finally adopted were $\alpha = 5\ \text{fm}^{-1}$ for the choice A functions (11)–(12) and $\alpha = 1.4\ \text{fm}^{-1}$ for the choice B functions (11) and (13). For the NN scattering problem we take $\hbar^2/2m = 41.47$ MeV fm^2.

In Table I we give elastic scattering phase shifts for the $^1S_0$ Reid soft core potential for both expansion functions and compare them with the best results obtained by the Schwinger v.p. taken from Ref. [4] (denoted choice A there). In Table II we give exactly the same quantities as in Table I, but for the alternate potential and compare them with the result of Schwinger v.p. taken from Ref. [4] (denoted choice 1 there).

From Tables I and II we see that the phase-shifts converge rapidly for both potentials and for both choices of expansion functions. However, convergence is easier to obtain in the case of the alternate potential than in the case of the Reid potential possibly because of the stronger repulsive core of the latter. In order to check the possible existence of any hidden systematic errors in all three calculations of Tables I and II, we also compared the present phase shifts with those calculated with entirely different methods such as by direct matrix inversion or by iteration whenever available [5, 11, 17, 18]. The agreement between our results and these calculations assured us of the absence of any systematic errors.

A point of technical importance is that as the functions used in this work are not orthogonalized, for large N they tend to be similar and the matrix J^{-1} of Eq. (15) tend to become singular and one faces numerical trouble in inverting it. In the present calculation, carried out in double precision—about 16 decimal places—numerical difficulty in matrix inversion appeared only for $N > 16$ (>10) for choice A (B) functions.

At higher energies, particularly at 176 MeV, the convergence is slower with the choice B function and the Schwinger (S) method. For the choice B function the

TABLE II

Same as in Table I for the Alternate Potential

$E_{c.m.}$ (MeV)	Choice	Results for $N=$ 4	6	8	10	14	16
	A	1.08659	1.09965	1.09972	1.099726	1.099728	1.099728
12	B	1.09944	1.09969	1.09973	1.099731		
	S	1.0982	1.0997	1.0997	1.0996		
	A	0.54891	0.54887	0.54998	0.550055	0.550055	0.550055
48	B	0.54940	0.54986	0.55004	0.550053		
	S	0.5457	0.5490	0.5498	0.5503		
	A	0.36501	0.37101	0.37300	0.373020	0.373023	0.373023
72	B	0.36943	0.37224	0.37293	0.373011		
	S	0.3515	0.3722	0.3728	0.3731		
	A	0.30073	-0.03090	-0.02931	-0.03112	-0.031140	-0.031140
176	B	0.37447	-0.01288	-0.03073	-0.02993		
	S	-0.1507	-0.0374	-0.0323	-0.0314		

Note. The Schwinger variational phase-shifts S are taken from Table II of Ref. [5], denoted choice 1 there.

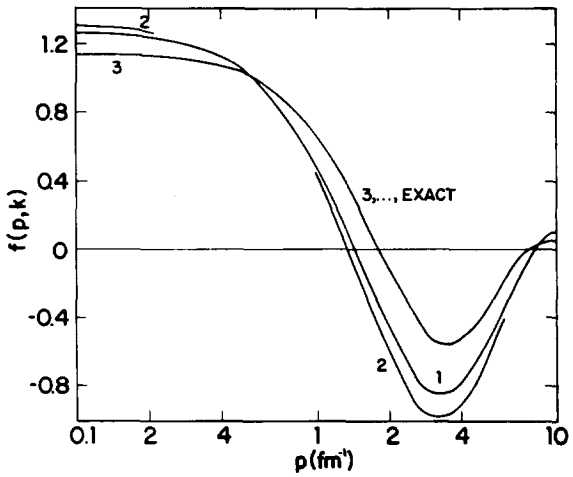

FIG. 1. Kowalski–Noyes half shell funcion $f(p, k)$ for different N for the Reid potential at $E_{c.m.} = 12$ MeV. The $N=3$ result is indistinguishable from the $N>3$ results.

TABLE III

Kowalski–Noyes Half-Shell Functions $f(p, k)$ for the Alternate Potential with Choice A Expansion Function for Various N at $E_{c.m.} = 48$ MeV.

	Results for $N=$				
p (fm^{-1})	1	4	6	10	$\geqslant 12$
0.5	$1.5872 + 10^{-1}i$	$1.34678 + 10^{-2}i$	$1.35216 + 10^{-3}i$	$1.350656 + 10^{-6}i$	$1.350652 + 10^{-7}i$
1.0	$1.0928 + 10^{-2}i$	$1.06418 + 10^{-3}i$	$1.06480 + 10^{-4}i$	$1.064598 - 10^{-7}i$	$1.064598 + 10^{-8}i$
1.5	$0.4699 - 10^{-1}i$	$0.56859 - 10^{-3}i$	$0.56648 - 10^{-4}i$	$0.567073 + 10^{-7}i$	$0.567071 + 10^{-7}i$
2.0	$-0.0354 - 10^{-1}i$	$0.04418 - 10^{-3}i$	$0.04204 + 10^{-4}i$	$0.042110 + 10^{-7}i$	$0.042110 + 10^{-7}i$
3.0	$-0.4365 - 10^{-1}i$	$-0.51694 + 10^{-3}i$	$-0.51718 - 10^{-4}i$	$-0.517571 + 10^{-7}i$	$-0.517571 + 10^{-7}i$
4.0	$-0.4102 - 10^{-1}i$	$-0.53945 + 10^{-3}i$	$-0.53825 - 10^{-3}i$	$-0.537611 - 10^{-7}i$	$-0.537609 + 10^{-7}i$
6.0	$-0.02045 - 10^{-1}i$	$-0.27233 + 10^{-3}i$	$-0.27065 - 10^{-4}i$	$-0.27068 + 10^{-7}i$	$-0.27069 + 10^{-7}i$
8.0	$-0.0914 - 10^{-1}i$	$-0.12186 + 10^{-3}i$	$-0.12067 + 10^{-4}i$	$-0.12090 - 10^{-7}i$	$-0.12098 + 10^{-7}i$
10.0	$-0.0414 - 10^{-1}i$	$-0.06206 + 10^{-4}i$	$-0.06083 + 10^{-4}i$	$-0.061037 - 10^{-7}i$	$-0.061031 + 10^{-7}i$

Note. Only the order of magnitude of the imaginary part has been shown. The method does not yield explicitly unitary results. The order of magnitude of the imaginary part of f is a good measure of unitary violation.

numerical difficulty with matrix inversion sets up before the result converges to desired accuracy.

In Table III we show the half-shell function for the alternate potential for the choice A functions at $E_{c.m.} = 48$ MeV for different N. At a given energy the half-shell function is defined by $f(p, k) = \langle p| t(E) |k\rangle / \langle k| t(E) |k\rangle$. This is to the best of our knowledge the first calculation of the half-shell function using the Kohn or the complex Kohn v.p.

From Tables I–III we find that both the phase shifts and the half-shell functions converge equally rapidly. The final convergence of the phase-shifts obtained with the complex Kohn v.p. is extremely good and is faster than that obtained with Schwinger v.p. or other degenerate kernel/separable expansion methods. The convergence obtained in the present study is much better than that obtained with the Schwinger v.p. denoted by S in Tables I and II. For $N = 14$ the $^1S_0$ Reid soft core (alternate potential) phase shifts of the Kohn v.p. with choice A expansion functions have converged to an estimated numerical accuracy of $< 0.005\%$ ($< 0.0005\%$).

In Fig. 1 we plot the half-shell function for the Reid potential for the choice A function at $E_{c.m.} = 12$ MeV for various N. It is realized that the half-shell function converges very rapidly.

The precision obtained with the present method is better than that obtained with any separable expansion [4, 5] or degenerate kernel methods [16] and is comparable to one of the best previous precision [17] obtained (for the Reid $^1S_0$ potential) with the use of the co-called iteration subtraction method.

In order to solve the LS equation the integral equation is basically transformed into a matrix equation which is then solved by matrix inversion, iteration, or otherwise. The infinite integral in momentum space of the LS equation, in other methods, is usually transformed into a discrete sum. In order to achieve a precision comparable to that of the present method one requires to take about 100 discrete mesh points. This procedure involves handling 100×100 matrices in momentum space [18]. The same precision is obtained in the present method via matrices of dimension 10–15.

Often claim has been made about the superiority of the Kohn v.p. over the Schwinger v.p. in atomic scattering problems [7, 10, 19]. In the present study we observe the superiority of the complex Kohn method over the Schwinger method in nuclear scattering problems. Usually, such a comparison is not to the point, because in these two methods different functions are expanded using a set of trial functions. In order to find a rapidly convergent expansion, the set of expansion funcions must be appropriately modified. From the observed superiority of the Kohn v.p. it seems that the choice of an optimal set of expansion functions in the Kohn or the complex Kohn method is under control, whereas the same in the Schwinger method is a more difficult task.

However, it is interesting to recall that in order to incorporate the correct outgoing wave boundary condition the expansion functions in the complex Kohn v.p. are not only energy dependent but include unnormalizable complex functions. The Schwinger v.p., on the other hand, employs only real normalizable functions. Hence it is not surprising that the larger degree of freedom associated with the choice of expansions functions of the Kohn method leads to rapid convergence.

5. SUMMARY

We have applied for the first time the complex Kohn v.p. for the solution of the LS equation for NN scattering with

two phenomenological potentials with soft core. We calculated both scattering phase shifts and Kowalski–Noyes half-shell functions. We find that the method leads to rapid convergence and high precision results. The rate of convergence obtained with the complex Kohn v.p. is superior to that obtained with the Schwinger v.p. Previously, the same conclusion was arrived at in atomic scattering problems. We realize that the higher flexibility in the choice of expansion functions in the Kohn method is responsible for the superior rate of convergence and high precision result obtained with this method.

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REFERENCES

1. J. Schwinger, Lecture notes, Harvard University, 1947, unpublished.
2. W. Kohn, *Phys. Rev.* **74**, 1763 (1948); L. Hulthén, *K. Fysiogr. Saéllsk., Lund Foér-n.* **14**, 257 (1944); *Ark. Mat. Astron. Fys.* **35A**, No. 25 (1948).
3. For reviews on variational principles, see J. Callaway, *Phys. Rev.* **45**, 89 (1978); M. A. Abdel-Rauof, *Phys. Rep.* **84**, 163 (1982); **108**, 1 (1984); R. R. Lucchese, K. Takatsuka, and V. McKoy, *Phys. Rep.* **131**, 147 (1986); E. Gerjuoy, A. R. P. Rau, and L. Spruch, *Rev. Mod. Phys.* **55**, 725 (1983); R. K. Nesbet, *Adv. At. Mol. Phys.* **13**, 315 (1979).
4. S. K. Adhikari and I. H. Sloan, *Phys. Rev. C* **11**, 1133 (1975); S. K. Adhikari and L. Tomio, *Phys. Rev. C* **36**, 1275 (1987).
5. S. K. Adhikari and K. L. Kowalski, *Dynamical Collision Theory and Its Applications* (Academic Press, Boston, 1991), Chapter 3.
6. I. H. Sloan and T. J. Brady, *Phys. Rev. C* **6**, 701 (1972).
7. K. Takatsuka, R. R. Lucchese, and V. McKoy, *Phys. Rev. A* **24**, 1812 (1981); K. Takatsuka and V. McKoy, *Phys. Rev. A* **23**, 2352 (1981).
8. B. A. Lippmann and J. Schwinger, *Phys. Rev.* **79**, 469 (1950).
9. C. Schwartz, *Phys. Rev.* **124**, 1468 (1961); R. K. Nesbet, *Variational Methods in Electron—Atom Scattering Theory* (Plenum, New York, 1980).
10. Y. Mito and M. Kamimura, *Prog. Theor. Phys.* **56**, 583 (1976); W. H. Miller and B. M. D. D. Jansen of de Haar, *J. Chem. Phys.* **86**, 6213 (1987); J. Z. H. Zhang, S.-I. Chu, and W. H. Miller, *J. Chem. Phys.* **88**, 6233 (1988); C. W. McCurdy, T. N. Rescigno, and B. I. Schneider, *Phys. Rev. A* **36**, 2061 (1987); B. I. Schneider and T. N. Rescigno, *Phys. Rev. A* **37**, 3749 (1988).
11. R. V. Reid, Jr., *Ann. Phys. (N.Y.)* **50**, 411 (1968); I. Afnan and J. M. Read, *Austr. J. Phys.* **26**, 449 (1973).
12. B. Apagyi, P. Lévay, and K. Ladányi, *Phys. Rev. A* **37**, 4577 (1988), C. Winstead and V. McKoy, *Phys. Rev. A.* **41**, 49 (1990).
13. S. K. Adhikari, *Phys. Rev. A* **42**, 6 (1990); *Chem. Phys. Lett.* **181**, 435 (1991).
14. R. R. Lucchese, *Phys. Rev. A* **40**, 6879 (1989); S. K. Adhikari, *Chem. Phys. Lett.* **189**, 340 (1992).
15. K. L. Kowalski, *Phys. Rev. Lett.* **15**, 798 (1965); **15**, 908 (E) (1965); H. P. Noyes, *Phys. Rev. Lett.* **15**, 538 (1965).
16. I. H. Sloan and S. K. Adhikari, *Nucl. Phys. A* **235**, 352 (1974); G. H. Rawitscher and G. Delic, *Phys. Rev. C* **29**, 747 (1984); G. H. Rawitscher, *Phys. Rev. C* **25**, 2196 (1982); S. K. Adhikari and I. H. Sloan, *Nucl. Phys.* **A241**, 429 (1975); K. Hartt and P. V. A. Yidana, *Phys. Rev. C* **36**, 475 (1987).
17. S. K. Adhikari and L. Tomio, *Phys. Rev. C* **33**, 467 (1986).
18. J. Horáček and T. Sasakawa, *Phys. Rev. C* **32**, 70 (1985).
19. G. Staszewska and D. G. Truhlar, *J. Chem. Phys.* **86**, 2793 (1987); J. Callaway, *Phys. Lett.* **77A**, 137 (1980).