Variational separable expansion scheme for two-body Coulomb-scattering problems

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We present a separable expansion approximation method for Coulomb-like potentials which is based on Schwinger variational principle and uses Coulomb-Sturmian functions as basis states. The new scheme provides faster convergence with respect to our formerly used nonvariational approach.

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Both variational approaches and separable expansion schemes are extensively used in solving few-body problems. Some time ago Adhikari and Tomio presented an unified treatment of separable expansion schemes based on Schwinger variational principles [1]. They proposed various approximation schemes for the transition operator t satisfying the Lippmann-Schwinger equation

$$t = v + v g^0 t, \tag{1}$$

where v is the potential and g^0 is the free Green's operator. It was found that using these schemes with appropriate choice of expansion functions a rapid convergence could be obtained. However, in this paper, not a single word was devoted to Coulomb-like potentials.

At about the same time in a series of papers [2] a separable expansion scheme for Coulomb-like potentials was proposed by one of us. The Coulomb interaction was kept in the Green's operator and only the short-range part of the potential was subject to the separable expansion. This approach uses Coulomb-Sturmian (CS) functions as basis, allowing an exact analytical calculation of the matrix elements of the Coulomb Green's operator (see [2] and, recently, [3]). Thereby only the short-range part of the interaction is approximated and the correct Coulomb asymptotic properties of all quantities are guaranteed. The method has also been applied in three-body Faddeev calculations for bound-state and low-energy scattering problems with Coulomb interactions [4].

In this paper we generalize one of the separable expansion schemes proposed by Adhikari and Tomio for two-body Coulomb-scattering problems.

The expansion schemes in Ref. [1] are based on a finite rank-N approximation of the product of operators

$$AB^{-1}C \approx \sum_{i,j}^{N} A|\eta_i\rangle D_{ij}\langle\zeta_j|C, \tag{2}$$

where

$$(D^{-1})_{ji} = \langle\zeta_j|B|\eta_i\rangle. \tag{3}$$

Here the sets $|\eta_i\rangle$ and $|\zeta_j\rangle$ are assumed to be complete sets of states in Hilbert space. If N tends to infinity, Eq. (2) becomes an identity.

From among the separable approximation schemes of Ref. [1] let us start with the form of t following from Eq. (1):

$$t = \mathbf{1}(v^{-1} - g_0)^{-1}\mathbf{1}. \tag{4}$$

Applying Eq. (2) we get

$$t \approx \sum_{i,j}^{N} |\eta_i\rangle D_{ij}\langle\eta_j|, \tag{5}$$

with

$$(D^{-1})_{ji} = \langle\eta_j|v^{-1}|\eta_i\rangle - \langle\eta_j|g_0|\eta_i\rangle. \tag{6}$$

The first term in Eq. (6) can again be approximated as before:

$$\langle\eta_j|v^{-1}|\eta_i\rangle = \langle\eta_j|\mathbf{1}v^{-1}\mathbf{1}|\eta_i\rangle \approx \sum_{i',j'}^{N} \langle\eta_j|\zeta_{j'}\rangle C_{j'i'}\langle\zeta_{i'}|\eta_i\rangle, \tag{7}$$

where

$$(C^{-1})_{i'j'} = \langle\zeta_{i'}|v|\zeta_{j'}\rangle. \tag{8}$$

As shown in Sec. III. of [1] this expansion scheme can be derived from the following variational form for the t:

$$\langle p|t|p'\rangle = \langle p|\xi_{p'}^{(+)}\rangle + \langle\xi_p^{(-)}|p'\rangle - \langle\xi_p^{(-)}|(v^{-1} - g_0)|\xi_{p'}^{(+)}\rangle, \tag{9}$$

where

$$|\xi_{p'}^{(+)}\rangle = v|p'\rangle + v g_0|\xi_{p'}^{(+)}\rangle, \tag{10}$$

$$\langle\xi_p^{(-)}| = \langle p|v + \langle\xi_p^{(-)}|g_0 v. \tag{11}$$

Equation (9) is a modified version of the original Schwinger variational form for the operator t and stationary with respect to first-order variations in $|\xi_{p'}^{(+)}\rangle$ and $\langle\xi_p^{(-)}|$ [5].

The scheme of Eqs. (5)–(8) can easily be generalized for Coulomb-like potentials. A Coulomb-like potential in some partial wave l can be written in the form

$$v_l = v^C + v_l^s, \tag{12}$$

where v^C is the pure Coulomb potential and v_l^s is short ranged. The Lippmann-Schwinger equation for the Coulomb-modified transition operator t^{sC} reads

$$t_l^{sC}=v_l^s+v_l^s g_l^C(E)t_l^{sC}, \tag{13}$$

where $g_l^C(E)=(E-h_l^0-v^C)^{-1}$ is the Coulomb Green's operator and h_l^0 is the free Hamiltonian. The solution of this equation can be given in a form analogous to Eq. (4),

$$t_l^{sC}=\mathbf{1}[(v_l^s)^{-1}-g_l^C(E)]^{-1}\mathbf{1}, \tag{14}$$

and the whole procedure of Eqs. (5)–(7) can be repeated. Only the free Green's operator has to be replaced by the Coulomb one.

As basis states we choose CS functions because they allow an exact analytical calculation of matrix elements of $g_l^C(E)$. In coordinate representation they have the form

$$\langle r|n;b\rangle=\left[\frac{n!}{(n+2l+1)!}\right]^{1/2}(2br)^{l+1}\exp(-br)L_n^{2l+1}(2br), \tag{15}$$

where $n=0,1,2,\ldots,$ L_n^{2l+1} are the Laguerre polynomials and b is a scaling parameter. They have an analogous simple form also in momentum representation:

$$\langle p|n;b\rangle=\frac{2^{l+3/2}l!(n+l+1)\sqrt{n!}}{\sqrt{\pi(n+2l+1)!}}\times\frac{b(2bp)^{l+1}}{(p^2+b^2)^{2l+2}}G_n^{l+1}\left(\frac{p^2-b^2}{p^2+b^2}\right), \tag{16}$$

where G denotes the Gegenbauer polynomials. Introducing the notation $\langle r|\widetilde{n;b}\rangle=\langle r|n;b\rangle/r$ we can express the orthogonality and completeness of the CS functions as

$$\langle n;b|\widetilde{n';b}\rangle=\delta_{nn'} \tag{17}$$

and

$$\mathbf{1}=\lim_{N\to\infty}\sum_{n=0}^{N}|\widetilde{n;b}\rangle\langle n;b|=\lim_{N\to\infty}\sum_{n=0}^{\infty}|n;b\rangle\langle\widetilde{n;b}|, \tag{18}$$

TABLE I. Convergence of the Coulomb-modified nuclear phase shift $\delta_0^{sC}(E)$ (in radians) in the potential of Eq. (26) at different energies with respect to the N number of basis states used in the separable expansion schemes, Eqs. (24) and (22).

N	$E=0.1$ MeV		$E=1$ MeV		$E=10$ MeV		$E=100$ MeV	
	Eq. (24)	Eq. (22)	Eq. (24)	Eq. (22)	Eq. (24)	Eq. (22)	Eq. (24)	Eq. (22)
2	-0.100682	-0.151364	-0.624200	-0.797903	1.546662	1.453638	0.163942	0.253576
3	-0.115923	-0.122391	-0.685037	-0.710521	1.506720	1.479076	0.365679	0.351795
4	-0.120857	-0.120468	-0.706248	-0.705228	1.480305	1.477592	0.430684	0.403522
5	-0.118844	-0.119136	-0.701335	-0.701377	1.473793	1.477278	0.415215	0.402637
6	-0.118655	-0.119182	-0.699997	-0.701573	1.481240	1.479584	0.411720	0.404552
7	-0.119150	-0.119165	-0.701393	-0.701565	1.483505	1.480309	0.408933	0.407128
8	-0.119166	-0.119165	-0.701534	-0.701549	1.481915	1.480743	0.408615	0.407224
9	-0.119147	-0.119164	-0.701390	-0.701523	1.481590	1.480921	0.409217	0.407345
10	-0.119155	-0.119164	-0.701439	-0.701519	1.481230	1.480945	0.408458	0.407467
11	-0.119157	-0.119162	-0.701462	-0.701508	1.481028	1.480958	0.407939	0.407487
12	-0.119158	-0.119162	-0.701472	-0.701507	1.480981	1.480957	0.407830	0.407488
13	-0.119160	-0.119162	-0.701490	-0.701505	1.480959	1.480957	0.407694	0.407497
14	-0.119160	-0.119162	-0.701492	-0.701504	1.480958	1.480957	0.407585	0.407499
15	-0.119161	-0.119162	-0.701498	-0.701504	1.480959	1.480957	0.407557	0.407499
16	-0.119161	-0.119162	-0.701499	-0.701504	1.480959	1.480957	0.407535	0.407499
17	-0.119161	-0.119162	-0.701501	-0.701504	1.480959	1.480957	0.407511	0.407499
18	-0.119161	-0.119162	-0.701502	-0.701504	1.480959	1.480957	0.407506	0.407499
19	-0.119161	-0.119162	-0.701502	-0.701504	1.480958	1.480957	0.407506	0.407499
20	-0.119162	-0.119162	-0.701503	-0.701504	1.480957	1.480957	0.407500	0.407499
21	-0.119162	-0.119162	-0.701503	-0.701504	1.480957	1.480957	0.407499	0.407499
22	-0.119162	-0.119162	-0.701503	-0.701504	1.480957	1.480957	0.407501	0.407499
23	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499
24	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499
25	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499
26	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499
27	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499
28	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499
29	-0.119162	-0.119162	-0.701504	-0.701504	1.480957	1.480957	0.407499	0.407499

respectively.

As $|\eta_i\rangle$ and $|\zeta_j\rangle$ we take CS bases with different b parameters:

$$t_l^{sC} \approx \sum_{n,n'=0}^{N} |\widetilde{n;b_1}\rangle D_{nn'} \langle\widetilde{n';b_1}|, \tag{19}$$

$$(D^{-1})_{n'n} = \sum_{m,m'=0}^{N} \langle n';b_1|\widetilde{m;b_2}\rangle C_{mm'} \langle\widetilde{m';b_2}|n;b_1\rangle - \langle n';b_1|g_l^C|n;b_1\rangle, \tag{20}$$

$$(C^{-1})_{m'm} = \langle m';b_2|v_l^s|m;b_2\rangle. \tag{21}$$

While the matrix elements of the potential and the overlap of CS functions should be calculated numerically either in configuration or momentum space the matrix elements of the Coulomb Green's operator can be calculated analytically [2,3].

This scheme is essentially equivalent with a twofold separable expansion for potential v_l^s:

$$v_l^s \approx \sum_{n,n',m,m'=0}^{N} |\widetilde{n;b_1}\rangle (\langle n;b_1|\widetilde{m';b_2}\rangle)^{-1} \langle m';b_2|v_l^s|m;b_2\rangle \times (\langle\widetilde{m;b_2}|n';b_1\rangle)^{-1} \langle\widetilde{n';b_1}|. \tag{22}$$

It is easy to verify that Eqs. (19)–(21) are the solutions of the Lippmann-Schwinger equation (13), with this approximate potential.

This scheme should be compared with the CS potential separable expansion scheme of Refs. [2,3] which is not supported by variational principle. It is based on the approximation of the unit operator

$$\mathbf{1} = \lim_{N\to\infty} \sum_{n=0}^{N} |\tilde{n}\rangle \sigma_n^N \langle n|, \tag{23}$$

with σ factors possessing the properties $\lim_{n\to\infty} \sigma_n^N = 0$ and $\lim_{N\to\infty} \sigma_n^N = 1$. Now, the approximation takes the form

$$v_l^s = \mathbf{1} v_l^s \mathbf{1} \approx \sum_{n,n'=0}^{N} |\tilde{n}\rangle \sigma_n^N \langle n|v_{sl}|n'\rangle \sigma_{n'}^N \langle\tilde{n'}|. \tag{24}$$

For σ_n^N the form

$$\sigma_n^N = \frac{1-\exp\{-[\alpha(n-N-1)/(N+1)]^2\}}{1-\exp(-\alpha^2)} \tag{25}$$

was used with $\alpha \sim 5$. This value of the arbitrary parameter α yielded the fastest convergence.

To show the relative power of these separable expansion schemes we have calculated the Coulomb-modified nuclear phase shifts δ_l^{sC} at $l=0$ and at various energies for a $p-p$ scattering. The short-range potential was taken in Malfliet-Tjon form

$$v_l^s = v_0 \exp(-\beta_0 r)/r + v_1 \exp(-\beta_1 r)/r, \tag{26}$$

with $v_0 = -626.885$ MeV, $\beta_0 = 1.55$ fm, $v_1 = 1438.720$ MeV, and $\beta_1 = 3.11$ fm. In the method of Eq. (24), the CS basis parameter $b = 3$ fm^{-1} was used, while in the expansion, Eq. (22), $b_1 = 3.8$ fm^{-1} and $b_2 = 2.5$ fm^{-1} were taken. It can be seen in Table I that in both approximation schemes it is possible to choose the b parameters so that the expansions give almost equally fast convergence over the whole spectrum and provide extremely accurate results. To reach six-digit accuracy the method of Eq. (22) needs 10–13 basis states, while the method of Eq. (24) needs 20–23 states. We have observed similar results over a wide range of b parameters. It should be noted, however, that the method of Eq. (22) is more complicated numerically, so the numerical effectivity of both methods are more or less the same.

In this Brief Report we have combined two separable expansion methods. One based on Schwinger variational principle has been proposed by Adhikari and Tomio in Ref. [1]. The other approach proposed by Papp in Refs. [2] is not variational and it was designed for Coulomb-like potentials. This new scheme is a variational separable expansion method and is applicable for Coulomb-like potentials. It converges considerably faster in terms of basis states than the nonvariational method of Eq. (24). This property could be useful in three-body calculations where the rank of the expansion is of crucial importance. The method of Eq. (24) has been generalized for solving Faddeev-type integral equations of three-body Coulombic systems. Whether or not the method of Eq. (22) can be extended in this direction is still an open question.

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