Use of Coulomb-Sturmian functions in calculating scattering quantities in Coulomb-like potentials

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An approximate solution to a scattering problem containing Coulomb and short-range potentials is presented. The method is based on a separable expansion of the short-range part of the interaction in terms of bound-state Coulomb-Sturmian functions. Similarly to the approximation based on the expansion of the scattering wave function on a scattering-state Coulomb-Sturmian basis, the method yields asymptotically correct wave functions. The convergence, however, is much faster in the potential separable-expansion method.

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Recently Shakeshaft [1] presented a method for calculating scattering quantities in a Coulomb plus short-range potential. The regular solution of the Schrödinger equation and the Coulomb-Green function at a given energy have been expanded in terms of scattering Coulomb-Sturmian (CS) functions belonging to the same energy. This choice of the CS functions ensures that, when the phase shift is sufficiently well approximated, the solution possesses the correct Coulomb-like asymptotic behavior. In the case of a Coulomb plus Yukawa–type potential an agreement up to two or three significant figures with the exact value was reached by the aid of a [12, 12] Padé approximation. To generate an $[N, N]$ Padé approximation roughly $2N$ terms in the wave-function expansion on CS basis are needed.

In the potential separable-expansion method, the bound-state CS functions have been used for solving single-channel bound-, resonant- [2, 3], and scattering-state [4, 5] problems. In this method the potential is expanded in a separable way, thus the solution of the Schrödinger equation falls back to the solution of a system of algebraic equations. In this Brief Report we show that if only the short-range potential is expanded the asymptotics will always be correct even if one uses bound-state CS functions, provided convergence in phase shift is reached. So, the potential separable-expansion method based on bound-state CS functions shares the most important advantage of the wave-function expansion method based on scattering-state CS functions.

First we sketch the potential separable-expansion method as it is applied in single-channel scattering-state calculations. A Coulomb-like potential V_l can be written in the form

$$V_l = V^C + V_l^s, \tag{1}$$

where V^C is the Coulomb potential and V_l^s is a short-range potential. The physical scattering wave function $\psi_l^{(+)}(k,r)$ corresponding to the regular physical Coulomb function $\psi_l^{(C)(+)}(k,r)$ satisfies the inhomogeneous Lippmann-Schwinger equation [6]

$$|\psi_l^{(+)}(k)\rangle = |\psi_l^{(C)(+)}(k)\rangle + G_l^{(C)(+)}(k)V_l^s|\psi_l^{(+)}(k)\rangle, \tag{2}$$

where $k = \sqrt{2mE/\hbar^2}$, m is the reduced mass, and $G_l^{(C)(+)}$ is the radial Coulomb-Green operator; the branch cut was taken along the positive E axis and k is positive when E is on the upper rim of the cut.

For the expansion of the short-range potential we choose the bound-state CS functions, the Sturm-Liouville solutions to the hydrogen problem at negative energy. In coordinate representation they are of the following form:

$$\langle r|nl;b\rangle = \left[\frac{n!}{(n+2l+1)!}\right]^{1/2} \times (2br)^{l+1}\exp(-br)L_n^{2l+1}(2br), \tag{3}$$

where n is the radial quantum number, L is the Laguerre polynomial, and b is a parameter, which is related to the energy in the Sturm-Liouville problem. The functions $\langle r|nl;b\rangle$ are orthogonal and form a complete set with respect to the weight function $\langle r|\Delta|r'\rangle = \delta(r-r')/r$. Introducing the notation $\langle r|\Delta nl;b\rangle = \langle r|nl;b\rangle/r$ we can write the unity operator $\mathbb{1}_l$ as

$$\mathbb{1}_l = \lim_{N\to\infty}\sum_{n=0}^{N}|\Delta nl;b\rangle\sigma_n^N\langle b;nl| = \lim_{N\to\infty}\sum_{n=0}^{N}|nl;b\rangle\sigma_n^N\langle b;nl\Delta|. \tag{4}$$

The σ factors, which have the property $\lim_{N\to\infty}\sigma_n^N = 1$, were introduced to suppress the Gibbs oscillations [7]. The choice of σ_n^N,

$$\sigma_i^N = \frac{1-\exp\{-[\alpha(n-N-1)/(N+1)]^2\}}{1-\exp(-\alpha^2)}, \tag{5}$$

has proved to be very successful in practical applications.

Let us write the short-range potential V_l^s as $V_l^s = \mathbb{1}_l V_l^s \mathbb{1}_l$ and then approximate the unity operator $\mathbb{1}_l$ by keeping N finite in (4). In this way the short-range potential V_l^s is approximated by a finite-rank separable potential,

$$V_l^s \approx \sum_{n,n'=0}^{N}|\Delta nl;b\rangle\sigma_n^N\langle b;nl|V_l^s|n'l;b\rangle\sigma_{n'}^N\langle b;n'l\Delta|, \tag{6}$$

and Eq. (2) appears as

$$|\psi_l^{(+)}(k)\rangle = |\psi_l^{(C)(+)}(k)\rangle + \sum_{n,n'=0}^{N} G_l^{(C)(+)}(k)|\Delta nl;b\rangle\ \sigma_n^N \langle b;nl|V_l^s|n'l;b\rangle \sigma_{n'}^N\ \langle b;n'l\Delta|\psi_l^{(+)}(k)\rangle. \quad (7)$$

Multiplying (7) by $\langle b;il\Delta|$ we get a set of algebraic equation for the overlap $(\underline{C})_n = \langle b;nl\Delta|\psi_l^{(+)}(k)\rangle$,

$$(\underline{1} - \underline{G}_l^{(C)(+)}\underline{V}_l^{s\sigma})\underline{C} = \underline{C}^{(C)}, \quad (8)$$

where $(\underline{G}_l^{(C)(+)})_{nn'} = \langle b;nl\Delta|G_l^{(C)(+)}(k)|\Delta n'l;b\rangle$ and $(\underline{V}_l^{s\sigma})_{nn'} = \sigma_n^N\langle b;nl|V_l^s|n'l;b\rangle\sigma_{n'}^N$ are the Green and potential matrices, respectively, and $(\underline{C}^{(C)})_n = \langle b;nl\Delta|\psi_l^{(C)(+)}(k)\rangle$. The wave function $\psi_l^{(+)}(k,r)$ derives as

$$\psi_l^{(+)}(k,r) = \psi_l^{(C)(+)}(k,r) + \sum_{n=0}^{N}(\underline{B})_n\mathcal{G}_{ln}^{(C)}(k,r), \quad (9)$$

where $\underline{B} = \underline{V}_l^{s\sigma}\underline{C}$ and $\mathcal{G}_{ln}^{(C)}(k,r) = \langle r|G_l^{(C)(+)}(k)|\Delta nl;b\rangle$.

The difference $\psi_l^{(+)}(k,r) - \psi_l^{(C)(+)}(k,r)$ should be regular at the origin and should tend to infinity as the Coulomb-Jost solution $f_l^{(C)(+)}(k,r)$, which is the solution to the Coulomb-Schrödinger equation with the boundary condition

$$\lim_{r\to\infty} f_l^{(C)(+)}(k,r)\ \mathrm{e}^{-i(kr-\gamma\ln 2kr)} = 1, \quad (10)$$

where $\gamma = Z_{12}e^2m/\hbar^2k$ is the Coulomb parameter. The Coulomb-Green function $G_l^{(C)(+)}(k,r,r')$ can be constructed from the functions $\psi_l^{(C)(+)}(k,r)$ and $f_l^{(C)(+)}(k,r)$ as

$$G_l^{(C)(+)}(k,r,r') = -\frac{e^{-1/2\pi l}}{k}\psi_l^{(C)(+)}(k,r_<)f_l^{(C)(+)}(k,r_>), \quad (11)$$

where $r_< = \min(r,r')$ and $r_> = \max(r,r')$ [6]. We can see now that the function $\mathcal{G}_{ln}^{(C)}(k,r)$, which is proportional to the integral

$$\int_0^\infty dr'\ \psi_l^{(C)(+)}(k,r_<)f_l^{(C)(+)}(k,r_>)\langle r'|\Delta nl\rangle, \quad (12)$$

behaves in the $r\to 0$ limit like $\psi_l^{(C)(+)}(k,r)$ and in the $r\to\infty$ limit like $f_l^{(C)(+)}(k,r)$. So, in the potential separable-expansion method the difference $\psi_l^{(+)}(k,r) - \psi_l^{(C)(+)}(k,r)$, which is a linear combination of the functions $\mathcal{G}_{ln}^{(C)}(k,r)$, possesses the correct Coulomb-like asymptotic behavior. This result is independent of the basis. The asymptotics is determined only by the Coulomb-Green function.

The advantage of using bound-state CS functions comes up in the calculation of the quantities $\langle b;nl\Delta|G_l^{(C)(+)}(k)|\Delta n'l;b\rangle$, $\langle b;nl\Delta|\psi_l^{(C)(+)}(k)\rangle$, and $\langle r|G_l^{(C)(+)}(k)|\Delta nl;b\rangle$. They can be calculated analytically or quasianalytically [2–5]. The short-range potential enters into the method via its CS matrix elements. The method thus becomes rather general: one has to calculate only the CS matrix elements of the short-range potential, which can be done, at least numerically, for all physically reasonable potentials no matter whether they are local, nonlocal, complex, etc., and then the rest is exact and quasianalytic.

This method is not variational. Convergence on a basis of reasonable size cannot be easily reached without the σ factors, which damp the rather large oscillations of the phase shift. We have experienced that the optimal α value in (5) is $\alpha \approx 6$ regardless of the potential and the state. The parameter b of the CS functions should be of the same order of magnitude as the characteristic range of the potential to be expanded. The rate of convergence is, however, nearly insensitive to the choice of b within a rather broad interval.

To demonstrate the power of the potential separable-expansion method based on bound-state CS functions in comparison with the method of [1] we calculate the

TABLE I. Convergence of the non-Coulombic $l = 0$ and $l = 1$ phase shifts for the potential $V_l = -2/r + 4\exp(-2r)/r$ with $k = 0.5$ as the function of the maximal radial quantum number N.

N	$\delta_0(k)$	$\delta_1(k)$
0	-1.509004	-0.5115865
1	1.185569	-0.7100061
2	1.352081	-0.6297025
3	1.353765	-0.5592434
4	1.331342	-0.5632251
5	1.348846	-0.5658368
6	1.359452	-0.5603505
7	1.361686	-0.5573900
8	1.362847	-0.5564093
9	1.363527	-0.5558843
10	1.363828	-0.5556103
11	1.364000	-0.5554950
12	1.364108	-0.5554414
13	1.364165	-0.5554106
14	1.364191	-0.5553928
15	1.364203	-0.5553834
16	1.364209	-0.5553787
17	1.364212	-0.5553760
18	1.364213	-0.5553745
19	1.364214	-0.5553736
20	1.364215	-0.5553731
21	1.364215	-0.5553728
22	1.364216	-0.5553727
23	1.364216	-0.5553726
24	1.364216	-0.5553724
Exact	1.364	-0.5554

same physical example: the $l = 0$ and 1 non-Coulombic phase shifts δ for the Coulomb-like potential $V_l = -2/r + 4\exp(-2r)/r$ at $k = 0.5$. The calculations were performed with the computer code of Ref. [5]. The parameter b was chosen as $b = 4$, which is about the optimum in this case. The results are shown in Table I. The convergence is considerably faster than in [1] and much higher accuracy has been achieved with the same number of basis functions; the best values in [1] are $\delta_0(k) = 1.35$ and $\delta_1(k) = -0.555$. Reference [1] gives the exact values up to four significant figures as $\delta_0(k) = 1.364$ and $\delta_1(k) = -0.5554$. The quasimonotonic nature of the convergence exhibited in Table I shows the power of the damping factor (5).

We can conclude by saying that the potential separable-expansion method based on the bound-state CS functions, similarly to the wave-function expansion method based on the scattering-state CS functions, preserves the correct Coulomb-like asymptotic behavior of the solution. From the numerical point of view it seems to be more advantageous. The codes of Refs. [3] and [5] are tailored for accurate and fast computations. The generalization of the method for multichannel problems with nonorthogonal channels is under way [8].

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