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Simple Contour Method for the Tail Correction in Long-Range Potentials

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The simple contour method used for the evaluation of integrals involving products of inverse powers of r and oscillatory wave functions in short-range potentials is extended to treat oscillatory wave functions in long-range potentials. Merits of various methods are assessed.

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I. INTRODUCTION

In the calculation of collision processes, integrals involving products of oscillatory wave functions and inverse powers of r have contributions from the inner region $0 \leq r \leq R$ and from the outer region $r \geq R$, where R is sufficiently large compared to the size of the collision region. The inner part is called the primary integral, and the outer part the tail correction. In general, the tail correction is significant but small compared with the primary integral. However for certain cases, e.g., integrals with wave functions of large angular momentum or of small *energy*, the tail correction is of the *same* order of magnitude as the primary integral such that the total sum of the integral may be far smaller than the primary integral because of a large cancellation between the primary integral and the tail correction.

A few numerical techniques have been developed for the evaluation of the tail correction. In the earlier attempt, Belling [1] calculated the tail correction as solutions to differential equations. More recently, Sil *et al.* [2] applied a complex contour integration method to convert the tail correction into an integral converging exponentially along a specific numerical path. In a previous paper [3], we considered specifically integrals with wave

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functions in short-range potentials and expanded the oscillatory wave functions in terms of spherical Bessel functions such that a simple contour is possible in the complex integration method. On the other hand, the phase amplitude method by Sil *et al.* [2] can also be improved upon by extending the phase-amplitude form to higher orders.

In this paper, we will extend the simple contour method to treat oscillatory wave functions in long-range potentials. Merits of various methods will be assessed. In Sec. II, we will discuss the simple contour method. The high-order phase amplitude method is reviewed in Sec. III. Results and discussion are given in Sec. IV.

II. THE SIMPLE CONTOUR METHOD

We shall extend the simple contour method developed previously [3] to treat the tail correction with oscillatory wave functions obtained in a long-range potential, which reduces to a Coulomb potential $V(r) = -Z/r$ beyond a characteristic range a_0. The oscillatory wave function in the region $R > a_0$ can be expanded in terms of the regular and irregular Coulomb functions F_l and G_l as

$$u_l(kr) = G_l(kr)\sin\varphi + F_l(kr)\cos\varphi\,, \tag{1}$$

where φ is the short-range phase shift. The tail correction can therefore be written as

$$\begin{aligned}\int_R^\infty \frac{u_{l'}(k'r)u_l(kr)}{r^n}dr &= \cos\varphi'\cos\varphi\int_R^\infty \frac{1}{r^n}F_{l'}(k'r)F_l(kr)dr \\ &\quad + \sin\varphi'\sin\varphi\int_R^\infty \frac{1}{r^n}G_{l'}(k'r)G_l(kr)dr \\ &\quad + \sin\varphi'\cos\varphi\int_R^\infty \frac{1}{r^n}G_{l'}(k'r)F_l(kr)dr \\ &\quad + \cos\varphi'\sin\varphi\int_R^\infty \frac{1}{r^n}F_{l'}(k'r)G_l(kr)dr\,,\end{aligned} \tag{2}$$

where $n \geq 1$, and we choose $k' \geq k$. To evaluate integrals in (2), we first define two complex integrals

$$M_{l'l} = \frac{1}{2}\int_R^\infty \frac{1}{r^n}H_{l'}^{(+)}(k'r)H_l^{(-)}(kr)dr\,, \tag{3}$$

$$N_{l'l} = \frac{1}{2}\int_R^\infty \frac{1}{r^n}H_{l'}^{(+)}(k'r)H_l^{(+)}(kr)dr\,, \tag{4}$$

where

$$H_l^{(\pm)}(x) = G_l(x) \pm iF_l(x)\,. \tag{5}$$

In terms of $M_{l'l}$ and $N_{l'l}$, we can rewrite the integrals in (2) as

$$\int_R^\infty \frac{1}{r^n} F_{l'}(k'r)F_l(kr)dr = \mathrm{Re}(M_{l'l} - N_{l'l}), \tag{6}$$

$$\int_R^\infty \frac{1}{r^n} G_{l'}(k'r)G_l(kr)dr = \mathrm{Re}(M_{l'l} + N_{l'l}), \tag{7}$$

$$\int_R^\infty \frac{1}{r^n} G_{l'}(k'r)F_l(kr)dr = -\mathrm{Im}(M_{l'l} - N_{l'l}), \tag{8}$$

$$\int_R^\infty \frac{1}{r^n} F_{l'}(k'r)G_l(kr)dr = \mathrm{Im}(M_{l'l} + N_{l'l}). \tag{9}$$

The complex integrals $M_{l'l}$ and $N_{l'l}$ have the general form

$$I = \int_R^\infty f(r)e^{iKr}dr. \tag{10}$$

By the complex contour integration, we can convert (10) into a complex integral converging exponentially

$$I = \left(\frac{i}{K}\right)e^{iKR}\int_0^\infty f(R + it/K)e^{-t}dt, \tag{11}$$

which can be evaluated easily. For Coulomb wave functions with complex arguments, we use a computer program by Thompson and Barnett[4].

There is a large cancellation between $M_{l'l}$ and $N_{l'l}$ when $kR < y + \sqrt{y^2 + l(l+1)}$ or $k'R < y' + \sqrt{y'^2 + l'(l'+1)}$, where $y = -Z/k$ and $y' = -Z'/k'$. In this case, we write (G)-(9) in the alternative forms:

$$\int_R^\infty \frac{1}{r^n} F_{l'}(k'r)F_l(kr)dr = \mathrm{Re}(K_{l'l}), \tag{12}$$

$$\int_R^\infty \frac{1}{r^n} G_{l'}(k'r)G_l(kr)dr = \mathrm{Re}(L_{l'l}), \tag{13}$$

$$\int_R^\infty \frac{1}{r^n} G_{l'}(k'r)F_l(kr)dr = -\mathrm{Im}(K_{l'l}), \tag{14}$$

$$\int_R^\infty \frac{1}{r^n} F_{l'}(k'r)G_l(kr)dr = \mathrm{Im}(L_{l'l}), \tag{15}$$

where

$$K_{l'l} = -i\int_R^\infty \frac{1}{r^n} H_{l'}^{(+)}(k'r)F_l(kr)dr, \tag{16}$$

$$L_{l'l} = \int_R^\infty \frac{1}{r^n} H_{l'}^{(+)}(k'r)G_l(kr)dr. \tag{17}$$

The evaluation of (16) and (17) is similar to that of (3) and (4) with $F_l(kr)$ and $G_l(kr)$ playing the roles of $H_l^{(-)}(kr)$ and $H_l^{(+)}(kr)$, respectively.

III. THE HIGH-ORDER PHASE AMPLITUDE METHOD

This approach has been given in a previous paper [3] for short-range potentials and follows basically that of Sil *el* al. [2], except that the phase and amplitude are calculated to high orders by a power series expansion. The oscillatory wave functions are taken to be solutions to the differential equation

$$\left\{\frac{d^2}{dx^2} + w(x)\right\}F(x) = 0, \tag{18}$$

where $x = kr$, and

$$w(x) = 1 - \frac{2y}{x} - \frac{l(l+1)}{x^2}. \tag{19}$$

Here $y =$ -Z/k, and Z and k are the corresponding nuclear charge and particle momentum, respectively. The solution for $w(x) > 0$ is assumed to be in the phase amplitude form [5]

$$F(x) = \frac{1}{\sqrt{A(x)}} e^{i\phi(x)}, \tag{20}$$

where

$$\phi = \int^x A(x')dx'. \tag{21}$$

The amplitude A satisfies the following equation,

$$A^2 = w + A^{1/2}\frac{d^2}{dx^2}(A^{-1/2}), \tag{22}$$

and an iterative evaluation of A is carried out to high orders in power series by

$$A_{j+1}^2 = w + A_j^{1/2}\frac{d^2}{dx^2}(A_j^{-1/2}) \tag{23}$$

We choose

$$A_0 = 1 - \frac{y}{x} - \frac{l(l+1) + y^2}{2x^2}, \tag{24}$$

and for A_j we retain the power series calculated from (23) to order x^{-2j-2} such that A_j has the form

$$A_j = \sum_{n=0}^{2(j+1)} C_n x^{-n}. \tag{25}$$

where $C_0 = 1$, $C_1 = -y, C_2 = -\frac{l(l+1)+y^2}{2}$, etc. The rest of the procedure follows that of Sil et al. We note that because of the requirement $w(x) > 0$, the phase amplitude method in general is not applicable for $kR < y + \sqrt{y^2 + l(l+1)}$ [5].

IV. RESULTS AND DISCUSSION

We have used the simple contour method and the phase amplitude method to evaluate integrals in (2) for various combinations of Z, R, n, l', l, and (k ' , k). For sufficiently large kR, both methods yield results which agree with each other. As kR decreases, the phase amplitude method begins to have convergence difficulties. When $kR < y + \sqrt{y^2 + l(l+1)}$, the phase amplitude method is no longer applicable. The simple contour method, on the other hand, is valid for the entire range of kR.

As demonstrations, we list in Table I the tail correction results for the integral (6) from the phase amplitude and simple contour methods for $l' = l$ and various pairs of (k ' , k) in the long-range potential with an attractive Coulomb tail $V(r) = -1/r$. We can see that, for $(k', k) = (1, 0.22)$, there is a convergence difficulty with the phase amplitude method when k is small. However for other cases, the ninth-order phase amplitude results represent significant improvements over the zeroth-order results. Similarly, in Table II, we present results for the long-range potential with a repulsive Coulomb tail $V(r)$ = l/r, which is appropriate, e.g., for the positron-atom collision. Here we note the few cases where the phase amplitude method is not applicable for $kR < y + \sqrt{y^2 + l(l+1)}$, and k is the smaller of k and k ' by definition.

To test the accuracy of the simple contour method, we investigate its consistency. We consider the integral

$$\int_{R_0}^{R} \frac{1}{r^n} f_{l'}(k'r) g_l(kr) dr = \int_{R_0}^{\infty} \frac{1}{r^n} f_{l'}(k'r) g_l(kr) dr - \int_{R}^{\infty} \frac{1}{r^n} f_{l'}(k'r) g_l(kr) dr, \qquad (26)$$

where $R > R_0$, and f_l and g_l may each be F_l or G_l. The left-hand side of (26) may be evaluated precisely by numerical integration, while the right-hand side is the difference between two separate tail correction results. We have compared the results for various combinations of Z, R, n, l', l, and (k', k), and the agreements are excellent.

In conclusion! we mention that the simple contour method for the evaluation of the tail correction may be applied to oscillatory wave functions in any potentials and for all kR. The high-order phase amplitude method on the other hand can also be used with the provision that $kR > y + \sqrt{y^2 + l(l+1)}$. For $Z = 0$, or $y = 0$, the present methods reduce to those for wave functions in short-range potentials reported previously [3]. We note, however, that Table I in Ref. [3] should be for $(2/\pi)(k'k)^{1/2} T_l$ instead of T_l defined in Eq. (3-L) of Ref. [3].

TABLE I. Numerical results of the tail correction given in (G) for $n = 1$, $l' = l$, and $R = 50$ in the long-range potential with a Coulomb tail $V(r)$ = -l/r, i.e., for $Z = 1$. Numbers in parentheses indicate powers of ten: $x(y) = x \cdot 10^y$. The phase amplitude method is not applicable for $kR < y + \sqrt{y^2 + l(l+1)}$.

			Phase amplitude method		Simple contour
k'	k	l	Zeroth-order	Ninth-order	method
1	0.22	0	−2.82701101(−03)	−3.85156673(−03)	−3.85121976(−03)
		2	−2.35365169(-02)	−2.38774222(-02)	−2.38781524(−02)
		4	−1.48661289(−02)	−9.01008237(-03)	−8.99726594(−03)
		6	−7.01722293(−03)	2.55433674(-03)	2.77859389(−03)
		S	−1.34750907(−02)	−7.54920475(−04)	3.85238214(−05)
		10	−2.79687237(−02)	5.30746582(-03)	−1.76261591(−02)
1	0.25	0	3.05165198(−03)	2.50025421(-03)	2.50025138(−03)
		2	−1.24985119(−02)	−1.45981039(-02)	−1.45980967(−02)
		4	−2.43913948(-02)	−2.40555150(−02)	−2.40555116(−02)
		6	−2.26988575(−02)	−1.98173582(−02)	−1.98130957(−02)
		S	−2.49512769(-02)	−2.20325912(−02)	−2.19972035(−02)
		10	−2.37802815(−02)	−2.71204248(−03)	−2.74002105(−03)
1	0.5	0	4.09893737(−04)	4.38927317(-04)	4.38927317(−04)
		2	1.19690060(−02)	1.20988990(-02)	1.20988990(-02)
		4	2.07595728(-02)	2.09298423(−02)	2.09298423(-02)
		6	2.19969550(-02)	2.21745840(−02)	2.21745840(−02)
		S	2.19131715(−02)	2.22247808(-02)	2.22247808(-02)
		10	1.98743492(-02)	2.05822365(-02)	2.05822365(-02)
1	0.9	0	5.82058202(-02)	5.82070313(−02)	5.82070314(−02)
		2	6.56280994(-02)	6.56375348(-02)	6.56375349(−02)
		4	6.66719640(−02)	6.66847587(−02)	6.66847587(−02 j
		6	6.64472205(-02)	6.64614692(−02)	6.64614693(−02)
		S	6.66143488(−02)	6.66372677(−02)	6.66372678(−02)
		10	6.69362575(-02)	6.69851641(−02)	6.69851641(−02)
10	4	0	3.26607731(−05)	3.26606178(-05)	3.26606178(−05)
		2	5.85881906(−05)	5.85891572(-05)	5.85891572(−05)
		4	6.91663912(-05)	6.91699347(−05)	6.91699347(−05)
		6	7.28840151(−05)	7.28910961(−05)	7.28910961(−05)
		8	7.20384709(−05)	7.20493086(-05)	7.20493086(-05)
		10	6.77499160(-0.5)	6.77637243(−05)	6.77637243(−05)

TABLE II. Numerical results of the tail correction given in (6) for $n = 1$, $l' = l$, and $R = 50$ in the long-range potential with a Coulomb tail $V(r) = 1/r$, i.e., for $Z = -1$. Numbers in parentheses indicate powers of ten: $x(y) = x \cdot 10^y$. The phase amplitude method is not applicable for $kR < y + \sqrt{y^2 + l(l+1)}$.

			Phase amplitude method		Simple contour
k'	k	l	Zeroth-order	Ninth-order	method
1	0.22	0	1.50470386(-02)	1.73918099(−02)	1.73920190(−02)
		2	2.30924902(-02)	2.82825743(-02)	2.82765052(-02)
		4	6.29888261(−04)	−2.64756990(−02)	−2.63852040(−02)
		6	a	a	1.03279033(-02)
		8	a	a	−1.24635266(-03)
		10	a	a	−4.20800575(-04)
1	0.25	0	1.27526869(-02)	1.11103656(−02)	1.11103628(−02)
		2	2.06574117(−02)	1.73946029(-02)	1.73946020(-02)
		4	−3.66737587(−02)	−3.76903580(−02)	−3.76896606(-02)
		6	7.41450520(-03)	2.57653706(-02)	2.58099004(-02)
		8	a	a	−5.24227916(-03)
		10	a	a	−2.00471295(-03)
1	0.5	0	−1.25136668(-02)	−1.25322891(−02)	−1.25322891(−02)
		2	−1.63550646(−02)	−1.64315118(−02)	−1.64315118(−02)
		4	−2.35900539(-02)	−2.34039187(−02)	−2.34039187(-02)
		6	−8.27154149(-03)	−7.36716740(-03)	−7.36716740(-03)
		8	4.18217375(−03)	5.14248797(−03)	5.14248797(−03)
		10	3.67061834(-03)	4.67790218(-03)	4.67790219(−03)
1	0.9	0	5.67935902(-02)	5.67935588(-02)	5.67935588(-02)
		2	5.80532081(-02)	5.80591174(−02)	5.80591174(−02)
		4	6.44957372(-02)	6.45052386(-02)	6.45052386(-02)
		6	6.52370994(-02)	6.52020650(-02)	6.52020650(−02)
		8	6.20446124(-02)	6.19407666(-02)	6.19407666(−02)
		10	6.01841726(−02)	6.01181445(−02)	6.01181444(-02)
10	4	0	1.22125370(-04)	1.22125084(−04)	1.22125084(-04)
		2	1.82739826(-04)	1.82741010(−04)	1.82741010(−04)
		4	2.04716744(−04)	2.04720530(-04)	2.04720530(−04)
		6	2.18574499(−04)	2.18581349(−04)	2.18581349(−04)
		8	2.28226660(-04)	2.28235911(−04)	2.28235911(-04)
		10	2.34115207(−04)	2.34124178(−04)	2.34124178(−04)

[a] $kR < y + \sqrt{y^2 + l(l+1)}$.

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