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Complex-correlation Kohn *T*-matrix method of calculating total and elastic cross sections: Electron-hydrogen elastic scattering

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We report on a study of electron-hydrogen scattering using a method [Bhatia, Schneider, and Temkin, Phys. Rev. Lett. **70**, 1936 (1993)] that allows for the *ab initio* calculation of total and elastic cross sections at higher energies. In its general form the method uses complex-"radial" correlation functions, in a (Kohn) *T*-matrix formalism. The complex-correlation Kohn *T*-matrix method is reviewed in the context of electron-hydrogen scattering, including the derivation of the equation for the (complex) scattering function, and the extraction of the scattering information from the latter. The calculation reported here is restricted to *S* waves in the elastic region, where the correlation functions can be taken, without loss of generality, to be real. Phase shifts are calculated using Hylleraas-type correlation functions with up to 95 terms. Results are rigorous lower bounds; they are in general agreement with those of Schwartz [Phys. Rev. **124**, 1468 (1961)], but they are more accurate and outside his error bounds at a couple of energies.

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I. INTRODUCTION

In a previous paper [1], we developed a method for calculating elastic and total cross sections for electron-atom scattering. Called "complex-correlation Kohn *T*-matrix," and abbreviated (CCKT) the method is intended for nonelastic scattering in low- and medium-energy range, by which we mean the energy domain where all the inelastic channels are open plus the continuum of ionization channels (up to a total available energy E, which is, say, less than five times the continuum threshold). Clearly, no method can specify all such open channels individually, and usual approximations such as the Born and Eikonal methods [2] are only reliable at high energies. Because our method is intended for the low continuum, it is a partial-wave method where the partial-wave expansion can still be expected to converge reasonably effectively.

The original formulation [1] was applied to an approximation of electron-hydrogen (e-H) scattering called the spherically symmetric model [3]. The S-wave part of that model reduces to the Temkin-Poet (TP) model [4,5], and it was only for the latter that the actual calculation was carried out. (The TP model was later generalized in a different and more incisive way in what was called the "generalized exchange approximation" [6]).

In this paper we deal with the real (i.e., physical) e-H problem. The method is reviewed in Sec. II. Specifically, a more detailed derivation of the (complex) optical potential and scattering equations is given. As opposed to Ref. [1], the emphasis here is on the numerical solution of the scattering equation by decomposing it into its coupled real and imaginary parts and from the solution extracting the T matrix.

An actual calculation in its full generality, however, is still a very extensive undertaking. We shall therefore confine ourselves, in this initial study, to elastic S-wave scattering. Here our aim is to check and increase the accuracy of the classic calculation of Schwartz [7]. Results are presented in Sec. III. Suffice it here to say that our results are rigorous lower bounds on the phase shifts. Thus where they exceed Schwartz' results, which they do at two energies, they are necessarily more accurate. In general, our results are within the stated uncertainty of his remarkable calculation (considering when it was done). Here, given the convergence of our results, we would only claim greater accuracy.

II. THE COMPLEX-CORRELATION KOHN *T*-MATRIX METHOD

A. General

Confined to the e-H partial wave (denoted by L) problem, the total spatial function is written:

$$\Psi_L^{(\pm)}(\mathbf{r}_1,\mathbf{r}_2)=\frac{u_L^{(\pm)}(r_1)}{r_1}Y_{L0}(\hat{\mathbf{r}}_1)\phi_{10}(r_2)Y_{00}(\hat{\mathbf{r}}_2)\pm(1\leftrightarrow 2)+\Phi_L^{(\pm)}(\mathbf{r}_1,\mathbf{r}_2). \tag{1}$$

The superscript $(\pm)$ above refers to singlet (upper sign) or triplet (lower sign) scattering, respectively. (This superscript will be dropped hereinafter, except where it is necessary.) Beyond the terms containing u_L explicitly (those are the terms giving rise to the exchange approximation), the function Φ_L is the correlation function, which is our concern here. For arbitrary L this function is most efficiently written in terms of symmetric Euler angles [8],

$$\Phi_L=\sum_{\kappa}[f_L^{\kappa,1}(r_1,r_2,r_{12})\mathcal{D}_L^{\kappa,1}(\theta,\phi,\psi)+f_L^{\kappa,-1}(r_2,r_1,r_{12})\mathcal{D}_L^{\kappa,-1}(\theta,\phi,\psi)]. \tag{2}$$

The $\mathcal{D}^{\kappa,\epsilon}$ functions $(\epsilon=+1,-1)$ are exchange-adapted combinations of Wigner functions. (The $\mathcal{D}$ functions, in general have been called *rotational harmonics* [9].) The f's above are generalized "radial" functions, which depend on the three residual coordinates that are required (beyond the Euler angles) to define the two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ (further technical details of the symmetry and other properties of the symmetric Euler angle description are given in [8]). What distinguishes this CCKT approach is the fact that the "radial" functions are taken to be complex, that is, different from ordinary variational methods, wherein the radial functions are taken to be real. In the latter case, when one forms the variational functional to be varied [cf. Eq. (5) below], one uses the function Ψ_L^*) on the left. That is so because the f functions would be real, so that only the $\mathcal{D}$ functions in Eq. (2) would be complex conjugated. When the radial functions are complex, however, then—in order to have a variational principle for the T matrix—only the $\mathcal{D}$ but *not* the radial functions are to be complex conjugated in the left-hand function. This is indicated by using the tilde rather than star for that function, which is used in the functional I_L of the variational principle (below). Explicitly,

$$\tilde{\Psi}_L = \frac{u_l^{(\pm)}(r_1)}{r_1} Y_{L0}^*(\hat{\mathbf{r}}_1)\,\phi_{10}(r_2)\,Y_{00}^*(\hat{\mathbf{r}}_2) \pm (1 \leftrightarrow 2) + \tilde{\Phi}_L, \tag{3}$$

where

$$\tilde{\Phi}_L = \sum_{\kappa} \{ f_L^{\kappa,1}(r_1,r_2,r_{12})[\mathcal{D}_L^{\kappa,1}(\theta,\phi,\psi)]^* + f_L^{\kappa,-1}(r_2,r_1,r_{12})[\mathcal{D}_L^{\kappa,-1}(\theta,\phi,\psi)]^* \} \tag{4}$$

The Kohn variational principle [10] for T_L reads

$$\delta[I_L - (-1)^L T_L] = 0, \tag{5}$$

where I_L is the (Kohn) functional

$$I_L = \int [\tilde{\Psi}_L (H-E)\Psi_L]\, d\mathbf{r}_1 d\mathbf{r}_2 . \tag{6}$$

Carrying out the variation leads to scattering equation for $u_L^{(\pm)}(r_1)$ (Rydberg units throughout) and letting $r_1 = r$,

$$\left[-\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + V_d \pm V_{ex} + \mathcal{V}_{op}^{(\pm)} - k^2 \right] u_L^{(\pm)} = 0, \tag{7}$$

where V_d and V_{ex} are the well-known direct and exchange potentials of the "exchange approximation" [11]. These potentials (the latter being nonlocal) are real, however the (remaining) optical potential acting on $u_L(r)$ is complex,

$$\mathcal{V}_{op} u_L = r \left\langle Y_{L0}^* PHQ \frac{1}{E - QHQ} QHP\Psi_L \right\rangle . \tag{8}$$

Thus, $u_L(r)$ is nontrivially complex and leads to a *nonunitary* T_L matrix, which is derivable from the asymptotic form of u_L

$$\lim_{r\to\infty} u_L(r) = \frac{i^L \sin(kr - \pi L/2)}{k} + T_L e^{ikr}. \tag{9}$$

In defining the optical potential we have used the Feshbach approach [12], involving projection operators P and Q, which for the hydrogenic (i.e., one-electron) target can be written expicitly [13]

$$P = P_1 + P_2 - P_1 P_2, \tag{10}$$

$$Q = 1 - P, \tag{11}$$

where the spatial projectors are

$$P_i = e^{-r_i} Y_{00}(\hat{\mathbf{r}}_i)\rangle\langle e^{-r_i} Y_{00}(\hat{\mathbf{r}}_i). \tag{12}$$

Note that P_1 and P_2 commute and are each idempotent, hence the complete P and Q operators are idempotent ($P^2 = P$; $Q^2 = Q$) and orthogonal ($PQ = 0$).

To complete this review of the CCKT method, the optical potental is expanded in terms of the eigenspectrum of the QHQ problem:

$$\delta\left[\frac{\langle \tilde{\Phi}_L QHQ \Phi_L \rangle}{\langle \tilde{\Phi}_L Q \Phi_L \rangle} \right] = 0. \tag{13}$$

This leads to complex radial eigenfunctions $\Phi_L^{(s)}$ and complex eigenvalues $\mathcal{E}_s$. Insertng a complete set of these functions (understood to be approximated by a discrete set arising from Eq. (13) using an ansatz with a finite number of variational parameters) allows the optical potential to be expanded:

$$\mathcal{V}_{op} u_L(\mathbf{r}_1) = r_1 \sum_{s}^{N\omega} \frac{\left\langle Y_{L0}^*(\hat{\mathbf{r}}_1)\,\phi_{10}(\mathbf{r}_2) \frac{2}{r_{12}} Q \Phi_L^{(s)} \right\rangle \left\langle Q \tilde{\Phi}_L^{(s)} \frac{2}{r_{12}} P \Psi_L \right\rangle}{E - \mathcal{E}_s}. \tag{14}$$

To repeat the main point of the CCKT method: because the radial functions $f_L^{\kappa,\epsilon}(r_1,r_2,r_{12})$ in Eq. (2) are complex, the resulting T_L matrix (which in this method is actually a number) will be complex and the associated S_L matrix will be nonunitary—$S_L = 1 - 2ikT_L$. This means that the elastic cross section, calculated from

$$\sigma_L(elastic) = 4\pi(2L+1)|T_L|^2, \tag{15}$$

will be different from the total cross section, calculated from

$$\sigma_L(total) = \frac{4\pi}{k}(2L+1)\,\mathrm{Im}(T_L). \tag{16}$$

The effect of a nonunitary S_L, is of course well known from the literature (cf., for example, Ref. [14]). What is new about the CCKT is that it provides an *ab initio* method for calculating the associated T_L, rather than parametrizing it, as was done, for example, in the "clouded crystal ball" model of neutron-nucleus scattering and reactions [15].

B. Some details of the CCKT method

The Kohn variational principle is generally applied in such a way, as in Ref. [1], that the function $u_L(r)$ of Eq. (7) is parametrized by an expansion in terms of known functions, and the functional in Eq. (6) is analytically evaluated; it is a bilinear expression in terms of the (linear) expansion coefficients. The (Kohn) principle then reduces to differentiation with respect to these parameters, which in turn leads to a set of linear equations, the last being an inhomogeneous equation from the differentiation with respect to T_L. The solution of the set of equations then provides values for all the (linear) constants plus the value of T_L. The latter can be improved by subtracting the value of the functional itself, which in general will not be zero when the calculation is performed in this way. In that case an improved T_L can be obtained by subtraction,

$$T_L^{improved}=T_L-I_L. \tag{17}$$

When, however, the calculation is carried out (as it is here) by solving directly for $u_L(r)$, then this is equivalent to making $I_L=0$. Thus the T_L that emerges is automatically the improved (i.e., the second order) result. What we shall now do is to outline briefly how the calculation is performed when the potentials and hence the solutions are complex. Specifically, the radial equation can be written

$$[\mathcal{L}_L^{(\pm)}+\mathcal{V}_{op}^{(\pm)}]u_L^{(\pm)}(r)=0, \tag{18}$$

where

$$\mathcal{L}_L^{(\pm)}=-\frac{d^2}{dr^2}+\frac{L(L+1)}{r^2}+V_d\pm V_{ex}-k^2. \tag{19}$$

The V_d is the (local) Hartree potential $[V_d(r)=-2\exp(-2r)(1+1/r)]$ and V_{ex} is the well-known (nonlocal) static exchange potential [11]. The remaining (nonlocal) potential is what is gererally called the optical potential, Eq. (5).

We now give a few details of how one solves the radial equation (18) in the general case. Dropping subscripts (superscripts), we write the solution of Eq. (4)

$$u(r)=u_R(r)+iu_I(r) \tag{20}$$

where $u_R(r)$ and $u_I(r)$ are real functions which, substituted in Eq. (18), lead to a coupled set of (real) differential equations:

$$(\mathcal{L}+\mathcal{V}_{op}^{(R)})u_R=\mathcal{V}_{op}^{(I)}u_I, \tag{21}$$

$$(\mathcal{L}+\mathcal{V}_{op}^{(R)})u_I=-\mathcal{V}_{op}^{(I)}u_R, \tag{22}$$

$\mathcal{V}_{op}^{(R)}$ and $\mathcal{V}_{op}^{(I)}$ above are the real and imaginary parts of the optical potential, respectively. (Both are real, nonlocal potentials.) The coupled Eqs. (21) and (22) have two sets of solutions (i.e., both regular at the origin), labeled $u_R^{(i)}(r)$, $u_I^{(i)}(r)$ where $(i=1,2)$. From these two solutions one determines two real constants C_1 and C_2 such that the real and imaginary parts of the asymptotic form (9) is satisfied; the equations for $L=0$ reduce to

$$\lim_{r\to\infty}[C_1u_R^{(1)}+C_2u_R^{(2)}]=\frac{\sin kr}{k}+T_R\cos kr-T_I\sin kr, \tag{23}$$

$$\lim_{r\to\infty}[C_1u_I^{(1)}+C_2u_I^{(2)}]=T_I\cos kr+T_R\sin kr. \tag{24}$$

The two linearly independent solutions will necessarily have the asymptotic form

$$\lim_{r\to\infty}u_R^{(i)}=A_R^{(i)}\sin(kr+\eta_R^{(i)}), \tag{25}$$

$$\lim_{r\to\infty}u_I^{(i)}=A_I^{(i)}\sin(kr+\eta_I^{(i)}), \tag{26}$$

in which one of the normalization constants, say $A_R^{(i)}$, is arbitrary. This is tantamount to letting $A^{(i)}=A_I^{(i)}/A_R^{(i)}$, which allows Eqs. (23) and (24) to be rewritten as

$$C_1\cos\eta_R^{(1)}+C_2\cos\eta_R^{(2)}=\frac{1}{k}-T_I, \tag{27}$$

$$C_1\sin\eta_R^{(1)}+C_2\sin\eta_R^{(2)}=T_R, \tag{28}$$

$$C_1A^{(1)}\cos\eta_I^{(1)}+C_2A^{(2)}\cos\eta_I^{(2)}=T_R, \tag{29}$$

$$C_1A^{(1)}\sin\eta_I^{(1)}+C_2A^{(2)}\sin\eta_I^{(2)}=T_I. \tag{30}$$

The η's and A's are extracted from the solutions of Eqs. (21) and (22); thus Eqs. (27)–(30) is a set of four equations for four real constants: C_1,C_2 and in particular the real and imaginary parts of T (i.e., T_R and T_I). From the latter one calculates the elastic and total cross sections, Eqs. (15) and (16).

TABLE I. Convergence [the phase shifts (in radians) have been optimized with respect to γ and δ for each $N(\omega)$] of *S*-wave phase shift as a function of $N(\omega)$ for $k=0.8$.

	^1S			^3S		
$N(\omega)$	$\gamma=\delta$	$\eta^{(+)}$	N(ω)	γ	δ	$\eta^{(-)}$
EA[a]		0.65127	EA[a]			1.61729
3(1)	1.23	0.79028				
7(2)	0.68	0.87536	10(2)	0.65	0.55	1.63845
13(3)	0.68	0.87684	20(3)	0.84	0.70	1.64205
22(4)	0.69	0.88362	35(4)	0.85	0.50	1.64294
34(5)	0.61	0.88584	56(5)	0.85	0.50	1.64344
50(6)	0.54	0.88616	84(6)	0.85	0.50	1.64379
70(7)	0.66	0.88687				
95(8)	0.72	0.88718				

[a] EA are the well-known exchange approximation phase shifts [11]; it corresponds to no correlation terms $[N(\omega)=0\to\mathcal{V}_{op}=0$ in Eq. (7)].

TABLE II. Phase shifts of ^1S for various k for $N=95$.

k	$\gamma=\delta$	η	$\eta_{Schwartz}$
0.1	0.53	2.55358	2.553(1)
0.2	0.60	2.06678	2.0673(9)
0.3	0.72	1.69816	1.6964(5)
0.4	0.70	1.41540	1.4146(4)
0.5	0.70	1.20094	1.202(1)
0.6	0.70	1.04083	1.041(1)
0.7	0.71	0.93111	0.930(1)
0.8	0.72	0.88718	0.886(1)

TABLE III. Phase shifts of ^3S for various k for $N=84$.

k	γ	δ	η	$\eta_{Schwartz}$
0.1	0.85	0.12	2.93853	2.9388(4)
0.2	0.84	0.39	2.71741	2.7171(5)
0.3	0.90	0.37	2.49975	2.4996(8)
0.4	0.91	0.38	2.29408	2.2938(4)
0.5	0.88	0.44	2.10454	2.1046(4)
0.6	0.77	0.52	1.93272	1.9329(8)
0.7	0.70	0.55	1.77950	1.7797(6)
0.8	0.86	0.50	1.64379	1.643(3)

III. CALCULATION

As stated in the Introduction we calculate here only S-wave (i.e., $L=0$) elastic scattering, specifically, phase shifts. This means, since $\mathcal{D}_L=$constant in Eq. (12), that the correlation function Φ_L is only a function of the "radial" coordinates. Here Φ_L is taken of Hylleraas form

$$\Phi^{(\pm)}_{L=0}=e^{-\gamma r_1-\delta r_2}\sum_{lmn}^{N_\omega} C_{lmn} r_1^l r_2^m r_{12}^n \pm(1\leftrightarrow 2), \tag{31}$$

where the sum includes all triples such that $l+m+n=\omega$ and $\omega=0,1,2,\ldots,8$. The total number of terms N_ω depends on spin and whether $\gamma=\delta$ or not. The values of N_ω as a function of l,m,n is given in the following simple array:

	ω	0	1	2	3	4	5	6	7	8
^1S	$N_\omega(\gamma=\delta)$	1	3	7	13	22	34	50	70	95
^3S	$N_\omega(\gamma\neq\delta)$	1	4	10	20	35	56	84	120	165

To summarize the calculation, the QHQ problem is solved (for a given γ and δ and N_ω). The result is a set of eigenvalues $\mathcal{E}_s$ $(s=1,2,\ldots N_\omega)$ and associated eigenfunctions $\Phi^{(s)}$. From them (the terms in) the optical potential, Eq. (14) is constructed, and the integro-differential Eq. (7) is solved noniteratively. Because all quantities are real, the solution is unique (up to an arbitrary normalization) with asymptotic form

$$\lim_{r\to\infty} u^{(\pm)}(r)\propto \sin(kr+\eta^{(\pm)}) \tag{32}$$

From $u^{(\pm)}(r)$ and its derivative the phase shift η is readily extracted.

Examples demonstrating the convergence of η for $k=0.8$ as a function of N_ω are given in Table I. By virtue of the fact that η's are rigorous lower bounds on the phase shift [13], the convergence then becomes a powerful indication of the accuracy of the result. Phase shifts as a function of k are given in Tables II and III. To repeat, they are rigorous lower bounds in all cases. They are compared to the results of Schwartz [7]. Our ^1S phase shifts are seen to exceed Schwartz' (including his estimated error) at $k=0.3$, 0.4. Otherwise our results for both ^1S and ^3S are within his estimated uncertainty, which we find to be quite impressive considering that his calculation was carried out over 40 years ago. Nevertheless we believe that our present calculation is more accurate. The difficulty in making a secure extrapolation is due to the difficulty of estimating quantitatively the effects of polarization and other long-range potentials at nonzero k. (In principle, one can optimally, rigorously include polarization by use of a polarization pseudostate [16]; however, in practice those corrections are small, yet require a much more extensive calculation than is worthwhile here for our present purpose.) The convergence of the results suggests that they are accurate to one or two units in the fourth place after the decimal point. (We have given five digits because to that accuracy they are rigorous lower bounds.)

Scattering lengths are not included in our calculation, because at $k=0$ the Kohn variational principle, which applies to Schwartz' calculation, is well known to provide rigorous (in this case upper) bounds [17]. It is worth recalling that one of us [18] had earlier deduced that long-range polarization would have decisive quantitative effect on the scattering length and had derived a formula

$$a=a(R)-\alpha\left(\frac{1}{R}-\frac{a}{R^2}+O\left(\frac{1}{R^3}\right)\right) \tag{33}$$

in which $a(R)$ represents the value of scattering length including only the region of configuration space $r\leqslant R$, and the remaining terms in Eq. (33) give the effect of the long-range polarization ($\alpha=$ polarizability of the hydrogen atom$=4.5$). Use of that formula led to the first correct estimate of the true scattering length [18]. Thus when Schwartz applied his calculation at $k=0$, he found it necessary to include the equivalent of long-range polarization terms, as predicted [18], in addition to the Hylleraas terms in order to get adequate convergence. For these reasons we believe his scattering lengths are sufficiently secure and accurate as not to require further calculation. His results are: $a(^1S)=5.965\pm0.003$, $a(^3S)=1.7686\pm0.0002$.

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