

Solving close-coupling equations in momentum space without singularities for charged targets

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Abstract

The analytical treatment of the Green's function in the convergent close-coupling method [Bray *et al.* Comp. Phys. Comm. **203** 147 (2016)] has been extended to charged targets. Furthermore, we show that this approach allows for calculation of cross sections at zero channel energy. For neutral targets this means the electron scattering length may be obtained from a single calculation with zero incident energy. For charged targets the non-zero excitation cross sections at thresholds can also be calculated by simply setting the incident energy to the exact threshold value. These features are demonstrated by considering electron scattering on H and He⁺.

1. Introduction

There has been immense progress in the field of atomic and molecular scattering theory during the last two decades. Computational methods such as R-matrix with pseudostates [1–3], exterior complex scaling [4, 5], time-dependent close-coupling [6], and convergent close-coupling (CCC) [7, 8] all set out to fully solve the underlying Schrödinger equation without approximation. Collisions involving electron, positron, or photon scattering on few-electron atoms and ions can now be routinely calculated accurately at any energy of interest. The CCC approach has also been recently extended to molecular targets [9] and heavy projectiles like antiprotons and protons [10–14].

Generally, further progress in the field comes from extending the capability to more complex collision systems. However, recently we found that a novel approach to the solution of the CCC equations yields greater utility when applied to ill-conditioned systems such as two-centre positron-atom scattering [15–17]. Starting with the electron-hydrogen S-wave model, it was shown that the Green's function in the CCC coupled Lippmann-Schwinger equations may be treated analytically, and thereby removing a somewhat problematic principal-value integral [18]. The full implementation [15] is applicable to electron or positron scattering on neutral targets. However, in the case of ionic targets there is considerable extra complexity due to the requirement for the inclusion of projectile bound states. Extension to ionic targets is useful in its own right, and is also a requirement for the application of the CCC method to photon scattering [19–22].

Another interesting consequence of the analytical approach is that the elimination of the singularity allows the application of the method at exact threshold energies. In the case of neutral targets this is useful when calculating the scattering length. However, for charged targets the excitation cross sections are non zero at threshold, and as we shall show, may be directly calculated. Atomic units are used throughout unless specified otherwise.

2. Theory

The general ideas behind the analytic treatment of the Green's function in the Lippmann-Schwinger equations have already been discussed earlier [15, 18]. Here we concentrate on the extra complexity associated with charged targets. In such cases the projectile asymptotic Hamiltonian contains the potential due to the asymptotic nuclear charge Z_a , leading to the projectile wave satisfying

$$\left(K + \frac{z_p Z_a}{r} - \varepsilon_k\right) |\mathbf{k}_p\rangle = 0, \quad (1)$$

where K is the projectile kinetic energy operator and \mathbf{k}_p is projectile momentum. In the case of electron scattering we have $z_p = -1$, and for the He⁺ target $Z_a = +1$. Consequently, the complete set in projectile space includes the countably infinite number of discrete states as well as the continuum. The resulting coupled Lippmann-Schwinger equations [23] take almost an identical form to the case of neutral targets except for the requirement to also include the bound states of the projectile of energy ε_k

$$\begin{aligned} \langle \mathbf{k}_f \phi_f | T_S | \phi_i \mathbf{k}_i \rangle &= \langle \mathbf{k}_f \phi_f | V_S | \phi_i \mathbf{k}_i \rangle \\ &+ \sum_{n=1}^N \int d\mathbf{k} \frac{\langle \mathbf{k}_f \phi_f | V_S | \phi_n \mathbf{k} \rangle \langle \mathbf{k} \phi_n | T_S | \phi_i \mathbf{k}_i \rangle}{E + i0 - \varepsilon_n - \varepsilon_k}. \end{aligned} \quad (2)$$

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Here \mathbf{k}_f (\mathbf{k}_i) is the projectile final (initial) momentum, the notation $i0$ is used to indicate the limit of ix as positive $x \rightarrow 0$ to ensure outgoing spherical wave boundary conditions, S is the total spin of the system, V_S are the interaction potentials and T_S are the required transition amplitudes. For He^+ the target wavefunctions ϕ_n of energy ϵ_n are obtained from the Hamiltonian in Eq. (1) with $Z_a=+2$.

Eq. (2) is solved by first taking the complex part of the integral analytically to yield the equation for the K matrix [7]

$$\begin{aligned} \langle \mathbf{k}_f \phi_f | K_S | \phi_i \mathbf{k}_i \rangle &= \langle \mathbf{k}_f \phi_f | V_S | \phi_i \mathbf{k}_i \rangle \\ &+ \sum_{n=1}^N \mathcal{P} \int \mathcal{D}\mathbf{k} \frac{\langle \mathbf{k}_f \phi_f | V_S | \phi_n \mathbf{k} \rangle \langle \phi_n | K_S | \phi_i \mathbf{k}_i \rangle}{E + i0 - \epsilon_n - \epsilon_k}, \end{aligned} \quad (3)$$

where the required T matrix is obtained from

$$\langle \mathbf{k}_f \phi_f | K_S | \phi_i \mathbf{k}_i \rangle = \sum_{n=1}^{N_o} \langle \mathbf{k}_f \phi_f | T_S | \phi_n \mathbf{k}_n \rangle (\delta_{ni} + i\pi k_n \langle \phi_n | K_S | \phi_i \mathbf{k}_i \rangle), \quad (4)$$

and where N_o is the number of open states such that $E - \epsilon_n = k_n^2/2 > 0$. The symbol \mathcal{P} indicates a principal value integral.

A partial-wave expansion is utilised to solve Eq. (3), with the numerical details for the original approach given in Ref. [24]. Briefly, the singularity in Eq. (3), whenever $E - \epsilon_n = k_n^2/2 > 0$, is treated using symmetric, about k_n , quadratures. This is problematic near excitation thresholds ($k_n \approx 0$), and whenever the system of equations is particularly ill-conditioned, such that the addition of large values either side of the singularity causes considerable precision loss. The latter circumstance is commonly the case for positron scattering treated within the two-centre formalism [25].

An alternative approach has been proposed, which treats the integral in the partial-wave expanded Eq. (3) analytically [15, 18]. For neutral targets, following the introduction of several complete sets of states, the integral can be isolated to

$$\begin{aligned} G_n^L(r', r'') &= \mathcal{P} \int_0^\infty dk \frac{\langle r' | kL \rangle \langle Lk | r'' \rangle}{E - \epsilon_n - \frac{1}{2}k^2} \\ &= \text{Re} \left[-\pi k_n^{-1} s_L(k_n r_{<}) (c_L(k_n r_{>}) + i s_L(k_n r_{>})) \right], \end{aligned} \quad (5)$$

where $s_L(k_n r) = \langle r | k_n L \rangle$ and $c_L(k_n r)$ are the regular and irregular Riccati-Bessel functions respectively, with $k_n = \sqrt{2(E - \epsilon_n)}$. Note that for closed channels $E - \epsilon_n < 0$, and k_n is purely imaginary.

The possibility of solving (2) at zero incident energy, so as to obtain the scattering length (via $\sigma_S = 4\pi a_S^2$) from a single calculation, was not considered previously, and we do so now. For $k_i^2/2 = 0$ we only require $L = 0$ for a non-zero cross section, and so Eq. (5) becomes

$$G_i^0(r', r'') = -\pi r_{<}. \quad (6)$$

There is no need to consider threshold excitation energies for neutral targets because the $(kr)^{(L+1)}$ behaviour of $s_L(kr)$ for small k ensures zero cross sections at threshold.

For charged targets the situation is somewhat more complicated. Now we utilise the result used in the coupled-channel optical approach [26, 27]

$$\begin{aligned} G_n^L(r', r'') &= \sum_{n'=1}^\infty \frac{\langle r' | n' L \rangle \langle L n' | r'' \rangle}{E - \epsilon_n + \frac{1}{2}Z_a^2/n'^2} + \mathcal{P} \int_0^\infty dk \frac{\langle r' | kL \rangle \langle Lk | r'' \rangle}{E - \epsilon_n - \frac{1}{2}k^2} \\ &= \text{Re} \left[-\pi k_n^{-1} f_L(k_n r_{<}) (g_L(k_n r_{>}) + i f_L(k_n r_{>})) \right], \end{aligned} \quad (7)$$

where $\langle r | nL \rangle$ are the bound states, with energy $-\frac{1}{2}Z_a^2/n^2$, and $f_L(k_n r) = \langle r | k_n L \rangle$ and $g_L(k_n r)$ are the corresponding regular and irregular Coulomb functions of energy $E - \epsilon_n = k_n^2/2$ (negative for closed channels), respectively.

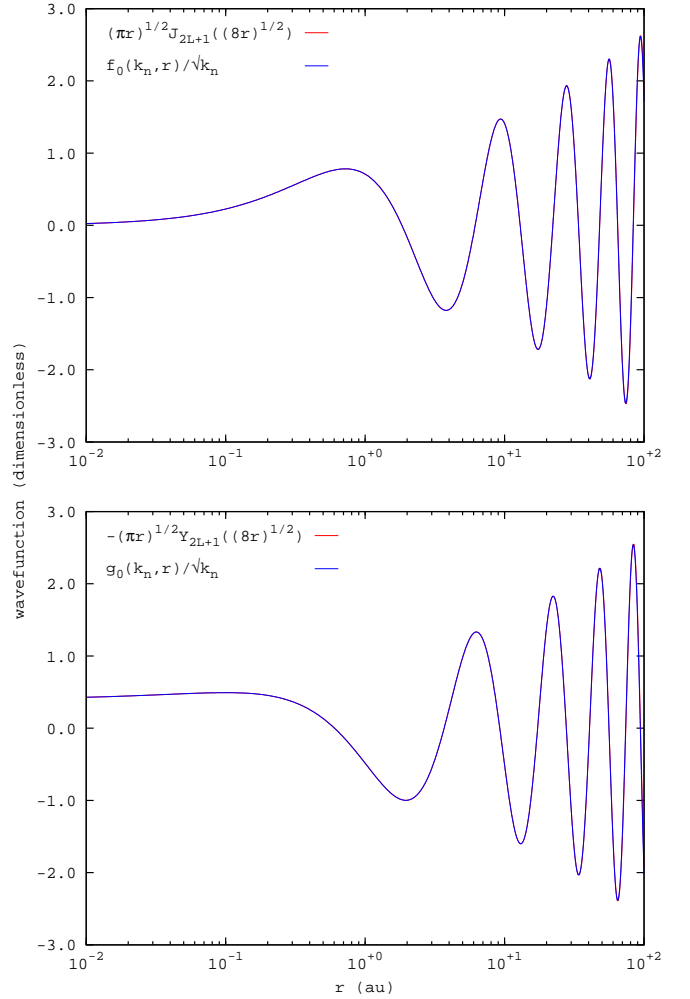


Figure 1: Regular (top) and irregular (bottom) $L = 0$ Coulomb waves for zero energy calculated using the RHS of Eq. (8) and the LHS with $k_n = 0.12$. The two results are almost indistinguishable over the full range of r .

For charged targets the elastic cross section diverges as $1/k_i^2$ and so the scattering length is infinite. However, the cross sections at excitation thresholds corresponding to $k_n = 0$ are finite for all L , and may be calculated in the following way. We use

$$\begin{aligned} \lim_{k_n \rightarrow 0} f_L(k_n r) / \sqrt{k_n} &= \sqrt{\pi r} J_{2L+1}(\sqrt{8r}), \\ \lim_{k_n \rightarrow 0} g_L(k_n r) / \sqrt{k_n} &= -\sqrt{\pi r} Y_{2L+1}(\sqrt{8r}), \end{aligned} \quad (8)$$

where J and Y are the cylindrical Bessel functions. This is demonstrated in Fig. 1, and allows us to eliminate the division by k_n in Eq. (7).

A further problem is that the cross section is defined as $\sigma_{fi} = k_f/k_i |T_{fi}|^2$, with $k_f = 0$ at threshold. Accordingly, we modify Eq. (4) by multiplying both sides by $\sqrt{k_f k_i}$, which allows the removal of explicit multiplication by k_n , leaving matrix elements of the form $T_{fi} \sqrt{k_f k_i}$, which are non-zero for ions as $k_f \rightarrow 0$. This leads to a non-zero cross section for $k_f = 0$ and $k_i > 0$.

Having defined G_n^L for all k_n , we first define N_k box-based states by solving Eq. (1) for each L with a specified box size R_k . For $Z_a > 0$ these will include as many bound states ($\varepsilon_k < 0$) as R_k allows. We then proceed as previously [15], and define

$$\begin{aligned} \langle L_f k_f l_f n_f | V_{S,J} | n l k'' L \rangle &= \int_0^\infty dr' \int_0^\infty dr'' \sum_{k'} \\ &\times \langle L_f k_f l_f n_f | V_{S,J} | n l k' L \rangle \langle L k' l' r' \rangle G_n^L(r', r'') \langle r'' | k'' L \rangle, \end{aligned} \quad (9)$$

with the final equation to be solved being

$$\begin{aligned} \langle L_f k_f l_f n_f | K_{S,J} | n_i l_i k_i L_i \rangle &= \langle L_f k_f l_f n_f | V_{S,J} | n_i l_i k_i L_i \rangle \\ &+ \sum_{l,L} \sum_{n=1}^N \sum_k \langle L_f k_f l_f n_f | V_{S,J} | n l k L \rangle \langle L k l n | K_{S,J} | n_i l_i k_i L_i \rangle, \end{aligned} \quad (10)$$

which has no singularities. Convergence in the solution of Eq. (10) is obtained with increasing N_k and R_k . Note that there are no substantially extra computational resources required in the evaluating Eq. (9) due to the near-separable nature of $G_n^L(r', r'')$.

3. Results

We begin by considering the e-H scattering system to demonstrate that both the numerical (nGF) and analytical (aGF) approaches to treating the Green's function in Eq. (2) yield the same results at all energies. Furthermore, only the analytical approach may be applied at exactly zero projectile energy. The zeroth partial wave suffices for our purposes. The target states are taken to have $l_{\max} = 2$ and $N_l = 10 - l$ with Laguerre exponential parameter $\lambda_l = 2$. An energy range varying over six orders of magnitude is considered, though no attempt is made to make it sufficiently dense to map out any resonance structures.

The e-H cross sections for elastic scattering and 2s, and 2p excitation are presented in Fig. 2. We see excellent agreement between the two approaches across all energies and for all transitions. For elastic scattering the arrows indicate the aGF calculation performed at exactly zero energy. As required, it is consistent with those performed at very small energies, and yields a scattering lengths $a_{S=0} = 6.0$ and $a_{S=1} = 1.8$, which are consistent with those of Schwartz [28]. Note that the cross sections are plotted against energy above threshold, which emphasizes the near-threshold behaviour, where they start from zero.

We next consider e-He⁺ scattering using the same parameters as for the e-H system, with the cross sections presented in

Fig. 3. The elastic cross sections have been multiplied by the incident energy to check the expected divergence. It is clear that the original nGF approach struggles to yield the correct behaviour close to thresholds in all presented cases. While we can improve the given nGF results, this requires going out to very large radial coordinates so as to incorporate more bound states. In the original formulation the approach to summation over the bound states and integration over the continuum are entirely separate. However, in the aGF approach increasing R_k systematically affects both. Furthermore, for excitation, the aGF approach is clearly consistent with calculations exactly at the thresholds, as indicated by the arrows. It should be said that the presentation deliberately emphasises the near threshold energies. Away from these regions the agreement between the nGF and aGF calculations is excellent. Though not presented, we have checked that the behaviour for higher partial waves is much the same as presented here for the zeroth partial wave.

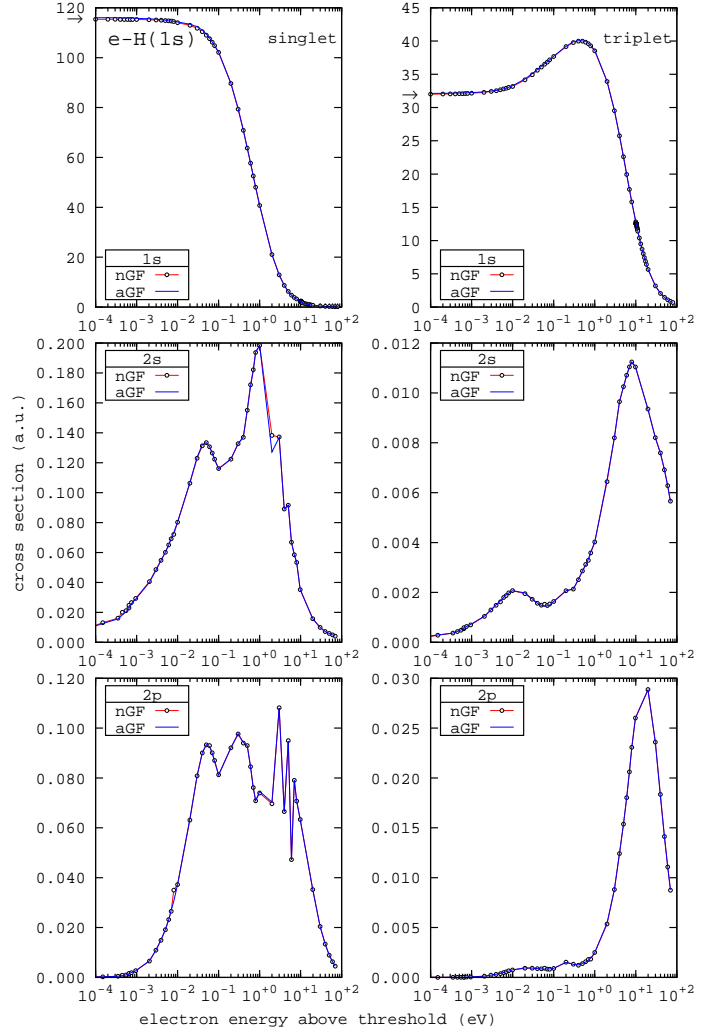


Figure 2: Electron-hydrogen scattering spin-weighted cross sections for the zeroth partial wave calculated with the numerical (nGF) and analytical (aGF) treatment of the Green's function in (3). The arrows indicate the $\frac{2S+1}{4}\sigma_S$ results when the projectile energy is set to zero, allowing for the determination of the scattering length a_S via $\sigma_S = 4\pi a_S^2$ from a single calculation. The calculations have been performed at the specified points connected by straight lines to help guide the eye.

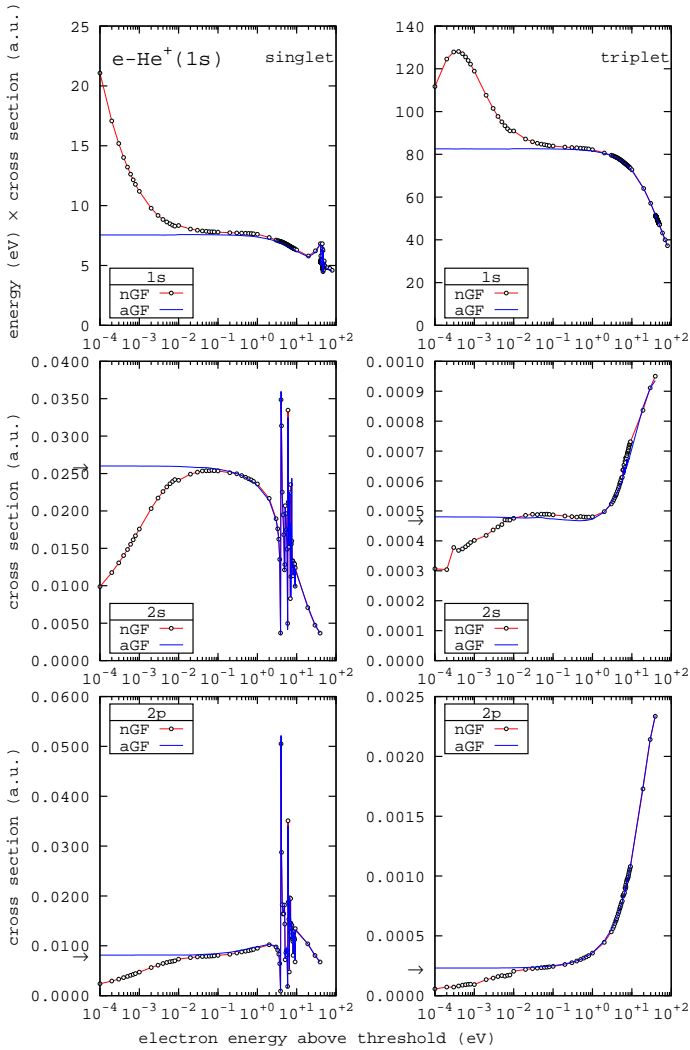


Figure 3: As for figure 2 except for the He^+ target. Now the arrows indicate the (non-zero) cross sections when the projectile energy is set to the threshold of excitation. Note that since the elastic cross section diverges as $1/E_p$, it has been multiplied by the incident projectile energy E_p .

4. Conclusions

The analytic approach to treating the Green's function in the coupled Lippmann-Schwinger equations of the CCC method has been implemented for charged targets, and at threshold energies. As a consequence it has the same utility as the original numerical approach for electron, positron or photon scattering. Earlier we have found that the analytical approach yields less ill-conditioned systems in the case of two-centre positron-atom scattering [15, 16]. Here we have demonstrated a more accurate treatment of the electron-ion collision system in the vicinity of thresholds.

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