A new theoretical approach to (e,2e) and (e,3e) processes

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Abstract. A new version of the J-matrix method is formulated for describing the (e,2e) and (e,3e) scattering of a fast projectile electron on a helium atom. The derived three-body final state wave function exactly satisfies two-body boundary conditions when one ejected electron is at large distances from while the other is close to the nucleus. The obtained results for differential cross sections of the He(e,2e)He$^+$ and He(e,3e)He$^{++}$ reactions are in a good agreement with experiment both in shape and absolute value.

1. Introduction

In this paper, we present a theoretical description of the multiple electron impact ionization experiments on helium which were carried out in the so-called dipolar coplanar geometry [1]. The kinematical conditions of these experiments are characterized by small momentum transfer and high incident and scattered energies (the projectile electron energy $E_i$ is approximately equal to its scattering energy $E_s$ in the range 5-8 keV), while the energies of the emitted electrons are of the order of few eVs. Such kinematics allow to employ the first Born approximation (FBA) and to describe the fast projectile electron as a plane wave. The triple differential cross section (TDCS) of the ionization-excitation reaction is (atomic units are used $m_e = e = \hbar = 1$)

$$\sigma^{(3)}_{n_0} \equiv \frac{d^3 \sigma_{n_0}}{d\Omega_s dE_1 dE_1} = \sum_{\ell_0 m} \frac{4p_s k_1}{p_i Q^4} \times \left| \left\langle \hat{\Psi}_{n_0\ell_0 m}^{-}(k_1) \right| \exp(iQr_1) + \exp(iQr_2) - 2|\Psi_0\rangle \right|^2,$$

(1)

where ($E_1, p_1$), ($E_s, p_s$), and ($E_1, k_1$) are the energies and momenta of, respectively, the incident (fast), the scattered (fast), and the ejected (slow) electrons; $Q = p_i - p_s$ is the transferred momentum. The quantum numbers $(n_0, \ell_0, m)$ designate the state of the residual ion He$^+$, $\Psi_0$ is the ground-state helium wave function.

The five-fold differential cross section (5DCS) of the He(e,3e)He$^{++}$ reaction is given by

$$\sigma^{(5)} \equiv \frac{d^5 \sigma}{d\Omega_s dE_1 dE_1 dE_2 dE_2} = \frac{4p_s k_1 k_2}{p_i Q^4} \times \left| \left\langle \hat{\Psi}^{-}(k_1, k_2) \right| \exp(iQr_1) + \exp(iQr_2) - 2|\Psi_0\rangle \right|^2,$$

(2)

where ($E_1, k_1$) and ($E_1, k_2$) are the energies and momenta of both ejected slow electrons.
2. General formulation: double electron continuum.
We consider the laboratory reference system assuming the nucleus mass \(m_3 \to \infty\) and \(r_3 = 0\). Particles 1 and 2 are electrons. The Schrödinger equation for the helium atom reads

\[
E + \frac{1}{2} \Delta_1 + \frac{1}{2} \Delta_2 + \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r_{12}} \Psi^{(-)}(k_0, p_0; r_1, r_2) = 0.
\]  
(3)

Using the Faddeev approach [2], we divide the Coulomb potentials into the short-range and long-range parts:

\[
\frac{Z}{r_i} = V_i^{(s)}(r_1, r_2) + V_i^{(l)}(r_1, r_2),
\]  
(4)

where

\[
V_i^{(s)}(r_1, r_2) = \frac{Z}{r_i} \zeta(r_i, r_j), \quad V_i^{(l)}(r_1, r_2) = \frac{Z}{r_i} \left[1 - \zeta(r_i, r_j)\right]
\]  
(5)

and

\[
\zeta(r_i, r_j) = \frac{2}{\{1 + \exp[(r_i/a)^\nu/(1 + r_j/b)]\}}.
\]  
(6)

We have three fitting parameters \(a, b\) and \(\nu > 2\). The role of the \(\zeta\)-function is to determine the border between the domain \(\Omega_0\) of so-called "true" three-body scattering (where \(r_1 \sim r_2\)), and the two-body domain \(\Omega_1 (r_1 \gg r_2)\), or \(\Omega_2 (r_2 \gg r_1)\).

Let us introduce the two functions \(\Psi_i^{(-)}(k_0, p_0; r_1, r_2)\) \((i = 1, 2)\) such that \(\Psi^{(-)} = 1/\sqrt{2} \left[\Psi_1^{(-)} + \Psi_2^{(-)}\right]\). Taking into account the symmetry of the two-electron wave function \(\Psi^{(-)}(k_0, p_0; r_1, r_2) = g\Psi_1^{(-)}(k_0, p_0; r_2, r_1)\) where \(g = +1 (-1)\) for a singlet (triplet) state, we demand

\[
\Psi_2^{(-)}(k_0, p_0; r_1, r_2) = g\tilde{P}_{12}\Psi_1^{(-)}(k_0, p_0; r_1, r_2).
\]  
(7)

We define now these new functions using the Faddeev-type reduction

\[
\left[ E + \frac{1}{2} \Delta_1 + \frac{1}{2} \Delta_2 + V_1^{(l)} + V_2^{(l)} - \frac{1}{r_{12}} \right] \Psi_1^{(-)} = -\sqrt{2} V_2^{(s)} \Psi^{(-)}
\]  
(8)

\[
\left[ E + \frac{1}{2} \Delta_1 + \frac{1}{2} \Delta_2 + V_1^{(l)} + V_2^{(l)} - \frac{1}{r_{12}} \right] \Psi_2^{(-)} = -\sqrt{2} V_1^{(s)} \Psi^{(-)}
\]  
(9)

or

\[
\left[ E + \frac{1}{2} \Delta_1 + \frac{1}{2} \Delta_2 + V_1^{(l)} + V_2^{(l)} - \frac{1}{r_{12}} \right] \Psi^{(-)} = -V_2^{(s)}(1 + g\tilde{P}_{12}) \Psi_1^{(-)}
\]  
(10)

because \(\Psi^{(-)} = 1/\sqrt{2} \left[1 + g\tilde{P}_{12}\right] \Psi_1^{(-)}\). In this way we obtain only one equation for the component \(\Psi_1^{(-)}(k_0, p_0; r_1, r_2)\), which is fully equivalent to Eq. (3).

Now we rewrite Eq. (10) as follows:

\[
\left[ E + \frac{1}{2} \Delta_1 + \frac{1}{2} \Delta_2 + \frac{Z - 1}{r_1} + \frac{Z}{r_2} \right] \Psi_1^{(-)} = V(r_1, r_2) \Psi_1^{(-)}
\]  
(11)

with

\[
V(r_1, r_2) = \frac{1}{r_{12}} - V_1^{(l)}(r_1, r_2) + \frac{Z - 1}{r_1} - gV_2^{(s)}(r_1, r_2)\tilde{P}_{12}.
\]  
(12)

It is straightforward to see that the potential \(V(r_1, r_2)\) is short-ranged in the two-body domain \(\Omega_1 (r_1 \gg r_2)\).

Eq. (11) is a basic one for our calculations. The operator in the l.h.s. of (11) acts on the two independent subspaces \(\{r_1\}\) and \(\{r_2\}\). Its free solution is a product of two Coulomb waves \(\varphi(k_0, r_2; Z) \varphi(p_0, r_1; Z - 1)\). This means that electron 2 "sees" the charge \(Z\), while electron 1
"sees" the screened charge \((Z - 1)\), i.e. one electron is much closer to the nucleus than the other one as it should do in the domain \(\Omega_1\).

Eq. (11) can be written in the integral form
\[
\Psi_1^{-}(k_0, p_0; \mathbf{r}_1, \mathbf{r}_2) = \varphi(k_0, \mathbf{r}_2; Z) \varphi(p_0, \mathbf{r}_1; Z - 1)
\]
\[+ \int d\mathbf{r}'_1 d\mathbf{r}'_2 \mathcal{G}^{-}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; E) V(\mathbf{r}'_1, \mathbf{r}'_2) \Psi_1^{-}(k_0, p_0; \mathbf{r}'_1, \mathbf{r}'_2).\]

In turn, the Green’s function of two independent sub-systems in (13) can be presented as a contour convolution integral
\[
\mathcal{G}^{-}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; E) = \frac{1}{2\pi i} \int \frac{dE}{E} \mathcal{G}^{-}(\mathbf{r}_2, \mathbf{r}'_2; E; Z) \mathcal{G}^{-}(\mathbf{r}_1, \mathbf{r}'_1; E - E; Z - 1).\]

The wave function \(\Psi_1^{-}(k_0, p_0; \mathbf{r}_1, \mathbf{r}_2)\) can be presented as the partial expansion
\[
\Psi_1^{-}(k_0, p_0; \mathbf{r}_1, \mathbf{r}_2) = \frac{2}{p_0 k_0} \sum_{LM_{\lambda\mu}} (\ell_0 m_0 \lambda_0 \mu_0|LM) i^{\ell_0 + \lambda_0} e^{-i(\sigma_0 + \sigma_{\lambda\mu})} X_{\ell_0 m_0}^{\lambda\mu}(k_0) Y_{\lambda\mu}(p_0) \psi_{L_{\lambda\mu}}^{M}(\mathbf{r}_1, \mathbf{r}_2).
\]

In turn, the wave function \(\psi_{LM}^{L_{\lambda\mu}}\) in (15) can be further expanded over the Laguerre basis plus bispherical harmonics series
\[
\psi_{L_{\lambda\mu}}^{LM}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\ell, \lambda, \nu, \mu} C_{\ell\lambda\nu\mu}(E) |n \ell \nu \lambda; LM\rangle,
\]
\[|n \ell \nu \lambda; LM\rangle = \frac{\phi_{\nu}(r_2)}{r_2} \frac{\phi_{\nu}(r_1)}{r_1} \chi_{\ell \lambda}(\mathbf{r}_1, \mathbf{r}_2)
\]
with
\[
\phi_{\nu}(r) = [(\nu + 1)(2\nu + 1)]^{-1/2} (2\nu r)^{\lambda + 1} e^{-\nu r} L_{\nu}^{2\lambda + 1}(2\nu r),
\]
and \(u\) is a scaling parameter.

Note that \(\varphi_{\ell}(r; Z) = \sum_{\nu} S_{\ell\nu}^{\alpha} Z_{\nu}(r) \phi_{\nu}(r)\) is the corresponding expansion of the Coulomb spectral state, and \(\alpha\) runs over the whole spectrum, both bound and continuous. Taking into account that the partial Coulomb Green’s function can be standardly factorized
\[
\mathcal{G}_{\ell}^{\pm}(r, r'; E; Z) = \frac{\varphi_{\ell}^{\alpha}(r; Z) \varphi_{\ell}^{\beta}(r'; Z)}{E - \varepsilon_{\alpha} \pm i\delta},
\]
and collecting all expansions together we obtain from (13)
\[
C_{\ell\nu\ell\mu}(E) = \delta_{(\ell\lambda)(\ell_0 \mu_0)} S_{\ell\ell_0}(k_0, Z) S_{\nu\mu}(p_0, Z - 1) +
\]
\[+ \sum_{\ell'\mu', \nu', \mu''} \sum_{L_{\lambda\mu}} \left[ \sum_{\alpha} S_{\ell'\mu'} S_{\nu'\mu''}^{*} \mathcal{G}_{\nu'\mu''}^{\lambda\mu}(E - \varepsilon_{\alpha}; Z - 1) \right] V_{LL'}^{(\ell\lambda)(\ell'\mu')}(E).
\]

The upper limit in the sum in (19) emphasizes that the short-range potential is zero if any index exceeds \(N\).

Eq. (19) is fully equivalent to eq. (35) in [3], or eq. (19) in [4]. The analogous mathematical formalism can be worked out for the single continuum wave function [5] which is even more
suitable to this approach. That is why we stop at this point and refer a reader to these papers for further details. Applying the J-matrix approach [7, 8, 9] we obtain finally the discrete analog of an integral equation of the Lipmann-Schwinger type [10] for their numerical calculations. No pseudostates are used in this theoretical scheme.

We also remind that the ground-state helium wave function \( \Psi_0 \) is obtained by diagonalizing the full Hamiltonian matrix using the basis set (17). For the results presented below we put \( \ell_{\text{max}} = 3 \) and \( n_{\text{max}} = \nu_{\text{max}} = 15 \). Choosing the basis parameter \( u_0 = 1.193 \) we obtain the ground state energy \( E_0 = -2.903256 \text{ a.u.} \).

3. Results and discussion

Due to the shortage of space we omit many powerful details of the method. The calculation details are as follows: \( L_{\text{max}} = 2 \), and \( \ell, \lambda \leq 5 \); the number of the basis functions (18) for each Jacobi coordinate \( r_1 \) and \( r_2 \) is \( N = 21 \); the optimal value of the basis parameter is found to be \( u = 0.3 \).

The angular distributions of the slow electron in the case of the \((e, 2e)\) reaction (TDCS) are shown in Fig. 1. \( \theta_1 \) is the in-plane emission angle with respect to the vector \( \mathbf{p}_i \). The displayed experimental data are due to [1]. It correspond to the general kinematic conditions \( n_0 = 2, E_s = 5500 \text{ eV} \), and three particular cases: \( E_1 = 5 \text{ eV}, \theta_s = 0.35^\circ \) (Fig. 1a); \( E_1 = 10 \text{ eV}, \theta_s = 0.32^\circ \) (Fig.1b); \( E_1 = 75 \text{ eV}, \theta_s = 1^\circ \) (Fig. 1c) \( (\theta_s \text{ is the scattering angle).} \)

**Figure 1.** TDCS for the ionization-excitation reaction \( \text{He}(e, 2e)\text{He}^+ \) when the helium ion is left in the state \( n_0 = 2 \). The fast scattered electron energy is \( E_s = 5500 \text{ eV} \), while the slow ejected electron energy is: a) \( E_1 = 5 \text{ eV} \); b) \( E_1 = 10 \text{ eV} \); c) \( E_1 = 75 \text{ eV} \). The scattering angle of the fast incident electron is fixed \( \theta_s = 0.35^\circ \), and the angle of the ejected electron \( \theta_1 \) varies relative to the incident electron direction. All electron velocities are disposed on the same plane. The CCC calculations [11] are depicted by the dashed lines. The experimental data are borrowed from [1].
The fully resolved five-fold differential cross section 5DCS of the electron-impact double ionization reaction \( \text{He}(e,3e)\text{He}^{++} \). The energy of the scattered electron is \( E_s = 5500 \text{ eV} \), and the energies of the slow ejected electrons are \( E_1 = E_2 = 10 \text{ eV} \). The scattering angle of the fast incident electron is fixed, \( \theta_s = 0^\circ \), and the angles of the ejected electrons are \( \theta_1 \) and \( \theta_2 \), where one angle is fixed while the other angle varies relative to the incident electron direction. All electron velocities are disposed on the same plane. The absolute measurements and CCC calculations (dashed line) are borrowed from [12].

The results for the FDCS, \( \sigma^{(5)} \), are presented in Fig. 2. The in-plane angle \( \theta_1 \) of one of the two slow electrons is fixed, while the in-plane angle \( \theta_2 \) of the other ejected slow electron is varied. The energy of the scattered electron \( E_s = 5500 \text{ eV} \), and its in-plane angle \( \theta_s = 0.45^\circ \) is also fixed in all experiments. The energies of the slow electrons are \( E_1 = E_2 = 10 \text{ eV} \). It is seen that our results quite satisfactorily describe the experimental distributions both in shape and
in magnitude. The latter circumstance favorably distinguish our calculations from the previous ones [12].

In summary, we can conclude that the proposed numerical scheme and the performed calculations demonstrate the importance of accounting for the whole two-body continuum spectrum. The method of pseudostates, which replaces the continuum by a finite number of states with positive energies, seems to be faced with serious difficulties as to the magnitude of the calculated differential cross sections, especially when the resulting final-state wave function is employed for the calculation of the (e,3e) matrix elements.

Acknowledgments

This work is partially supported by the scientific program "Far East - 2008" of the Russian Foundation for Basic Research (regional grant 08-02-98501).

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