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ELASTIC CROSS SECTIONS CALCULATIONS FOR e — He(3^3L) LOW-ENERGY SCATTERING

D. KOLEDIN

Institute of Physics, PO Box 57, 11001 Belgrade, Yugoslavia and Department of Biophysics, Faculty of Medicine, University of Belgrade, Belgrade, Yugoslavia

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A simple analytical procedure, proposed by Grujić and Koledin, essentially based on the exact resonance method, has been applied in calculating elastic cross sections for scattering process e — He (3^3L), within the noquenching approximation, in the low-energy region.

One of the main achievements in atomic physics during the last twenty years has been the development of systematic, precise quantitative calculations in electron — atom scattering, in parallel with more and more extensive and high quality experiments in this field. However, among the numerous many body techniques developed to deal with complex atomic systems, there is no exact analytical treatment of a complete scattering process. A number of semianalytical approximate methods[1], combined with the progress in computational facilities, are able to provide rather accurate cross sections for various scattering phenomena[2] but often at the very high price of a computing time consumed. On the other hand, in some problems in atomic physics, such accurately calculated cross sections (or the corresponding scattering matrix elements) are not required, approximate analytical forms being sufficient[3].

In calculating various cross sections for electron — hydrogen-like targets scattering, in the low-energy region where high-energy methods, like the Born approximation, are not valid, it is very convenient to apply the exact resonance method[4]. However, in the case of a non-hydrogenic target this method is not applicable, because the splitting of the sublevels cannot be neglected. On the other hand, as proposed by Grujić and Koledin[5)], the exact resonance method can be extended to the nondegenerate target, for the impact electron energy much larger than a typical separation of the excited atom sublevels with the same principal quantum numbers. Unfortunately, this extension to the nondegenerate atomic systems is not able ensure convergence in the case of inelastic cross sections. Namely, the cross sections for $s - p$ and $p - d$ transitions behave as l^{-1} (l being the total angular momentum quantum number).

Applicability of this method to the quantum theory of Stark broadening of nonhydrogenic lines from plasmas is envisaged in particular. Namely, in the formula for the half-width and shift of an isolated nonhydrogenic line[3)] quantity $1 - S_i S_f$ is met, where $S_{i(f)}$ are the diagonal scattering matrix elements for the initial (final) state of the transition. This is of special importance at low impact energy, when second and higher order processes make significant contributions to $S_{i(f)}$ [6)].

This approximative analytical treatment is applied to the case of e — He (3^3L) scattering in the energy region $0.7 < E_e < 3.7$ eV. Expression for the scattering matrix is given by[5)]

$$\hat{S} = \hat{K}^{1/2} \exp(\mathrm{i}\, \pi\, l_2)\, \hat{U} \exp(\mathrm{i}\, \gamma) \hat{U}^{+} \hat{K}^{-1/2} \tag{1}$$

where $\hat{K}^2 = ||k_i^2 \delta_{ij}||$ is the impact energy matrix, l_2 is angular momentum of colliding electron and $\hat{U}$ is unitary matrix which diagonalizes the dipole potential matrix, $\hat{V}$, including corresponding centrifugal terms ($\hat{V} = ||[v_{ij}(1 - \delta_{ij}) + l_2 (l_2 + 1)\, \delta_{ij}] r^{-2}||$, v_{ij} being the multipole components of the direct interaction potential for e — He). Diagonal matrix $\hat{U}^{+} \hat{V} \hat{U} = \mu\, (\mu + 1)$ determines real numbers:

$$\gamma_j = \begin{cases} -\pi\, \mu_j, & \mu_j = \mu_j^* \\ 2\delta_j + \pi/2 & \mu_j \neq \mu_j^* \end{cases}, \quad j = 1, 2, \ldots, N, \tag{2}$$

N being the number of channels incorporated. When μ-s take complex values, $\mu_j = -0.5 + \mathrm{i}\, \lambda_j$, ($\lambda_j$ — real), we have

$$\tan \delta_j = \tanh(\pi\, \lambda_j/2) \cot\left(\lambda_j \ln \frac{\tilde{k}_j}{K_o}\right) \tag{3}$$

where K_0 is given by: $K_0 = 2\,(E - E_r)$, E and E_r being the energies of the resonant parent state and corresponding negative ion, respectively; the momenta $\tilde{k}_j$ are defined in the following way

$$\hat{U}^{+} \hat{K}^2 \hat{U} = \hat{k}^2 + \hat{\Delta},\ \hat{k}^2 = \overline{k}_i^2\, \hat{I}$$

$$\tilde{k}^2 = \hat{k}^2 + \hat{\Delta}',\ \hat{\Delta} = \hat{\Delta}' + \hat{\Delta}'' \tag{3a}$$

where $\overline{k}_i^2$ is relative to the arithmetic mean of two mutually most separated sublevels and $\hat{\Delta}'$ is diagonal part of the matrix $\hat{\Delta}$. Eq. (1) follows, and, therefore, the method is valid under assumption $|k^2 + \Delta_{ii}| \gg \Delta_{ij}$.

In calculating the dipole potential matrix elements, the multipole expansion method[7] is applied. Analytical orbital wave functions for the two-electron atom, based on the »frozen core« approximation and more convenient in many applications than numerical Hartree — Fock orbitals of a comparable accuracy, are used[8,9]. For $l > 3$ (l being the total angular momentum) all μ-s turn out to be real (as opposite to the case $l \leq 3$). We have made use of experimental data[10] for evaluating $K_0 - s$ (see Table 1).

Table 1.

State	E_r (eV)	K_0 (au)
(3^2S)	22.460	0.13895
(3^2P)	22.650	0.16474
(3^2D)	22.885	0.11784
(3^2F)	23.090	0.12116

Bound state energies and K_0 wave numbers of He^-.

Since Heddle[10] has experimentaly observed three bound states: He^- (3^2S), He^- (3^2P) and He^- (3^2D), the last value in the Table 1, for K_0 (3^2F), as a pseudostate, is obtained by the linear extrapolation of the experimental data.

Defining nine scattering channels (see Table 2) and using Eq. (1) for the scattering matrix, we have calculated elastic partial cross sections by the standard formula

$$Q^l (i \to j) = \frac{\pi}{k_i^2} \sum_{l_i} \frac{2l+1}{2l_i+1} \left| S_{ij}^{l_i l_j} - \delta_{l_i l_j} \right|^2 \tag{4}$$

where k_i is the impact momentum in the corresponding channel and l_i denotes the initial value of the atomic electron orbital quantum number. Summing over l values, the total cross sections for scattering on $n = 3$ states (see Fig. 1) are finally obtained.

Table 2.

	parity $(-)^l$			parity $(-)^{l+1}$	
atomic electron	$3s$	$3p$	$3d$	$3p$	$3d$
impact electron	l	$l-1$ $l+1$	$l-2$ l $l+2$	l	$l-1$ $l+1$

The channels of e — He (3^3L) scattering.

As can be seen from Fig. 1, all cross sections exhibit similar monotoneous behaviour, which is mainly determined by k_l factor in Eq. (4). Since the method applied is valid if $|\hat{k}^2 + \hat{\Delta}'| \gg |\hat{\Delta}''|$, cross sections shown in Fig. 1 should be reliable for $E_e \geq 1$ eV, as indicated by the broken line in the figure. Below 1 eV the actual elastic cross sections may differ from these shown here, but the overall behaviour should be the same.

Up to now no measurements of the cross sections calculated have been reported, nor other theoretical calculations have been done to our knowledge.

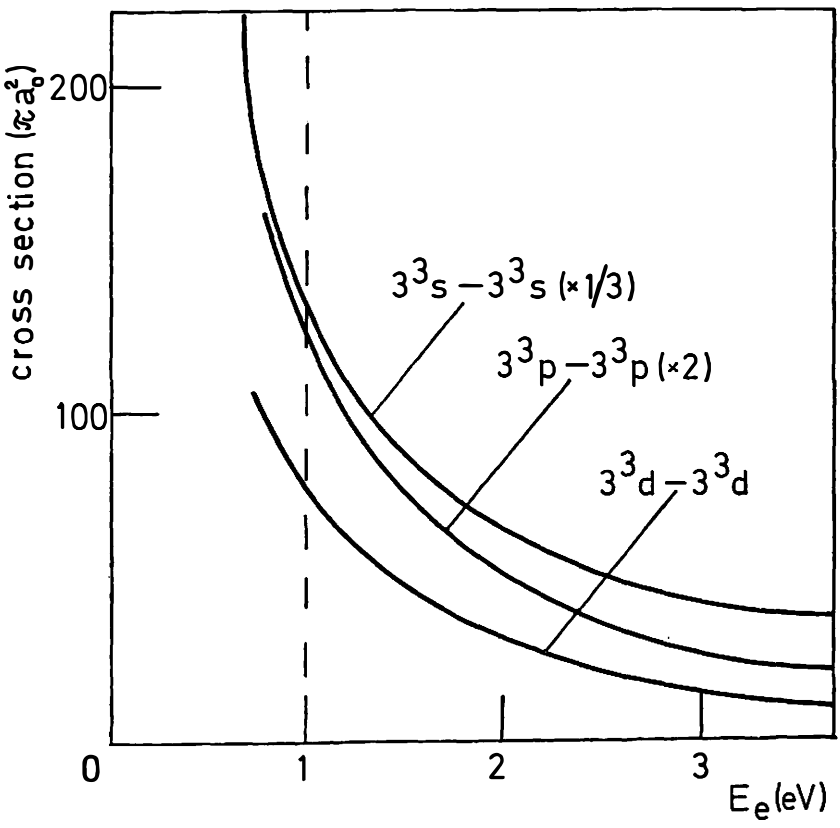

Fig. 1. Elastic cross sections for the scattering on $n = 3$ triplet states of helium. E_e is electron energy relative to 3^3S threshold.

It is worth to note that this simple analytical method may be useful for indicating of resonant (or virtual) states in the corresponding channel. Namely, the very appearance of the complex angular momentum quantum numbers in the rotated functional space indicates the presence of bound states, as demonstrated by Gailitis and Damburg[11]. In this respect, our results are consistent (except for $l = 3$) with experimental data[10].

The principal shortcoming of the method employed is the neglect of exchange potential, which may be crucial for lower partial waves, in the close vicinity of the threshold. However, in some applications, as is the case with the quantum theory fo Stark broadening[3], the main contributions come from higher partial waves at the relatively large energies above the threshold.

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IZRAČUNAVANJE EFIKASNIH PRESEKA ZA ELASTIČNO NISKO-ENERGETSKO RASEJANJE e — He(3^3L)

D. KOLEDIN

Institut za fiziku, p. f. 57 Beograd i Medicinski fakultet, Beograd

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Jednostavan analitički postupak, u osnovi zasnovan na metodu tačne rezonance, koji su postavili Grujić i Koledin, iskorišćen je za izračunavanje elastičnih efikasnih preseka za rasejanje niskoenergetskih elektrona na pobuđenom atomu helijuma, u stanju He (3^3L).