THEORETICAL CALCULATION FOR THE DOUBLE EXCITATION OF HELIUM TO THE $(2p2p)^1S$ STATE

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Abstract. Double excitation cross sections of the helium to the $(2p2p)^1S$ state by proton and antiproton impact have been evaluated. We have used a perturbation expansion in the projectile-electron interaction, and have been included in our calculations the first-order and the time ordered second-order (TS2) terms. Our results are compared with other theoretical calculations.

Introduction

In the theoretical study of two-electron transitions helium is the most investigated atom, because no other electrons are involved in the process. Various groups have studied two-electron transitions in the past several years theoretically and experimentally.

The experimental study of Andersen *et al* and of Hvelplund *et al* [1-3] on the double ionization of helium has shown unambiguously the dependence of the cross sections on the sign of the projectile charge. For the double ionization of helium they have obtained, that the cross sections for antiprotons are up to a factor of two higher than for the equivelocity protons over a wide velocity range. A similar dependence has been reported by Bailey *et al* [4] for the ionization-excitation.

The situation is not so clear for the double excitation of helium. The doubly excited states of the helium atom are not stationary discrete states; they are all autoionizing states, their energy lying above the single-ionization limit. In these conditions, information about the population of the doubly excited states can be obtained by

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the analysis of the energy spectra of the ejected electron, the different autoionizing states appearing as resonances. The theoretical interpretation of these experimental spectra is difficult, because of the interference of the direct and resonant ionization processes and the three-body Coulomb interaction in the final state between the scattered projectile, ejected electron and residual ion.

There have been published some experimental [5,6] and theoretical [7-9] studies on the double excitation process. The different calculations of the double excitation cross sections of the helium atom usually do not agree with each other.

The complete theoretical description of the resonant ionization processes at intermediate projectile energies (100 keV/u) performed by Godunov *et al* [10] made it possible for Moretto-Capelle *et al* [11] to extract double excitation cross sections from their experimental spectra of the ejected electron, obtained with a high resolution spectrometer. These cross sections not only complete the experimental data of Giese *et al* [6] to lower energies, but are also stated to be exact.

Our previous study on the double excitation of the helium [7] has produced cross sections in very good agreement with these latest experimental data. The considered transitions have been to the $(2s2p)^1P$, $(2p2p)^1D$ and $(2s2s)^1S$ states.

In the present paper we complete our previous work [7], by calculating the cross sections for the double excitation of helium to the $(2p2p)^1S$ state. Beside the proton projectiles we have also performed calculations for antiprotons and we analyze the dependence of the cross section on the sign of the projectile charge. We have considered a wide range of the impact energy (from 100 keV to 10 MeV) in order to discuss the importance of different mechanisms as a function of energy. Our results are compared with other theoretical cross sections. There are no experimental data for this state.

Theory

The theoretical method applied for the present calculation has been discussed in detail in the previous papers of one of the authors [13,14]. This is the impact-parameter (semiclassical) method, applying second-order perturbation approximation.

For the calculation of the double-excitation cross section of the helium by proton and antiproton impact we treat the projectile as a classical particle which moves on a straight-line trajectory. The interaction of the projectile with the two electrons

$$V(t) = V_1(t) + V_2(t) \tag{1}$$

is considered as a perturbation. The wave function of the two-electron system is approximated as a product of one-electron wave functions. The unperturbed Hamiltonian of the two electrons is

$$H^0 = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{Z_T}{r_1} - \frac{Z_T}{r_2} + \frac{1}{r_{12}}. \tag{2}$$

Applying time-dependent perturbation theory, the first-order probability amplitude for the transition of the electrons can be written as

$$a^{(1)} = -i\int_{-\infty}^{+\infty} dt e^{i(E_f - E_i)t} \langle f \,|[V_1(t) + V_2(t)]\,| i\rangle. \tag{3}$$

Here $|i\rangle$ and $|f\rangle$ are the initial and final two-electron states, respectively, E_i and E_f the energies of these states, while $V_1(t)$ and $V_2(t)$ stand for the two time-dependent projectile-electron interactions. The second-order amplitude is obtained to be:

$$a^{(2)} = -\sum_k \int_{-\infty}^{+\infty} dt e^{i(E_f - E_k)t} \langle f \,|V_1(t)\,| k\rangle \int_{-\infty}^{t} dt' e^{i(E_k - E_i)t'} \langle k \,|V_2(t')\,| i\rangle -$$

$$-\sum_k \int_{-\infty}^{+\infty} dt e^{i(E_f - E_k)t} \langle f \,|V_2(t)\,| k\rangle \int_{-\infty}^{t} dt' e^{i(E_k - E_i)t'} \langle k \,|V_1(t')\,| i\rangle. \tag{4}$$

For the description of the initial and final states we have used configuration-interaction (CI) wave-functions, which are written as a sum of products of one-electron orbitals:

$$|i\rangle = \sum_l c_l \,|i_1^l\rangle\,|i_2^l\rangle.$$

$$|f\rangle = \sum_j d_j \,|f'^j_1\rangle\,|f'^j_2\rangle. \tag{5}$$

Introducing the initial- and final-state CI wave-functions in the first-order amplitude (3), one obtains a sum of products of overlap integrals and one-electron transition amplitudes:

$$a^{(1)} = -i\sum_l \sum_j c_l d_j^* \langle f'^j_2 \,|\, i_2^l\rangle \int_{-\infty}^{+\infty} dt e^{i(E_f - E_i)t} \langle f'^j_1 \,|V_1(t)\,| i_1^l\rangle$$

$$-i\sum_{l}\sum_{j} c_l d_j^{*} \langle f'^{j}_{1} \mid i^{l}_{1}\rangle \int_{-\infty}^{+\infty} dt e^{i(E_f - E_i)t} \langle f'^{j}_{2} \mid V_2(t) \mid i^{l}_{2}\rangle. \qquad (6)$$

In our second order term the transition is caused by two consecutive projectile-electron interactions. We keep track of the time ordering: the energy transfer to the individual electron depends on the order of the interactions. In order to calculate the second-order amplitude, from the infinite number of intermediate states we keep only the most important ones. These are assumed to be those reachable from the initial and the final state by a single-electron transition. Simplified, in the considered intermediate states one of the electrons is in its initial state and the other one have reached the final state. In this approximation one obtains for the second order amplitude:

$$\begin{aligned} a^{(2)} = & -\sum_{j,k,l,} d_j^{*} c_l \langle f'^{j}_{2} \mid f^{k}_{2}\rangle\langle i'^{l}_{1} \mid i^{l}_{1}\rangle \int_{-\infty}^{+\infty} dt e^{i(E_f - E_{k2l1})t} \langle f'^{j}_{1} \mid V_1(t) \mid i'^{l}_{1}\rangle \\ & \times \int_{-\infty}^{t} dt' e^{i(E_{k2l1} - E_i)t'} \langle f^{k}_{2} \mid V_2(t') \mid i^{l}_{2}\rangle \\ & -\sum_{j,k,l} d_j^{*} c_l \langle f'^{j}_{1} \mid f^{k}_{1}\rangle\langle i'^{l}_{2} \mid i^{l}_{2}\rangle \int_{-\infty}^{+\infty} dt e^{i(E_f - E_{k1l2})t} \langle f'^{j}_{2} \mid V_2(t) \mid i'^{l}_{2}\rangle \\ & \times \int_{-\infty}^{t} dt' e^{i(E_{k1l2} - E_i)t'} \langle f^{k}_{1} \mid V_1(t') \mid i^{l}_{1}\rangle. \end{aligned} \qquad (7)$$

Here E_{k2l1} stands for the energy of the intermediate state when one electron is in the $|i'^{l}_{1}\rangle$ state and the other one in $|f^{k}_{2}\rangle$, while E_{j1l2} represents the energy of the intermediate state described by the $|f^{k}_{1}\rangle|i'^{l}_{2}\rangle$ configuration.

For the description of the bound state of helium we have used the CI wave-functions of Nesbet and Watson [14]. The wave-functions for the excited *(2p2p)^{1}S* state have been generated by us. We have used a variational method to obtain the coefficients for each configuration, namely *2s^2*, *2p^2*, *2s3s* and *2p3p*. All these configurations have been taken into account in the first-order amplitude. The second-order amplitude has been calculated by using only the basic *1s^2* configuration for initial state and *2s2s, 2p2p* configurations for the final state.

For this given state, the first-order amplitude is purely imaginary. The second-order amplitude, because of the time-ordering term, is complex. Interference occurs between first-order and second-order amplitudes, so we obtain different cross sections for positively and negatively charged projectiles.

The cross section can be calculated by integrating the square of the amplitude over the impact parameters:

$$\sigma = 2\int | a^{(1)} + a^{(2)} |^2 \, d^2b \qquad (8)$$

Results and discussion

Our calculated cross sections for the double excitation of helium for proton and antiproton projectiles as a function of the impact energy are plotted in Figure 1. Our results are compared with the theoretical cross sections calculated by Fritsch and Lin [8] in a close-coupling approximation, and with those of Moribayashi *et al* [9], calculated both by a close-couplin method (CC) and by a second-Born approximation. As Figure 1. shows, we have obtained higher cross sections for antiprotons than for protons in contradiction with the other theoretical predictions, but in accordance with the usual trend, proven experimentally, for most of the two-electron transitions in helium [1-4]. For example at 100 keV impact energy the cross section for antiproton projectile is more than 2.5 times higher than for the proton projectile. This large ratio, above 2 MeV projectile energy, tends to decrease.

The second-order amplitude has a real, non-time-ordered part and an imaginary part due to the time ordering. The non time-ordered part corresponds to two independent one-electron transitions from *1s* to *2p.* The imaginary part gives with the first-order amplitude a large interference term in transition probability, proportional to Z^3 (where Z is the charge of projectile), leading to a large difference in cross sections for protons and antiprotons. This difference decreases with the energy, because at high energies the second-order contribution becomes negligable, and so does the interference term.

In Figure 2. we have plotted the first- and second-order contribution to the cross section for the excitation of the $(2p2p)^1S$ state as a function of the projectile energy. At lower energies, the second-order contribution is larger than the first-order contribution. At around 300 keV they become equal, and at higher energies the first-order contribution dominates.

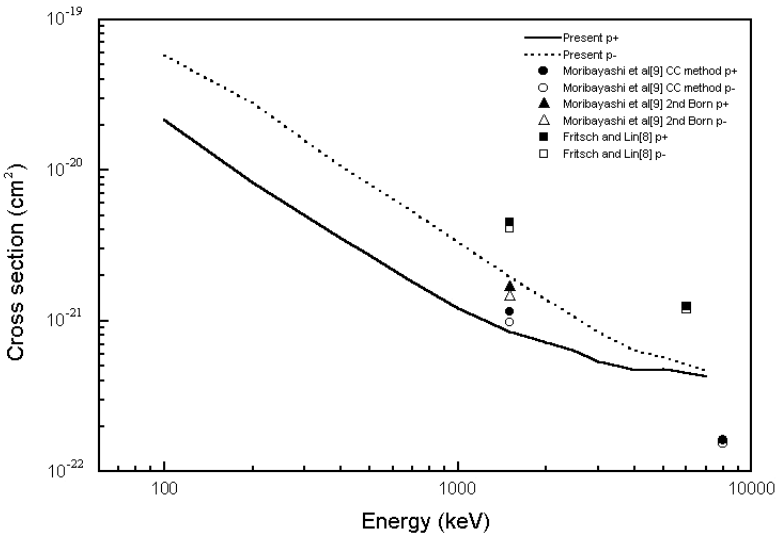

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Figure. 1. Cross sections for the double excitation of helium to the *(2p2p)*^{1}*S* state as a function of the projectile energy by proton and antiproton impact.

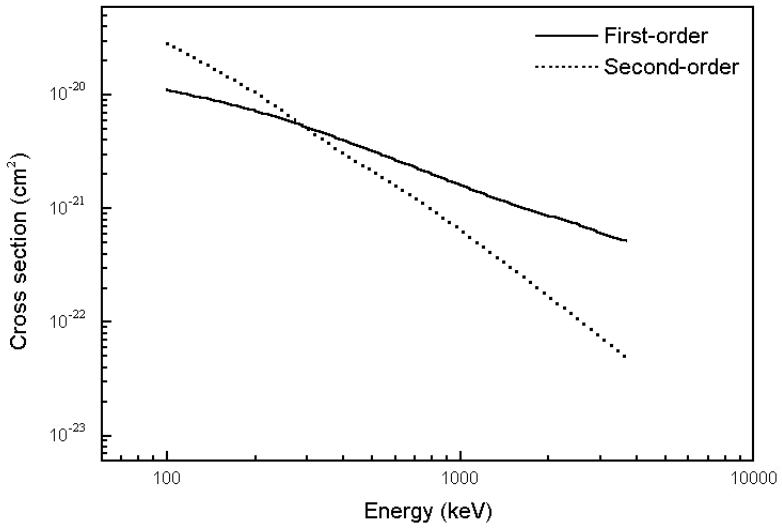

Figure. 2. First-order and second-order contribution to the cross sections for the double excitation of the helium atom to the *(2p2p)*^{1}*S* state as a function of the projectile energy.

Conclusions

We have calculated with a well-tested method the cross sections for the double excitation of helium to the $(2p2p)^1S$ state by proton and antiproton impact. Electron correlation is taken into account by the use of CI wavefunctions in the initial an final states. We obtain higher cross sections for antiprotons than for protons, in contradiction with other theoretical results, but in accordance with the general trend observed for two-electron transitions.

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