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Theoretical study of the simultaneous ionization and excitation of helium by fast charged projectiles

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Abstract

Cross sections for the simultaneous ionization and excitation to the 2s state of the helium atom by fast proton and antiproton impact have been calculated. We apply the impact parameter method and use a second-order perturbation approximation. Electron correlation is taken into account in the initial state but is neglected in the final state. The cross sections obtained for protons are higher than those obtained for antiproton projectiles, in accordance with the theoretical findings of Sidorovich (V.A. Sidorovich, J. Phys. B 30 (1997) 2187).

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1. Introduction

The multi-electron transitions have attracted much interest in the past, both on the theoretical [1–9] and on the experimental [10–15] side. It has been made clear that taking into account the electron correlation is essential for a correct theoretical description of these transitions [16].

The less studied two-electron transition in the helium atom is the ionization–excitation. A few experimental data are available for the excitation of the *n*p states [12–14] for proton and electron projectiles. Similarly to the double ionization, the cross sections obtained for negative projectiles are higher than those obtained for equivelocity positive projectiles. Most of the theoretical calculations are made only for electrons [2–4] and do not deal with the dependence of the cross sections on the sign of the projectile charge. The only published study on this dependence [17] qualitatively reproduces the experimental findings.

The ionization–excitation to an *n*s final state of the residual ion has not been investigated experimentally because of the difficulties in measuring the population of these excited state ($n\text{s} \rightarrow 1\text{s}$ is an optically not allowed transition). Recently Sidorovich has published a theoretical study on the simultaneous ionization and excitation of helium to the 2s state by fast protons and antiprotons [5]. He has found that the cross sections for protons are higher than those for antiprotons, opposite relative to other two-electron transitions. On the

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other hand, his cross sections for antiprotons are not in agreement with other theoretical results for equivelocity electrons [2,3].

In this paper we present our calculated cross sections for the ionization–excitation of the helium to the 2s state induced by fast protons and antiprotons. We compare our results with other theoretical data, and investigate the importance of different mechanisms in the considered transition.

2. Theory

The framework of our calculation is the impact parameter method. In this model the projectile moves on a classical straight-line trajectory. This method is suitable for proton and antiproton projectiles above 1 a.u. velocity (25 keV), but for electrons, because of its lower mass, this approximation gives reliable results only, if the energy of the projectile is much higher than the energy transfer. The average energy transfer in case of the ionization–excitation of the helium is around 100 eV. The impact parameter approximation can be taken to be valid for electrons with velocities above 5 a.u. (350 eV). This is the reason why direct comparison with other theoretical results for electrons below 350 eV energy is not possible.

For the study of the evolution of the two-electron system we have applied the second-order time dependent perturbation theory. The method we use has been described in detail elsewhere [8,9] and has been applied for the double ionization [9] and the double excitation [18] of the helium, and also for the ionization–excitation to the np states [17,19].

The first-order probability amplitude for the transition of the electrons can be written as

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

Here $|i\rangle$ and $\langle f|$ are the initial respective the final two-electron states, E_i and E_f are 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

$$\begin{aligned} a^{(2)} = &-\sum_k \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{i(E_f-E_k)t}\langle f \mid V_1(t) \mid k\rangle \\ &\times \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{i(E_k-E_i)t'}\langle k \mid V_2(t') \mid i\rangle \\ &-\sum_k \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{i(E_f-E_k)t}\langle f \mid V_2(t) \mid k\rangle \\ &\times \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{i(E_k-E_i)t'}\langle k \mid V_1(t') \mid i\rangle. \end{aligned} \tag{2}$$

Here we have to sum up over the intermediate states $|k\rangle$ with energies E_k, the infinite number of eigenstates of the two-electron unperturbed Hamiltonian.

For the description of the initial state we have used configuration-interaction (CI) wavefunctions [20], which are written as a sum of products of one-electron orbitals

$$|i\rangle = \sum_l c_l |i_1^l\rangle |i_2^l\rangle. \tag{3}$$

The final state is described by a properly symmetrized product of two one-electron wavefunctions

$$|f\rangle = \frac{1}{\sqrt{2}}\left(|f_c'(1)\rangle|f_e'(2)\rangle + |f_e'(1)\rangle|f_c'(2)\rangle\right). \tag{4}$$

Here $|f_c'\rangle$ stands for the state of the ejected electron, while $|f_e'\rangle$ represents the excited state of the electron in the residual ion. The wavefunction of the bound electron is calculated neglecting the effect of the ejected electron, but the wavefunction of the free electron is calculated taking into account the screening potential created by the other electron.

Introducing the initial and final state wavefunctions into the first-order amplitude (1), one gets a sum of products of overlap integrals and one-electron transition amplitudes

$$a^{(1)} = -i\frac{1}{\sqrt{2}}\sum_l c_l \times \left[\langle f'_e(2)|i'^l_2\rangle \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_i)t}\langle f'_c(1)|V_1(t)|i'^l_1\rangle + \langle f'_e(1)|i'^l_1\rangle \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_i)t}\langle f'_c(2)|V_2(t)|i'^l_2\rangle + \langle f'_c(2)|i'^l_2\rangle \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_i)t}\langle f'_e(1)|V_1(t)|i'^l_1\rangle + \langle f'_c(1)|i'^l_1\rangle \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_i)t}\langle f'_e(2)|V_2(t)|i'^l_2\rangle\right]. \quad (5)$$

The first two terms can be interpreted as the shake-up, and the last two as the shake-off contributions to the first-order amplitude.

In order to calculate the second-order amplitude, from the infinite number of the 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. Because in the case of the second-order amplitude the correlation is only a small correction (while the first-order amplitude of the two-electron transition is nonzero only because of the electron–electron interaction), in the calculation of the second-order amplitude we have taken into account only the basic, $1s^2 \equiv |i'^1_1\rangle|i'^1_2\rangle$ configuration for the description of the initial state. In this approximation one obtains for the second-order amplitude

$$a^{(2)} = -\frac{1}{\sqrt{2}}\langle f'_e(2)|f_e(2)\rangle\langle i'_1|i'^1_1\rangle \times \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_{ie})t}\langle f'_c(1)|V_1(t)|i'_1\rangle \times \int_{-\infty}^{t} dt'\, e^{i(E_{ie}-E_i)t'}\langle f_e(2)|V_2(t')|i'^1_2\rangle - \frac{1}{\sqrt{2}}\langle f'_c(2)|f_c(2)\rangle\langle i'_1|i'^1_1\rangle \times \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_{ic})t}\langle f'_e(1)|V_1(t)|i'_1\rangle \times \int_{-\infty}^{t} dt'\, e^{i(E_{ic}-E_i)t'}\langle f_c(2)|V_2(t')|i'^1_2\rangle - \frac{1}{\sqrt{2}}\langle f'_e(1)|f_e(1)\rangle\langle i'_2|i'^1_2\rangle \times \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_{ie})t}\langle f'_c(2)|V_2(t)|i'_2\rangle \times \int_{-\infty}^{t} dt'\, e^{i(E_{ie}-E_i)t'}\langle f_e(1)|V_1(t')|i'^1_1\rangle - \frac{1}{\sqrt{2}}\langle f'_c(1)|f_c(1)\rangle\langle i'_2|i'^1_2\rangle \times \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_{ic})t}\langle f'_e(2)|V_2(t)|i'_2\rangle \times \int_{-\infty}^{t} dt'\, e^{i(E_{ic}-E_i)t'}\langle f_c(1)|V_1(t')|i'^1_1\rangle. \quad (6)$$

Here E_{ie} stands for the energy of the intermediate state when one electron is in the $|i'_1\rangle$ (unscreened) initial state and the other one in the $|f_e(2)\rangle$ excited state, while E_{ic} represents the energy of the intermediate state described by the $|i'_1 > |f_c(2)\rangle$ configuration. The unprimed one-electron states are calculated with the other electron in the initial state, while the primed ones with the other electron in the final state, so the change in the screening (the relaxation of the orbitals [21]) is taken into account.

3. Results

Cross sections for the ionization of the helium with the simultaneous excitation of the 2s state as a function of the projectile velocity are represented in Fig. 1. We have made our calculations in a wide velocity range between 1 and 80 a.u. Above 2 a.u. projectile velocity the cross sections obtained for protons are higher than those for antiprotons. The difference reaches almost a factor of 2 between 5 and 8 a.u. At very high velocities this difference becomes negligible.

The ionization–excitation to the 2s state is the first two-electron transition, where higher cross sections are predicted for the positive projectiles than for the negative ones. Unfortunately, there are no experimental data for this transition, but our conclusion agrees with the findings of Sidorovich [5]. Furthermore, the agreement between these two theoretical calculations is also quantitatively good

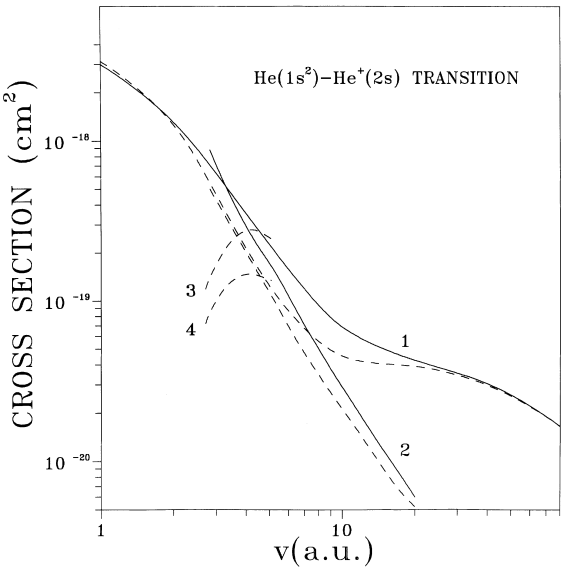

Fig. 1. Cross sections for the ionization–excitation to the 2s state of the helium by proton and antiproton impact as a function of the projectile velocity. Our results (curves 1) are compared with the cross sections computed by Sidorovich [5] (curves 2), and the cross sections for electron projectiles of Rudge [2] (curve 3) and of Raeker et al. [3] (curve 4). The solid and the dashed lines stand for proton and antiproton (or electron) projectiles, respectively.

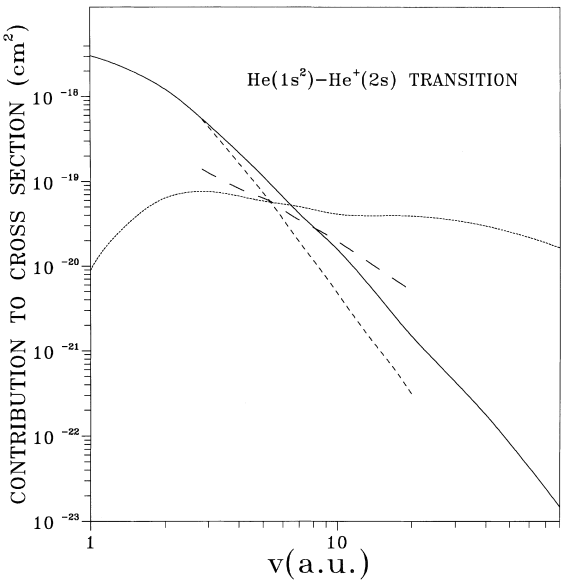

Fig. 2. The contributions of the first- and second-order amplitudes to the ionization–excitation cross section of the helium by proton or antiproton impact. The solid and the dotted line represent the second- and the first-order contributions calculated in the present work, respectively. The short-dashed and the long-dashed line stand for the same quantities computed by Sidorovich [5].

below 7 a.u. projectile velocity. At higher velocities our cross sections are larger. In the same Fig. 1 we have plotted the electron impact cross sections of Rudge [2] and of Raeker et al. [3]. The direct comparison of our results with these calculations is difficult, because electrons behave identically with equivelocity antiprotons only at high velocities, where these authors did not make calculations.

The first- and second-order contributions to the cross section are plotted in Fig. 2. As expected, at low velocities the second-order term, and at high velocities the first-order term dominates. Since the dependence of the cross section on the sign of the projectile charge is due to the interference of the first- and second-order amplitudes, at low and high velocities, where one of the two terms dominates, the interference effect is negligible. This is the reason why we have obtained for these extreme velocities similar cross sections for protons and antiprotons. Comparing our first- and second-order contributions with those obtained by Sidorovich [5], one observes that his data decrease more rapidly with the increasing velocity. The difference in behavior is more striking for the first-order contribution, where our data decrease very slowly.

The first-order amplitude (5) is a sum of two different types of terms. The shake-up contribution is due to the ionization of the target by a projectile–electron interaction, and the excitation of the other electron by electron–electron interaction. In case of the shake-off the projectile excites one electron, and the other leaves the atom due to the interaction with the first one. In order to investigate, why the first-order amplitude decreases so slowly, we have separated the shake-off and the shake-up contributions (Fig. 3). In this figure one can see, that the shake-off mechanism is responsible for the peculiar velocity behavior of the first-order contribution. The shake-off term increases up to 20 a.u. projectile velocity, and begin to decrease only above this.

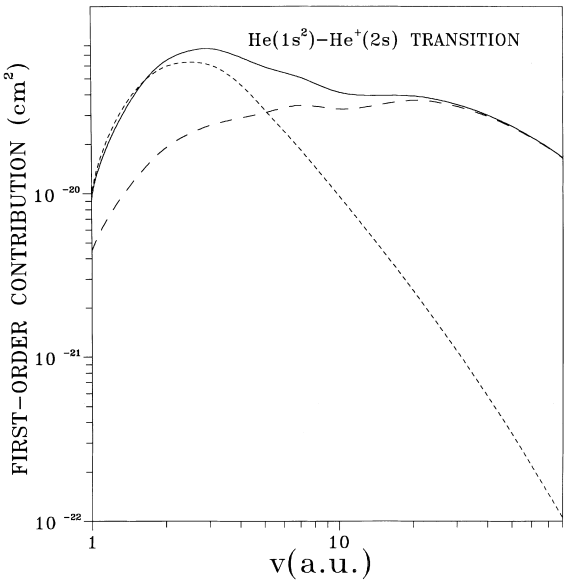

Fig. 3. The two different mechanisms leading to the first-order cross section. Shake-up: short-dashed line; shake-off: long-dashed line; total first-order cross section: solid line.

4. Conclusion

We have performed second-order perturbation theory calculations for the ionization–excitation of the helium to the 2s state induced by proton and antiproton impact. The cross sections obtained for protons are higher than those obtained for antiprotons in a wide projectile velocity range, in accordance with the results of Sidorovich [5]. The quantitative agreement between these two calculations is not very good, mainly because of the shake-off mechanism taken into account by us.

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