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Double-differential cross sections for the ionization-excitation of the helium by fast proton and antiproton impact

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Abstract

Calculated double differential cross sections are presented for the simultaneous ionization and excitation into the 2p state of the helium atom by fast proton and antiproton impact. We have used the semiclassical impact parameter method and the transition amplitude was calculated in second-order perturbation approximation. We have investigated the dependence of the cross sections on the sign of the projectile charge, and have analyzed the influence on the results of the inclusion of electron correlation in the initial state. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Ionization-excitation of the helium by charged particle impact have been investigated both experimentally [1–7] and theoretically [8–13]. Typically the calculated total cross sections disagree with each other, and only one of the calculations [9] lead to results in reasonable agreement with the experimental data. On the other hand, the theoretical cross sections in the references above are calculated only for electron projectiles, while one of the most interesting features in the experimental data is, that in a wide velocity range cross sections for negative projectiles are by a factor of two larger than the cross sections for equivelocity positive projectiles.

This large difference, observed earlier also for the double ionization of the helium, can be explained (as suggested by McGuire [14]) by the interference between the first-order and second-order processes (Z^3 effect). Based on a second-order perturbation approximation [15,16] one of us has calculated the ionization-excitation cross sections of the helium for proton and antiproton impact in a wide velocity range. This calculation has been done, first using a Hartree–Fock wavefunction for the initial state, taking into account in the first-order amplitude only the shake-off mechanism [17], than using a multi-configuration description of the ground state, including the ground-state correlation mechanism, too [18]. Although we have obtained larger cross sections for

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antiproton projectiles than for protons in qualitative accordance with the experimental data, none of our model has reproduced quantitatively the large experimental ratio of the cross sections obtained with negative and positive projectiles.

In the present Letter we investigate the behavior of the double-differential cross section of the ionization-excitation of the helium. There have been published experimental [6,7] and theoretical [12,13] triple-differential cross sections, but only for electron projectiles. Our specific aim is to study the dependence of the cross sections on the sign of the charge of the projectile, and on the correlation interaction in the initial state.

2. Theory

In our calculations we use the semiclassical impact parameter method, considering the projectile moving on a linear trajectory and we apply second-order time-dependent perturbation theory. The first-order amplitude for the transition from the initial state $|i\rangle$ to the final state $|f\rangle$ is obtained to be

$$a^{(1)} = -i\int_{-\infty}^{+\infty} dt\, \mathrm{e}^{i(\Delta E)t} \langle f | \left[V_1(t) + V_2(t) \right] | i \rangle , \quad (1)$$

where $\Delta E = E_\mathrm{f} - E_\mathrm{i}$ is the energy transfer to the electron system. The time-dependent perturbation potentials $V_j(t) = -Z_\mathrm{p}/|\boldsymbol{R}(t) - \boldsymbol{r}_j(t)|$, $j = 1,2$, are evaluated from the position vectors $\boldsymbol{R}(t)$ and $\boldsymbol{r}_j(t)$ of the projectile ion and the active target electrons, respectively. These projectile-electron interactions can be developed in multi-pole series

$$V_j(t) = -Z_\mathrm{p} \sum_{l'm'} \frac{4\pi}{2l'+1} \frac{r_<^{l'}}{r_>^{l'+1}} Y_{l'}^{m'*}(\hat{R}) Y_{l'}^{m'}(\hat{r}_j) , \quad (2)$$

where $r_< = \min\{R, r_j\}$, $r_> = \max\{R, r_j\}$, and $j = 1,2$.

For the second-order amplitude one gets

$$\begin{aligned} a^{(2)} = &- \sum_k \int_{-\infty}^{+\infty} dt\, \mathrm{e}^{i(E_\mathrm{f} - E_k)t} \langle f | V_1(t) | k \rangle \\ &\times \int_{-\infty}^{t} dt'\, \mathrm{e}^{i(E_k - E_\mathrm{i})t'} \langle k | V_2(t') | i \rangle \\ &- \sum_k \int_{-\infty}^{+\infty} dt\, \mathrm{e}^{i(E_\mathrm{f} - E_k)t} \langle f | V_2(t) | k \rangle \\ &\times \int_{-\infty}^{t} dt'\, \mathrm{e}^{i(E_k - E_\mathrm{i})t'} \langle k | V_1(t') | i \rangle , \end{aligned} \quad (3)$$

including a sum over the intermediate states $|k\rangle$, with energies E_k. The two-electron wavefunctions $|i\rangle$, $|k\rangle$ and $|f\rangle$ are the same with those used in Ref. [18]. Electron correlation is taken into account in the evaluation of the first-order amplitude, by using the configuration-interaction wavefunctions of Nesbet and Watson [19] to describe the initial state:

$$|i\rangle = \sum_l c_l \phi_{il}(1) \phi_{il}(2) . \quad (4)$$

Here ϕ_{il} are one-electron orbitals. The final state is written as:

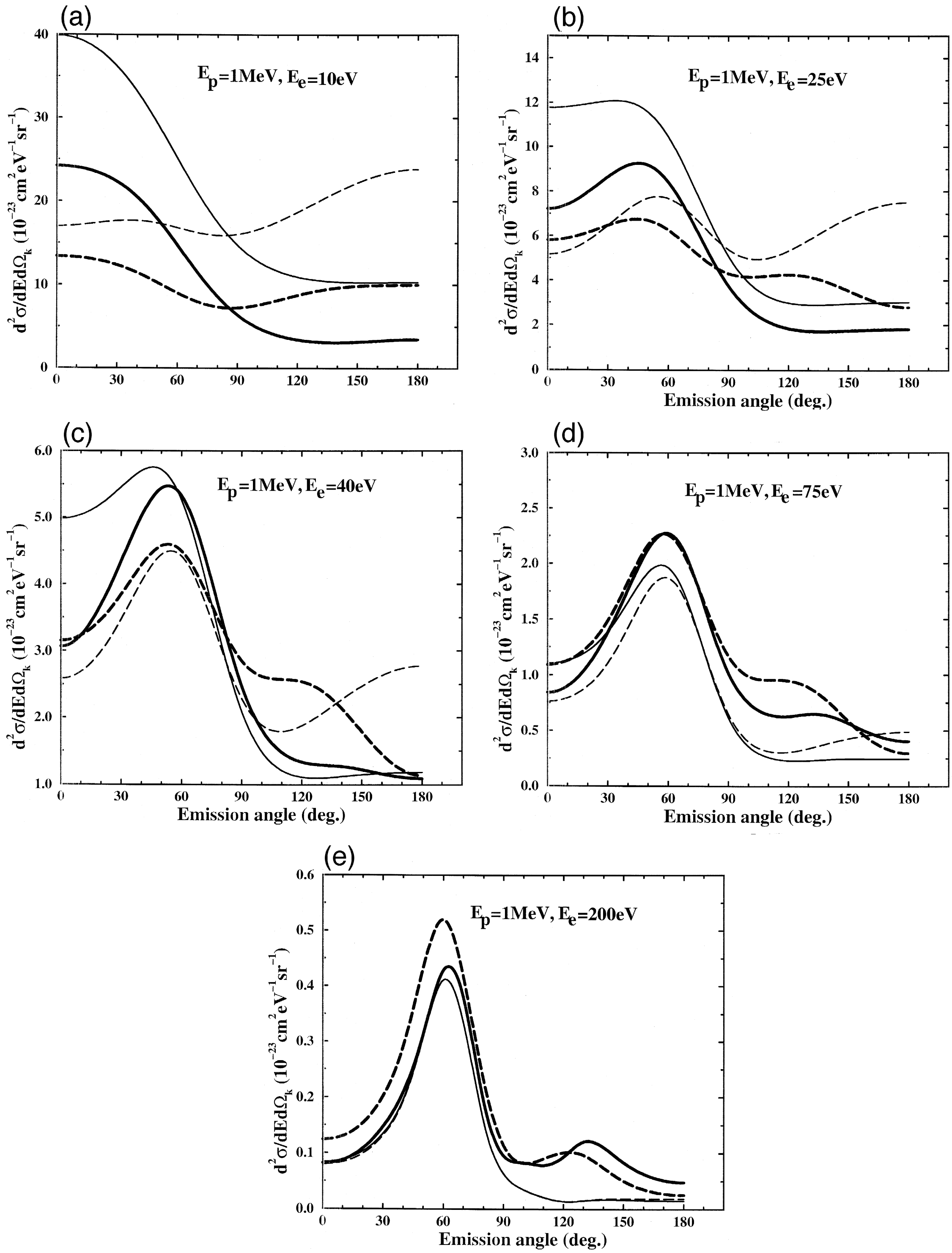
$$|f\rangle = \frac{1}{\sqrt{2}} \left[f_\mathrm{c}'(1) \phi_{2\mathrm{p}}'(2) + \phi_{2\mathrm{p}}'(1) f_\mathrm{c}'(2) \right] , \quad (5)$$

where $\phi_{2\mathrm{p}}'$ stand for the bound electron in the final 2p excited state. The ejected electron is described by a numerically evaluated wavefunction, developed into partial waves:

$$f_\mathrm{c}'(\boldsymbol{k}, \boldsymbol{r}) = \sum_{l_\mathrm{f} m_\mathrm{f}} i^{l_\mathrm{f}} \mathrm{e}^{i(\sigma_{l_\mathrm{f}} + \delta_{l_\mathrm{f}})} R_{kl_\mathrm{f}}'(r) Y_{l_\mathrm{f}}^{m_\mathrm{f}*}(\hat{k}) Y_{l_\mathrm{f}}^{m_\mathrm{f}}(\hat{r}) , \quad (6)$$

where $R_{kl_\mathrm{f}}'(r)$ is the radial function normalized with respect to the momentum, σ_{l_f} is a Coulomb phase-shift, and δ_{l_f} is the phase shift arising from the short range potential. The $R_{kl_\mathrm{f}}'(r)$ wavefunction is calculated in the field of the nucleus and of the bound electron. Electron-electron interaction in the final

Fig. 1. Double-differential cross sections for the ionization-excitation of the helium to the 2p state, for $E_\mathrm{p} = 1$ MeV projectile energy and $E_\mathrm{e} = 10$ eV (a), 25 eV (b), 40 eV (c), 75 eV (d) and 200 eV (e) ejected electron energies, as a function of the ejection angle of the electron. Solid lines stand for proton projectiles and long-dashed lines for antiproton projectiles, while thick lines represent the results using multi-configuration wavefunctions for the initial state and thin lines the results obtained with single-configuration wavefunctions.


(a)
Ep=1MeV, Ee=10eV
(b)
Ep=1MeV, Ee=25eV
(c)
Ep=1MeV, Ee=40eV
(d)
Ep=1MeV, Ee=75eV
(e)
Ep=1MeV, Ee=200eV
d2σ/dEdΩk (10-23cm2eV-1sr-1)
Emission angle (deg.)

state is taken into account only as a mean-field effect, correlation is neglected. This approximation is justified if the outgoing electron is fast, but may introduce some errors, if the electron leaves the atom with low velocity.

Substituting (4) and (5) into the expression of the first-order amplitude (1), and performing the integrals on the matrix elements, one gets:

$$a^{(1)}(\boldsymbol{k},b)$$
$$= (4\pi)^{1/2} \sum_{lml'm'} \sum_{l_f m_f} \sum_{m_e=-1}^{1} (-i)^{l_f} e^{-i(\sigma_{l_f}+\delta_{l_f})}$$
$$\times \sqrt{\frac{2l+1}{(2l_f+1)(2l'+1)}}\, C_{l0l'0}^{l_f 0}\, C_{lml'm'}^{l_f m_f}$$
$$\times Y_{l_f}^{m_f *}(\hat{k}) \int_{-\infty}^{+\infty} dt\, e^{i(E_f-E_i)t}\, Y_{l'}^{m' *}(\hat{R})$$
$$\times \left[M_{l'l}^{2p} A_l^{l_f} + A_l^{2p} M_{l'l}^{l_f} \right], \qquad (7)$$

where $A_l^{l_f}$, A_l^{2p}, $M_{l'l}^{2p}$ and $M_{l'l}^{l_f}$ are radial integrals

$$A_l^{l_f} = \int R'_{kl_f}(r_1) R_{il}(r_1) r_1^2 dr_1 = A_l \delta_{l_f l},$$

$$M_{l'l}^{2p} = \int R'_{2p}(r_2) \frac{r_<^{l'}}{r_>^{l'+1}} R_{il}(r_2) r_2^2 dr_2$$

$$A_l^{2p} = \int R'_{2p}(r_2) R_{il}(r_2) r_2^2 dr_2 = A_{2p} \delta_{1l},$$

$$M_{l'l}^{l_f} = \int R'_{kl_f}(r_1) \frac{r_<^{l'}}{r_>^{l'+1}} R_{il}(r_1) r_1^2 dr_1 . \qquad (8)$$

The terms R_{il} and R'_{2p} stand for the radial part of the wavefunctions ϕ_{il} and ϕ'_{2p}, respectively, and the overlap integrals $A_l^{l_f}$ and A_l^{2p} are non-zero only when the quantum number l equals l_f or l equals 1, respectively. In expression (7) we have considered that the first electron is ejected and the second is excited. For the reverse case one can write a similar expression.

In case of the second-order amplitude, the electron correlation is not so significant [15], thus we use only the basic $\phi_{i0}(1)\phi_{i0}(2)$ configuration to describe the initial state. The intermediate states $|k\rangle$ are eigenstates of the two-electron unperturbed Hamiltonian, and we have kept only the most important ones, considering an intermediate state as a two-electron state, where one electron is in its initial state, and the other is in its final state. Following this approximation, the sum over the intermediate states reduces to two terms.

In this approximation the second-order amplitude (3), considering the first electron ionized, and the second excited, becomes

$$a^{(2)}(\boldsymbol{k},b)$$
$$= \frac{(4\pi)^2}{3} \sum_{l_f m_f} \sum_{m_e=-1}^{1} (-i)^{l_f} e^{-i(\sigma_{l_f}+\delta_{l_f})}$$
$$\times \frac{1}{2l_f+1} Y_{l_f}^{m_f *}(\hat{k}) \Big[\langle \phi'_{2p}(2) | \phi_{2p}(2) \rangle$$
$$\times \langle \phi'_{i0}(1) | \phi_{i0}(1) \rangle \int_{-\infty}^{+\infty} dt\, e^{i(E_f - E_{ie})t}$$
$$\times M'_{l_f} Y_{l_f}^{m_f *}(\hat{R}) \int_{-\infty}^{t} dt'\, e^{i(E_{ie}-E_i)t'}$$
$$\times M_{2p} Y_1^{m_e *}(\hat{R}') + \langle f'_c(1) | f_c(1) \rangle$$
$$\times \langle \phi'_{i0}(2) | \phi_{i0}(2) \rangle \int_{-\infty}^{+\infty} dt\, e^{i(E_f - E_{ic})t}$$
$$\times M'_{2p} Y_1^{m_e *}(\hat{R}) \int_{-\infty}^{t} dt'\, e^{i(E_{ic}-E_i)t'}$$
$$\times M_{l_f} Y_{l_f}^{m_f *}(\hat{R}') \Big], \qquad (9)$$

where E_{ie} and E_{ic} is the energy of the intermediate states $\phi_{2p}(2)\phi'_{i0}(1)$ and $\phi'_{i0}(2) f_c(1)$, respectively. ϕ'_{i0} stands for an unscreened initial state, while the other electron is in the ϕ_{2p} excited state or in the f_c continuum. The $f'_c(\boldsymbol{k},\boldsymbol{r})$ wavefunction (6) is computed in the potentials of the He^+ ion in 1s state (denoted with $f_c(1)$, and corresponding to an intermediate state), and in 2p state (denoted with $f'_c(1)$ in the final wavefunction). So, the change of the screening potential [20] is also taken into account. A similar expression is valid for the other case also, when the second electron is the ionized one, and the first the excited one. The terms denoted with M_{2p}, M'_{2p}, M_{l_f} and M'_{l_f} are:

$$M_{2p} = \int R_{2p}(r_2)\frac{r_<}{r_>^2}R_{i0}(r_2)r_2^2dr_2,$$

$$M_{l_f} = \int R_{kl_f}(r_2)\frac{r_<^{l_f}}{r_>^{l_f+1}}R_{i0}(r_2)r_2^2dr_2$$

$$M'_{2p} = \int R'_{2p}(r_1)\frac{r_<}{r_>^2}R'_{i0}(r_1)r_1^2dr_1,$$

$$M'_{l_f} = \int R'_{kl_f}(r_1)\frac{r_<^{l_f}}{r_>^{l_f+1}}R'_{i0}(r_1)r_1^2dr_1. \quad (10)$$

Here R'_{i0} stands for the radial part of the unscreened initial state ϕ'_{i0}, while R_{2p} is the radial part of the wavefunction ϕ_{2p}. Expression (7) and (9) show the dependence of the first- and second-order amplitudes on the emission angle, through the spherical harmonics.

The probability of the ionization-excitation process, at a given impact parameter can be written as

$$P(b) = |a^{(1)}(\boldsymbol{k},b) + a^{(2)}(\boldsymbol{k},b)|^2. \quad (11)$$

Integrating over the impact parameter b, we obtain double differential cross sections for ejection of electrons at given energy and angle:

$$\frac{d^2\sigma}{dEd\Omega_k} = 2\pi k\int_0^\infty P(b)bdb \quad (12)$$

3. Results and discussion

We have calculated double differential cross sections for the ionization-excitation of the helium to the 2p state by proton and antiproton impact, using single-configuration and multi-configuration wavefunctions for the ground state. In Fig. 1 we present our results for 1 MeV projectile (proton and antiproton) energy, at different ejected electron energies as a function of the ejected electron angle.

At low energy of the ejected electron (10–40 eV) in the forward direction, cross sections are obtained higher for proton projectiles, while in backward direction are higher for antiprotons. This is valid for correlated (multi-configuration) and uncorrelated wavefunctions, but correlation reduces overall the absolute value of the cross sections. Knowing that experimentally the total cross sections for protons are by a factor-of-two lower than for negative projectiles [4], our method probably lead to wrong results for ejection in the forward direction. The problem could be the neglecting of the dynamic and final-state correlation between the two electrons.

For higher energies of the ejected electron differential cross sections have the same shape and magnitude for proton and antiproton projectiles, both in case of correlated and uncorrelated ground-state wavefunctions. This result suggests that electron correlation and Z^3 effects are not important when the ejected electron energy is above 200 eV. However, we can note an interesting feature in the differential cross section at $E_e = 200$ eV (Fig. 1e). Electron correlation introduces a second maximum of the cross section at 130 degree ejection angle.

4. Conclusions

We have calculated double-differential ionization-excitation cross section of the helium in collisions with fast charged projectiles. We have analyzed for the first time the dependence of these cross sections on the sign of the projectile charge. Comparing our results with the experimental data for the total cross sections, we can conclude that our model might be correct for the description of the electron ejection in backward direction, while for the correct description of the forward ejection the inclusion of dynamic and final-state correlation would be desirable. Electron correlation and Z^3 effects are more important for low ejection energies. At 200 eV ejected electron energy the cross sections for proton and antiproton projectiles have almost the same value and behavior.

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