Nuclear Instruments and Methods in Physics Research B 124 (1997) 401–404

ELSEVIER

NIM B
Beam Interactions
with Materials & Atoms

Electron correlation in the double excitation of the helium atom by fast charged particles

L. Nagy, D. Bodea

Department of Physics, Babeş-Bolyai University, str. Kogălniceanu nr. 1, 3400 Cluj, Romania

Abstract

Double excitation cross sections to the $2s2p$ state of the helium atom by fast proton and antiproton impact are calculated by perturbation expansion through second order. The initial and the final states are described by correlated wavefunctions. The importance of different mechanisms and of the electron correlation is analyzed. Cross sections for negative projectiles are found to be higher than those for positive projectiles. The present results are compared with other theoretical calculations and with the experimental data.

1. Introduction

The double excitation of the helium atom by fast charged particles have been investigated in the past few years both experimentally [1–3] and theoretically [4–10]. The study of the double excitation of the most simple two-electron target can provide useful information about the mechanisms of the two-electron processes and the role of electron correlation in these transitions. An important consequence of the electron correlation is the dependence of the two-electron process cross sections on the sign of the projectile charge. It has been made clear, that for the double ionization and ionization-excitation, the cross sections obtained with negative projectiles are higher than those obtained with positive projectiles [11,12]. In the case of the double excitation different theoretical and experimental results are contradictory.

The situation is not simple, because the doubly excited states of the helium are autoionizing states, and are observed only as resonances in the energy spectrum of the ejected electron in the single ionization process. Some experimentalists, like Pedersen and Hvelplund [1] and Giese et al. [2], have extracted from the obtained spectra the cross sections for different doubly excited states. Others, like Bordenave-Montesqueu et al. [3] give only the Shore and Fano parameters, which characterize directly the resonances. From the theoretical point of view, Martín and Salin [9,10] follow the last procedure. Their opinion is that due to the strong post-collision interactions, double excitation cross sections cannot be rigorously extracted from the measured spectra. They have calculated, using a coupled-channel method, the parameters characterizing the resonance structure of the doubly differential ionization cross section. Their results are in fair agreement with the experimental data of Bordenave-Montesqueu et al. [3].

Other coupled-channel calculations of Fritsch and Lin [6], Moribayashi et al. [7] and of Winter [8], and perturbation expansion calculation of Straton et al. [5], neglect the single ionization channel, assuming that the extraction of the double excitation cross sections from the measurements is possible. The problem is that these theoretical results in general do not agree with each other. Because of the difficulties in the extraction of the cross sections from experiments, the comparison with the experimental data is difficult.

In the present paper, like most of the authors above, we neglect the single ionization channel in the study of the double excitation. We compare our results for the excitation of $2s2p$ state with the double excitation cross sections extracted from the experiments [1,2], and with the existent theoretical calculations [5–7]. Previously we have published our results obtained using simple Hartee–Fock wavefunctions for the initial and the final states [13]. Now we investigate the role of initial-state and final-state correlations in the double excitation process.

2. Theory

Most of the theoretical work on the study of the double excitation have been made using the coupled-channel method. In the present paper we have applied a perturbation expansion up to second order, which can provide useful information about the role of some simple mechanisms in the double excitation process. As it was stated by Martín and Salin [10] and by Fritsch and Lin [6], the second-order Born approximation for proton and antiproton impact above 1 MeV projectile energy is fully justified.

0168-583X/97/$17.00
PII S0168-583X(96)01046-4

We have adopted the semiclassical (impact parameter) approximation, where the projectile moves on a classical straight-line trajectory. The projectile-electron interaction is considered a time-dependent perturbation. The first-order transition probability amplitude is given by

$$a^{(1)} = -i \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{i(E_f - E_i)t} \langle f|V(t)|i\rangle, \tag{1}$$

where $|i\rangle$ and $|f\rangle$ represent the initial and the final states of the two electrons, E_i and E_f stand for the initial and the final energy of the target, while $V(t)$ is the interaction potential of the projectile with the electrons.

In the second-order amplitude the time-ordering of the two interactions is taken into account, namely t' is restricted to be less than t

$$a^{(2)} = -\sum_k \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{i(E_f - E_k)t} \langle f|V(t)|k\rangle \times \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{i(E_k - E_i)t'} \langle k|V(t')|i\rangle. \tag{2}$$

The above expressions contain electron correlations through the wavefunctions in the initial, final and intermediate (k) states.

Electron correlation is essential in the first-order amplitude, because one can obtain a two-electron transition with a single projectile-electron interaction only through electron–electron interaction. In the calculation of this amplitude we have used correlated two-electron wavefunctions for the initial [14] and for the final states [15]. These are configuration-interaction (CI) wavefunctions.

Taking into account only the basic configurations for the initial and the final states one obtains the simple shake amplitude [16]. Applying the CI wavefunction only for the final state, we get the contribution of the final-state correlation alone, neglecting the initial-state (ground-state) correlation. Thus, the effect of these correlations can be separated.

In the second-order amplitude electron correlation is less important, because the transition is caused by two consecutive projectile-electron interactions. In the calculation of the second-order amplitude we have neglected the initial-state and final-state correlations. The two-electron wavefunctions become products of one-electron functions, and electron–electron interaction is taken into account by the change of the screening for the second electron after the transition of the first. As it have been shown previously [17], in this approximation the sum over the intermediate states collapses, and the second-order amplitude becomes

$$a^{(2)} = -\int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{i(\epsilon'_{f_2} - \epsilon'_{02})t} \langle f'_2|V_2(t)|i'_2\rangle \times \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{i(\epsilon_{f_1} - \epsilon_{01})t'} \langle f_1|V_1(t')|i_1\rangle - \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{i(\epsilon'_{f_1} - \epsilon'_{01})t} \langle f'_1|V_1(t)|i'_1\rangle \times \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{i(\epsilon_{f_2} - \epsilon_{02})t'} \langle f_2|V_2(t')|i_2\rangle. \tag{3}$$

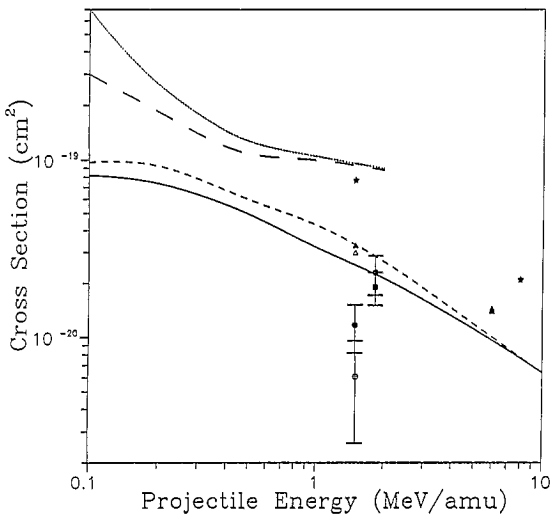

Fig. 1. Cross sections for the double excitation of the helium to the $2s2p$ state as a function of the projectile energy by proton and antiproton (or equivelocity electron) impact. Our calculated cross sections (solid line: p^+, short-dashed line: p^-) are compared to the theoretical results of Straton et al. [5] (dotted line: p^+, long-dashed line: p^-), of Fritsch and Lin [6] (triangles), of Moribayashi et al. [7] (stars) and to the experimental data of Giese et al. [2] (circles), and of Pedersen and Hvelplund [1] (squares). Open symbols stand for proton impact, while closed symbols for antiproton (equivelocity electron, in case of the experiments) impact.

Indices 1 and 2 refer to the two electrons. Unprimed wavefunctions and energies are calculated with the other electron in the initial state, while the primed ones are calculated with the other electron in the final state. The energy transfers to the individual electrons depend on the order of the interactions.

When calculating the double excitation cross sections, the interference between the first-order and second-order amplitudes give rise to the Z^3 term, which is responsible for the dependence of the cross sections on the sign of the projectile charge.

3. Results and discussion

In Fig. 1 we have plotted the cross sections for the double excitation of the helium atom to the $2s2p$ state by proton and antiproton impact as a function of the projectile

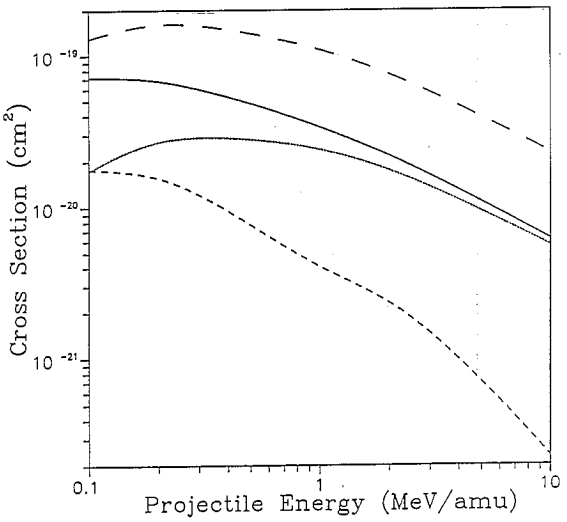

Fig. 2. The contribution of different mechanisms to the cross section for the double excitation of the helium atom to the $2s2p$ state as a function of the projectile energy. THe dotted line stands for the contribution of the simple shake, while the long-dashed line represents final-state correlation added to the simple shake. The solid line stands for the total contribution of the first-order amplitude (with the inclusion of the ground-state correlation), and the short-dashed line for the second-order (TS2) contribution.

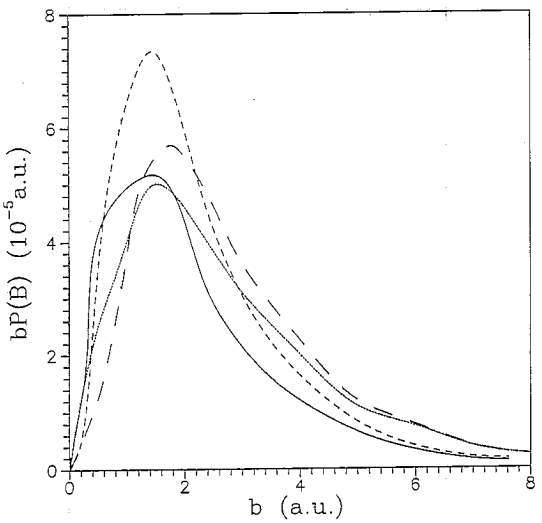

Fig. 3. The impact parameter dependence of the transition probability of the helium atom to the $2s2p$ doubly excited state at 1.5 MeV/amu projectile energy. Our results (solid line: p^+, short-dashed line: p^-) are compared to those of Fritsch and Lin [6] (dotted line: p^+, long-dashed line: p^-).

energy. Our calculated cross sections for antiproton impact (short-dashed line) are higher than those obtained for protons (solid line) in the impact energy range up to 8 MeV. This result is contradictory to the calculations of Straton et al. [5] (dotted lines: p^+ and long-dashed lines: p^-), Moribayashi et al. [7] (stars), but agrees with the theoretical results of Fritsch and Lin [6] (triangles) and with the experimental data of Giese et al. [2]. (Open symbols stand for proton impact and full symbols for antiproton or electron impact. The experiments were made for equivelocity electrons.) The comparison to the data of Pedersen and Hvelplund [1] (squares) is more difficult, because they give only the sum of the cross sections for the excitation of the $2s2p$ and $2p^2(^1D)$ states. We think, that our results and those of Fritsch and Lin are reliable, because for the other two-electron processes (double ionization, ionization-excitation), cross sections for negative projectiles are higher than those for positive projectiles. It is likely that the situation is the same in case of the double excitation, too.

As for the absolute value of the cross sections, the agreement with the coupled-channel results of Fritsch and Lin [6] is also good. These theoretical results overestimate the experimental data of Giese et al. [2] by a factor of 3, but we have to keep in mind that the extraction of the double excitation cross sections from the measurements is quite difficult.

Fig. 2 represents the contribution of different mechanisms to the double excitation cross section. (Results for protons and antiprotons are identical.) If we add to the simple shake cross section (dotted line) the contribution of the final-state correlation, the corresponding cross section (long-dashed line) becomes almost by an order of magnitude larger. Taking into account the ground-state correlation, too, it cancels partly the previous large amplitude, and we obtain for the total first-order cross section (solid line) lower values. The TS2 (second-order) contribution to the cross section (short-dashed line) is below the first-order contribution in the whole energy range, decreases more rapidly with the projectile energy (as it was expected), and becomes negligible at 10 MeV.

In Fig. 3 the impact parameter dependence of the transition probability is represented for proton (solid line) and antiproton (short-dashed line) impact at 1.5 MeV/amu projectile energy. Our results are compared with those of Fritsch and Lin [6] (dotted line: p^+, long-dashed line: p^-). Both calculations lead to higher probabilities for protons at small impact parameters (below $0.3a_0$ in our results), and to higher probabilities obtained with antiproton impact for the rest.

4. Conclusions

We have calculated the cross sections for the double excitation to the $2s2p$ state of the helium atom by proton and antiproton impact by a perturbation expansion through second order. We do obtain higher cross sections for antiprotons than for protons in the energy range between 0.1 and 8 MeV. Our results are in close agreement with the calculations of Fritsch and Lin [6].

Both initial-state and final-state correlations proved to be very important in the calculation of the first-order amplitude. The second-order amplitude becomes negligible at 10 MeV projectile energy.

References

[1] J.O.P. Pedersen and P. Hvelplund, Phys. Rev. Lett. 62 (1989) 2373.
[2] J.P. Giese, M. Schultz, J.K. Swenson, H. Schöne, M. Benhenni, S.L. Varghese, C.R. Vane, P.F. Dittner, S.M. Shafroth and S. Datz, Phys. Rev. A 42 (1990) 1231.
[3] A. Bordenave-Montesqueu, P. Moretto-Capelle, A. Gleizes, S. Andriamonje, F. Martín and A. Salin, J. Phys. B 28 (1995) 653.
[4] J.H. McGuire and J.C. Straton, Phys. Rev. A 43 (1991) 5184.
[5] J.C. Straton, J.H. McGuire and Zheng Chen, Phys. Rev. A 46 (1992) 5514.
[6] W. Fritsch and C.D. Lin, Phys. Rev. A 41 (1990) 4776.
[7] Kengo Moribayashi, Ken-ichi Hino, Michio Matsuzawa and M. Kimura, Phys. Rev. A 44 (1991) 7234.
[8] T.G. Winter, Phys. Rev. A 43 (1991) 4727.
[9] F. Martín and A. Salin, J. Phys. B 28 (1995) 639.
[10] F. Martín and A. Salin, J. Phys. B 28 (1995) 2159.
[11] H. Knudsen, L.H. Andersen, P. Hvelplund, G. Astner, H. Cederquist, H. Danared, L. Liljeby and K.G.Rensfelt, J. Phys. B 17 (1984) 3545.
[12] J.F. Reading and A.L. Ford, Phys. Rev. Lett. 58 (1987) 543; J. Phys. B 20 (1987) 347.
[13] L. Nagy and D. Bodea, Studia UBB Ser. Physica, in press.
[14] R.K. Nesbet and R.E. Watson, Phys. Rev. 110 (1958) 1073.
[15] Lester Lipsky and M.J. Conneely, Phys. Rev. A 14 (1976) 2193.
[16] J.H. McGuire, Adv. At. Molec. Opt. Phys. 29 (1992) 217.
[17] L. Nagy, J. Wang, Jack C. Straton and J.H. McGuire, Phys. Rev. A 52 (1995) R902.