



ELSEVIER

# Two-electron processes in fast collisions with charged particles

L. Nagy

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

## Abstract

Theoretical and experimental results for double ionization, ionization-excitation and double excitation of some simple targets by fast charged-particle impact are reviewed. The dependence of the cross sections on the sign of the projectile charge is discussed. A relatively simple perturbational method is presented, which takes into account electron correlations and time-ordering.

## 1. Introduction

The many-electron processes in atomic and molecular collisions, like double ionization, ionization-excitation, double excitation, double capture, transfer excitation, have attracted much interest in the last decade. A review of the topic was made by McGuire [1]. In the present paper we will focus on two-electron transitions induced by charged particles of high velocities, and we will neglect electron capture.

The single-electron transitions (such as ionization, excitation) are relatively well understood. Especially at high projectile velocities, the theoretical description of the single-electron process is simple. The use of the Born approximation leads to good results for projectile velocities  $v > v_{\text{orbit}}$ . The theory predicts that at these velocities the cross sections are proportional to  $Z_p^2/v^2$ , where  $Z_p$  is the charge of the projectile. This implies that cross sections for single-electron transitions do not depend on the sign of the projectile charge, and must be the same for equivelocity electrons and protons. Experimental data for single ionization and single excitation of different atomic targets have confirmed this prediction. In conclusion, electron correlation may be neglected in the description of these one-electron processes, the independent-electron approximation (IEA) [2] is valid.

In case of the many-electron processes the situation is not so simple. In the framework of the IEA, the cross sections for two-electron transitions (double ionization, ionization-excitation, double excitation) for high-velocity projectiles, should scale as  $Z_p^4/v^4$ . Experimental studies, especially for the double ionization of helium [3-11], have revealed a more complicated velocity dependence of the cross sections, and consequently gave a higher double ionization probability when using electron projectiles compared to those obtained with equivelocity protons. At the beginning of the '80s it was not clear that the difference in cross sections for protons and electrons is due to the different charge or the different

mass of the projectiles. The experiments of Andersen et al. [12-14] made with antiproton projectile were conclusive in this sense. They have shown unambiguously that in case of the double ionization by high-velocity projectiles, the cross section does not depend on the mass of the projectile, but on the charge sign. A similar dependence was reported in the case of the double excitation [15,16] and ionization-excitation [17-21] of the helium atom, and different two-electron processes for molecular hydrogen [22].

The dependence of the cross sections on the sign of the projectile charge for some two-electron processes was treated theoretically by several groups [23-31]. Using a perturbation expansion in terms of the projectile-electron interaction, McGuire [23] has suggested that the interference between the first-order (shake) and the second-order (TS2) amplitudes gives rise of a  $Z^3$  term in the cross section, and this is the cause of the difference. Becker [32], assuming that the collision is dipole dominated, has shown that because the shake mechanism is monopole in character, the two amplitudes do not interfere.

Reading and Ford [24] have made the first elaborate calculations for a two-electron transition, the double ionization of the helium atom, using the forced impulse method. They have shown that for the double ionization, even for relatively high energies, there are significant non-dipole contributions, and the  $Z^3$  terms are important. They have obtained the observed difference in the cross sections for positively and negatively charged projectiles. In a recent, more complete work [25] they have reported very good quantitative agreement with experimental data for the double ionization cross section of the helium atom by charged particles. From these complicated calculations one cannot separate the contributions of different simple mechanisms.

For the double excitation of the helium atom there are several theoretical calculations. Fritsh and Lin [28], Moribayashi et al. [29] and Winter [33] made close-coupling

calculations. Their results do not agree with each other. The cross sections of Fritsch and Lin are closer to the experimental data. Martín and Salin [34,35] has pointed out that the double excitation cross sections cannot be experimentally separated from the single ionization. Their close-coupling calculations give directly the resonance structure of the single ionization.

Returning to the perturbation expansion, McGuire and Straton [30] and Stolterfoht [36,37] have shown that in order to obtain interference between the first-order and second-order processes to explain the difference in the cross sections for two-electron transitions by negatively and positively charged projectiles, one must go beyond the IEA. This is obvious for the first-order processes (shake, TS1 or ground-state correlation), because one can get a two-electron transition with one projectile–electron interaction only with some electron–electron correlation. But even the second-order (TS2) amplitude cannot be taken as a product of one-electron amplitudes as described in [2,36]. Using the IEA for the second-order amplitude it can be easily shown [37], that the shake and TS2 amplitudes are 90° out of phase, and do not interfere. In order to obtain the interference term, when calculating the TS2 amplitude, one has to take into account the time-ordering of the interactions [30,37]. Stolterfoht [37] and Végh et al. [38] have concluded that the time-ordered TS2 differs from the IEA amplitude only, if the orbitals are “relaxed”, the change in the screening and orbital energy during the collision is taken into account. If the orbitals are “frozen”, the energy transfer does not depend on the order of the interactions, time-ordering is lost. Experimental studies were made [39,40] on the effect of time-ordering.

Straton et al. have applied the theory for the double excitation of the helium atom [41] using correlated two-electron wave functions. The difference in cross sections obtained for positive and negative projectiles has proved to be very small. Nagy and Bodea [42,43], using the same perturbation expansion, but a different method for the calculations, has obtained results closer to the experimental data. This method was applied for the ionization-excitation of the helium atom, too [31]. In this case the calculations reflect only partly the observed difference in cross sections for positive and negative projectiles. Godunov and Shipakov [44] made second-order perturbation calculations for the double excitation of the beryllium. The study of this target has the advantage that the doubly excited states are discrete, and therefore there is no interference with the continuum.

Although the most reliable calculations for two-electron transitions [25,28,34] use other methods, perturbational calculations could describe these processes in terms of some simple mechanisms. In the present paper first we describe a method for the calculation of the first-order and second-order amplitudes, and the many-body perturbation corrections to this approximation. In the third section, theoretical results and experimental data for some two-electron processes of the helium atom and the hydrogen molecule in collision with

charged particles, are presented and discussed.

## 2. Mechanisms in the two-electron transitions

The perturbation expansions in terms of the projectile–electron or/and the electron–electron interactions allow us to define some simple mechanisms in order to interpret the many-electron processes. If the perturbation potential is taken to be only the projectile–electron interaction then the mechanisms can be classified as first order (one projectile–electron interaction), second order (two projectile–electron interactions) and so on. The electron–electron interaction is taken into account (at least in principle) to all orders.

If the electron–electron interaction is considered a perturbation, too, then the many-body perturbation theory (MBPT) may be applied. To obtain a two-electron transition, one has to have at least two interactions, so the lowest-order MBPT amplitude is of second order. Through this order, the mechanisms for a two-electron transition are the following [1,22,45,46]: (i) TS2, meaning two projectile–electron interactions. This is the term appearing in the IEA, the double collision process. (ii) TS1, if one projectile–electron interaction is followed by an electron–electron interaction. This term is sometimes regarded as a final-state correlation [1], but it can be considered also as the effect of the electron–electron interaction during the collision process (scattering correlation). (iii) Ground-state correlation, meaning an electron–electron interaction preceding the projectile–electron interaction. (iv) The shake term can be interpreted as the interaction of the second electron (following a projectile–electron interaction) with the hole left by the first electron. In other words, after the transition of the first electron, the screening potential for the second one is changed, causing its transition to another state (the wavefunction collapses [1]). The separation of the TS1 and shake processes is not unique, it depends on the choice of the unperturbed Hamiltonian.

We show some useful formulae suitable for applications.

### 2.1. Impact parameter (semiclassical) formulation

If the wavelength of the projectile is less than the atomic dimension, the projectile can be considered as moving on a classical trajectory. In case of energetic projectiles, when the energy transfer to the electrons is negligible versus the energy of the projectile, they can be regarded as moving on a straight-line trajectory with constant velocity.

The cross section for a given process can be obtained by integrating the transition probability (the square of the modulus of the probability amplitude) over the impact parameter

$$\sigma = \int d^2B |a(B)|^2. \quad (1)$$

The probability amplitude is the overlap of the particular final state  $|f\rangle$  with the quantum-mechanical state in which

the initial state  $|i\rangle$  has evolved

$$a(B) = \langle f|U(-\infty, +\infty)|i\rangle, \quad (2)$$

where  $U(-\infty, +\infty)$  is the evolution operator of the electron system. Several methods have been applied in calculating this amplitude.

## 2.2. Perturbation expansion

The evolution operator from (2) can be obtained by solving the time-dependent Schrödinger equation in the interaction picture

$$i \frac{\partial}{\partial t} U(t, t_0) = V_I(t) U(t, t_0) \quad (3)$$

with the condition  $U(t_0, t_0) = 1$ . The solution can be written as an expansion in the powers of the perturbative interaction and it is equivalent to the Born series

$$U(t, t_0) = 1 + \sum_{n=1}^{\infty} (-i)^n \int_{t_0}^t dt_n V_I(t_n) \times \int_{t_0}^{t_n} dt_{n-1} V_I(t_{n-1}) \dots \int_{t_0}^{t_2} dt_1 V_I(t_1). \quad (4)$$

Switching to the Schrödinger picture, the evolution operator through second order will read as

$$U(t, t_0) = 1 - i \int_{t_0}^t dt_1 e^{iH_0 t_1} V(t_1) e^{-iH_0 t_1} + (-i)^2 \int_{t_0}^t dt_2 e^{iH_0 t_2} V(t_2) e^{-iH_0 t_2} \times \int_{t_0}^{t_2} dt_1 e^{iH_0 t_1} V(t_1) e^{-iH_0 t_1} + \dots \quad (5)$$

## 2.3. Projectile perturbation

The unperturbed Hamiltonian for the two-electron system is taken

$$H^0 = \sum_{i=1}^2 \left[ -\frac{\nabla_i^2}{2} - \frac{Z_T}{r_i} \right] + \frac{1}{r_{12}}, \quad (6)$$

and the perturbation is the sum of the two projectile-electron interactions

$$V = V_1 + V_2. \quad (7)$$

Now we introduce the perturbation expansion (5) of the evolution operator in the expression (2) of the amplitude.

Taking into account that the initial and final states are eigenstates of the unperturbed Hamiltonian, the first-order amplitude is read as

$$a^{(1)} = -i \int_{-\infty}^{+\infty} dt e^{i(E_f - E_i)t} \langle f|[V_1(t) + V_2(t)]|i\rangle. \quad (8)$$

Here  $|i\rangle$  and  $|f\rangle$  are two-electron wavefunctions.

In the expression of the second-order amplitude we insert a complete set of intermediate states  $\sum |k\rangle \langle k| = 1$ , and we get

$$a^{(2)} = - \sum_k \int_{-\infty}^{+\infty} dt e^{i(E_f - E_k)t} \langle f|[V_1(t) + V_2(t)]|k\rangle \times \int_{-\infty}^t dt' e^{i(E_k - E_i)t'} \langle k|[V_1(t') + V_2(t')]|i\rangle. \quad (9)$$

The above expressions contain electron correlations through the wavefunctions in the initial, final and intermediate states. If one knows exactly these wavefunctions, the first-order and second-order contributions to the cross sections can be calculated.

Straton et al. [41] have applied this method for the double excitation of the helium atom. They have used correlated wavefunctions for the initial and the final states. For the intermediate states in the second-order amplitude they have applied the closure approximation, i.e. the intermediate energy  $E_k$  is fixed arbitrary to a constant, and the intermediate states sum up to 1. In (9) the terms in  $(V_1)^2$  and  $(V_2)^2$  usually are neglected in a second-order theory, because they do not cause alone two-electron transitions, only with additional electron-electron interaction.

In order to simplify the problem and make it tractable for more complicated cases one may use the independent electron approximation. Usually, the unperturbed Hamiltonian is approximated to be a sum of one-electron Hamiltonians

$$H^0 \approx h_1 + h_2. \quad (10)$$

Here  $h_i$  may contain only the nuclear potential, or may be a Hartree-Fock Hamiltonian

$$h_i = -\frac{1}{2} \nabla_i^2 + V_{N-1}(r_i), \quad (11)$$

where

$$V_{N-1}(r_i) = -\frac{Z_N}{r_i} + \sum_{j \neq i} \int d\mathbf{r}_j \frac{|\phi_j(\mathbf{r}_j)|^2}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (12)$$

is the nuclear plus the screening potential.

The wavefunctions corresponding to the Hamiltonian (10) can be expressed with Slater determinants. In order to simplify the writing we use simple products of one-electron wavefunctions. However, if in the initial state the spatial

wavefunctions for the two electrons are identical, this is allowed.

The energies corresponding to a sum of one-electron Hamiltonians are sums of single-electron energies:  $E_f = \epsilon_{f_1} + \epsilon_{f_2}$ ,  $E_i = \epsilon_{i_1} + \epsilon_{i_2}$ .

The first-order amplitude for a two-electron process in the IEA is zero, because of the orthogonality of the initial and final one-electron states. As for the second-order amplitude, the sum over the intermediate states collapses, because using  $|k\rangle = |k_1 k_2\rangle$ ,

$$\begin{aligned} \langle k_1 k_2 | V_1(t) | i_1 i_2 \rangle &= \delta_{k_2 i_2} \langle k_1 | V_1(t) | i_1 \rangle, \\ \langle f_1 f_2 | V_1(t) | k_1 k_2 \rangle &= \delta_{f_2 k_2} \langle f_1 | V_1(t) | k_1 \rangle. \end{aligned} \quad (13)$$

It can be easily shown [37] that in this approximation the time-ordering is lost in the second-order amplitude and it becomes a product of one-electron amplitudes

$$\begin{aligned} a^{(2)} &= - \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f_1} - \epsilon_{i_1})t} \langle f_1 | V_1(t) | i_1 \rangle \\ &\quad \times \int_{-\infty}^{+\infty} dt' e^{i(\epsilon_{f_2} - \epsilon_{i_2})t'} \langle f_2 | V_2(t') | i_2 \rangle. \end{aligned} \quad (14)$$

It is clear that this approximation is not valid for the two-electron transitions at high energies, because electron correlation is important.

We take partly into account the electron-electron interaction by letting the orbitals to relax during the collision. This means that the screening potential is changed during the collision and the energy transfer to the individual electron depends on the order of the interactions. This changes the unperturbed Hamiltonian.

We treat the case when the order of the interactions with the projectile is  $V_2(t)V_1(t')$  with  $t > t'$ . The one-electron Hamiltonians are written as

$$\begin{aligned} h_1 &= -\frac{1}{2}\nabla_1^2 + V_{N-1}(\mathbf{r}_1), \\ h_2 &= -\frac{1}{2}\nabla_2^2 + V'_{N-1}(\mathbf{r}_2). \end{aligned} \quad (15)$$

$V'_{N-1}$  is calculated with the first electron in the final state. In case of ionization, when the first electron leaves the atom, instead of  $V'_{N-1}(\mathbf{r}_2)$  we can take  $V_{N-2}(\mathbf{r}_2)$  (screening approximation). For the initial state the wavefunctions for both electrons are calculated in the  $V_{N-1}$  potential (Hartree-Fock wavefunctions), because both electrons are in the ground state. Thus the initial state of electron 2 is not orthogonal to the final state, because the final state is calculated in  $V'_{N-1}$ . In the following formulae the eigenstates of the Hamiltonian containing the initial screening potential will be unprimed, and the eigenstates of the Hamiltonian with  $V'_{N-1}$  or the  $V_{N-2}$  Hamiltonian will be labeled prime. The initial state  $|i_1 i_2\rangle$  is not an eigenstate of the  $H^0 = h_1 + h_2$  Hamiltonian, but because usually the overlap integral between  $|i_2\rangle$  and the

proper eigenstate of the  $h_2$  ( $|i'_2\rangle$ ) is large, approximately we can write

$$(h_1 + h_2)|i_1 i_2\rangle \approx (\epsilon_{01} + \epsilon'_{02})|i_1 i'_2\rangle \approx E_0|i_1 i_2\rangle, \quad (16)$$

where  $E_0$  is the ground-state energy of the two electrons.

Let us express the transition amplitudes in this approximation. If the change in the screening during the two-electron transition is taken into account, because of the non-orthogonality of the initial and final states, the first-order amplitude is non-zero. Considering both interactions, we obtain

$$\begin{aligned} a^{(1)} &= -i \langle f'_2 | i_2 \rangle \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t} \langle f_1 | V_1(t) | i_1 \rangle \\ &\quad -i \langle f'_1 | i_1 \rangle \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t} \langle f_2 | V_2(t) | i_2 \rangle. \end{aligned} \quad (17)$$

This term is the shake amplitude (shake-off or shake-up).

Using the  $H^0 = h_1 + h_2$  Hamiltonian in the second-order amplitude where  $h_1$  and  $h_2$  are given by (15), one obtains

$$\begin{aligned} a^{(2)} &= - \sum_k \int_{-\infty}^{+\infty} dt \int_{-\infty}^t dt' e^{i(\epsilon_{f_1} + \epsilon_{f_2})t} \\ &\quad \times \langle f_1 f'_2 | V_2(t) | k_1 k'_2 \rangle e^{iE_k(t'-t)} \\ &\quad \times \langle k_1 k'_2 | V_1(t') | i_1 i_2 \rangle e^{-iE_0 t'}, \end{aligned} \quad (18)$$

where for simplicity we have taken only one possible order of the interactions.

The following matrix element reduces to a one-electron integral:

$$\langle f_1 f'_2 | V_2(t) | k_1 k'_2 \rangle = \delta_{f_1 k_1} \langle f'_2 | V_2(t) | k'_2 \rangle, \quad (19)$$

because  $|f_1\rangle$  and  $|k_1\rangle$  are both eigenstates of the  $h_1$  Hamiltonian. In case of the other matrix element

$$\langle k_1 k'_2 | V_1(t') | i_1 i_2 \rangle = \langle k'_2 | i_2 \rangle \langle k_1 | V_1(t') | i_1 \rangle, \quad (20)$$

$|i_2\rangle$  is calculated in the  $V_{N-1}$  potential, while  $|k'_2\rangle$  is the eigenstate of  $h_2$ . But the overlap integral of the  $|i_2\rangle$  state is much more larger with the ground state of the  $h_2$ ,  $|i'_2\rangle$ , than with the excited and continuum states, and so  $\langle k'_2 | i_2 \rangle \approx \delta_{k'_2 i'_2}$ . In these conditions we neglect the other possible intermediate states, and retain only one, in which one electron is in the final state, and the other in the modified ground state  $|i'_2\rangle$ . The unperturbed energy of this intermediate state is obtained by

$$\begin{aligned} H^0 |f_1 i'_2\rangle &= h_1 |f_1\rangle |i'_2\rangle + |f_1\rangle h_2 |i'_2\rangle \\ &= (\epsilon_{f_1} + \epsilon'_{02}) |f_1 i'_2\rangle. \end{aligned} \quad (21)$$

Considering only the above intermediate state with one electron in the final state and the other in the ground state, but

taking into account both of the possible order of the interactions, the second-order amplitude can be expressed as

$$\begin{aligned}
 a^{(2)} = & - \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f2} - \epsilon'_{02})t} \langle f'_2 | V_2(t) | i'_2 \rangle \\
 & \times \int_{-\infty}^t dt' e^{i(\epsilon_{f1} - \epsilon'_{01})t'} \langle f'_1 | V_1(t') | i_1 \rangle \\
 & - \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f1} - \epsilon'_{01})t} \langle f'_1 | V_1(t) | i'_1 \rangle \\
 & \times \int_{-\infty}^t dt' e^{i(\epsilon_{f2} - \epsilon'_{02})t'} \langle f'_2 | V_2(t') | i_2 \rangle. \quad (22)
 \end{aligned}$$

This term is the TS2 amplitude. Since  $\epsilon_{0i} \neq \epsilon'_{0i}$ , the transition energies depend on the order of the interactions.

In these conditions the second-order amplitude is not reduced to a product of one-electron amplitudes, as in (14) for IEA, because the energy transfers and wave functions depend on the order of the interactions. This amplitude for all final states has a real and imaginary part, leading to interference with the first-order amplitude. This interference term is responsible for the  $Z^3$  effect, the dependence of the cross section on the sign of the projectile charge.

The method described above has been applied by us for the ionization-excitation [31], double excitation [42] and double ionization [47] of the helium atom. Improvement can be obtained by using correlated wavefunctions for the ground state (including the ground-state correlation to all orders).

#### 2.4. Many-body perturbation

The treatment of electron correlations in the model presented in the previous subsection is not simple. Especially for the continuum final states, the use of fully correlated wavefunctions is a serious problem. In order to improve the method, the electron–electron interaction (entirely or partly) may be included in the perturbation potential. It is likely that the Hamiltonian in the screening approximation is closer to the exact one than the sum of the Hartree–Fock Hamiltonians. In the first case, the first-order corrections of MBPT are the only important corrections, the higher orders can be neglected.

The correction  $v$  in the potential is the difference between the exact unperturbed Hamiltonian (6) and the considered  $H^0$  (15). For the two-electron case

$$v = \frac{1}{r_{12}} - \int d\mathbf{r}_1 \frac{|\phi_{1f}(\mathbf{r}_1)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} - \int d\mathbf{r}_2 \frac{|\phi_{2f}(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (23)$$

where  $\phi_{ji}$  and  $\phi_{jf}$  are the wavefunctions of electron  $j$  in the initial and the final state, respectively. The perturbative interaction will read as

$$V(t) = V_1(t) + V_2(t) + v. \quad (24)$$

The correlation potential alone does not cause electron transitions. In the second-order probability amplitude the following terms causes two-electron transitions:

$$\begin{aligned}
 & V_1(t) V_2(t') + V_2(t) V_1(t') \\
 & + v V_1(t) + v V_2(t) + V_1(t)v + V_2(t)v. \quad (25)
 \end{aligned}$$

The first two terms lead to the already treated TS2 amplitude. The terms  $vV_i(t)$  means transitions caused by a projectile–electron interaction followed by an electron–electron interaction. This mechanism is commonly called TS1. The terms  $V_i(t)v$  lead to the ground-state correlation amplitude: a projectile–electron interaction preceded by an electron–electron interaction.

Further, we shall write the TS1 and ground-state correlation amplitudes only for the interaction of the projectile with one electron, those for the other electron can be obtained similarly.

The TS1 amplitude for the two-electron transition caused by the interaction of the projectile with electron 1 is

$$\begin{aligned}
 a_{\text{TS1}} = & - \int_{-\infty}^{+\infty} dt \int_{-\infty}^t dt' \\
 & \times \langle f_1 f_2 | e^{iH^0 t} v e^{-iH^0(t-t')} V_1(t') e^{-iH^0 t'} | i_1 i_2 \rangle. \quad (26)
 \end{aligned}$$

Because  $v$  does not depend on  $t$ , we can integrate analytically over  $t$ . But before this we have to change the order of the two integrals. Taking the eigenvalues (approximate for the initial state) of the  $H^0$  and introducing a complete set of intermediate states we can write

$$\begin{aligned}
 a_{\text{TS1}} = & - \sum_k \int_{-\infty}^{+\infty} dt \int_{-\infty}^t dt' \langle f_1 f_2 | e^{i(\epsilon_{f1} + \epsilon_{f2})t} v | k_1 k_2 \rangle \\
 & \times e^{-iE_k(t-t')} \langle k_1 k_2 | V_1(t') e^{-iE_0 t'} | i_1 i_2 \rangle \\
 = & - \sum_k \int_{-\infty}^{+\infty} dt' \int_{t'}^{+\infty} dt e^{i(\epsilon_{f1} + \epsilon_{f2} - E_k)t} \langle f_1 f_2 | v | k_1 k_2 \rangle \\
 & \times \langle k_1 k_2 | V_1(t') | i_1 i_2 \rangle e^{i(E_k - E_0)t'}. \quad (27)
 \end{aligned}$$

In order to obtain a convergent integral over  $t$  we introduce in the exponent a dumping factor  $+i\eta$ , and after performing the integration we make  $\eta \rightarrow 0$ . So we get

$$a_{\text{TS1}} = -i \sum_k \int_{-\infty}^{+\infty} dt' \langle f_1 f_2 | v | k_1 k_2 \rangle \frac{1}{\epsilon_{f1} + \epsilon_{f2} - E_k + i0}$$

$$\times e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t'} \langle k_1 k_2 | V_1(t') | i_1 i_2 \rangle. \quad (28)$$

In the last matrix element, as we have previously shown, the  $\langle k_2 | i_2 \rangle$  integral is significantly different from zero only for the ground eigenstate of the  $h_2$  Hamiltonian  $|i_2'\rangle$ . Thus

$$\langle k_2 | i_2 \rangle \approx \langle k_2 | i_2' \rangle = \delta_{k_2 i_2'}, \quad (29)$$

and the sum over  $k_2$  collapses and  $E_k = \epsilon_{k_1} + \epsilon_{0_2}'$ . The TS1 amplitude will read

$$a_{\text{TS1}} = -i \sum_{k_1} \int_{-\infty}^{+\infty} dt' \frac{1}{\epsilon_{f_1} + \epsilon_{f_2} - \epsilon_{k_1} - \epsilon_{0_2}' + i0} \times e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t'} \langle f_1 f_2 | v | k_1 i_2' \rangle \langle k_1 | V_1(t') | i_1 \rangle. \quad (30)$$

Because of the complex denominator the  $a_{\text{TS1}}$  amplitude has real and imaginary parts for each parity of the initial and the final states. Taking into account that the "sum over the  $k_1$  intermediate states" is a sum over the bound states and an integral over the continuum states, the real and imaginary parts can be separated as follows:

$$a_{\text{TS1}} = -iP \sum_{k_1} \int d\mathbf{k}_1 \frac{1}{\epsilon_{f_1} + \epsilon_{f_2} - \epsilon_{k_1} - \epsilon_{0_2}'} \langle f_1 f_2 | v | k_1 i_2' \rangle \times \int_{-\infty}^{+\infty} dt' e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t'} \langle k_1 | V_1(t') | i_1 \rangle + \pi \int k_1^z d\hat{\mathbf{k}}_1 \langle f_1 f_2 | v | k_1^z i_2' \rangle \times \int_{-\infty}^{+\infty} dt' e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t'} \langle k_1^z | V_1(t') | i_1 \rangle. \quad (31)$$

The first term, where we have a principal-value integral over the momenta of the intermediate states, is the off-shell part of the amplitude, energy is not conserved for the intermediate states. The second term is the energy-conserving or on-shell part, where  $\epsilon_{k_1^z} = \epsilon_{f_1} + \epsilon_{f_2} - \epsilon_{0_2}'$ .

If instead of the Hamiltonian given by (15) we use usual Hartree-Fock Hamiltonians as in (10), the second term of the perturbation potential given by (23) would contain the wavefunction  $\phi_{1i}(\mathbf{r}_1)$  of electron 1 in the initial state, creating the potential of the hole left after its transition. Including only this term in the formula of the amplitude (31), we obtain the shake amplitude from the MBPT. Because  $\langle f_1 | k_1 \rangle = \delta_{f_1 k_1}$ , the on-shell part is zero, and the sum in the first term collapses, leading to

$$a_{\text{shake}} = -i \frac{1}{\epsilon_{f_2} - \epsilon_{0_2}'} \left\langle i_1 f_2 \left| \frac{-1}{r_{12}} \right| i_1 i_2' \right\rangle \times \int_{-\infty}^{+\infty} dt' e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t'} \langle k_1 | V_1(t') | i_1 \rangle. \quad (32)$$

This formula is similar to that of Hino et al. [45]. In our formulation, presented in the previous subsection, we have included the shake term to all orders.

The ground-state correlation amplitude, if the interaction of the projectile with electron 1 is considered, is read as

$$a_{\text{GSC}} = - \int_{-\infty}^{+\infty} dt \int_{-\infty}^t dt' \times \langle f_1 f_2 | e^{iH_0 t} V_1(t) e^{-iH_0(t-t')} v e^{-iH_0 t'} | i_1 i_2 \rangle = - \sum_k \int_{-\infty}^{+\infty} dt \int_{-\infty}^t dt' e^{i(\epsilon_{f_1} + \epsilon_{f_2})t} \times \langle f_1 f_2 | V_1(t) | k_1 k_2 \rangle e^{-iE_k(t-t')} \langle k_1 k_2 | v | i_1 i_2 \rangle e^{-iE_0 t'}. \quad (33)$$

Integrating over  $t'$  we obtain

$$a_{\text{GSC}} = i \sum_k \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t} \langle f_1 f_2 | V_1(t) | k_1 k_2 \rangle \times \frac{1}{E_k - E_0} \langle k_1 k_2 | v | i_1 i_2 \rangle. \quad (34)$$

Because  $\langle f_2 | k_2 \rangle = \delta_{k_2 f_2}$ , the sum over  $k_2$  collapses, and the ground-state correlation amplitude becomes

$$a_{\text{GSC}} = i \sum_{k_1} \int_{-\infty}^{+\infty} dt e^{i(\epsilon_{f_1} + \epsilon_{f_2} - E_0)t} \langle f_1 | V_1(t) | k_1 \rangle \times \frac{1}{\epsilon_{k_1} + \epsilon_{f_2} - E_0} \langle k_1 f_2 | v | i_1 i_2 \rangle. \quad (35)$$

This amplitude has always the same phase as the shake amplitude.

Using a CI wavefunction for the ground state, one can take into account the ground-state correlation to all orders.

MBPT calculations were performed by Hino et al. [45] for the double photoionization of the helium atom. No MBPT calculations for charged-particle impact were made.

### 3. Analysis of some theoretical results and experimental data

#### 3.1. Double ionization of the helium atom

The double ionization is experimentally the most studied two-electron process. For fast charged-particle-helium collisions a series of experimental cross sections were published. Adamczyk et al. [4], P. Nagy et al. [8], Stephan et al. [9], Andersen et al. [12] and others measured the double ionization cross section of the helium atom by electron impact, and Wexler et al. [5], Puckett and Martin [6], Shah and

Gilbody [11], Knudsen et al. [10] and Andersen et al. [12] by proton impact. It was puzzling, why above 1 MeV/amu projectile energy up to 10 MeV/amu the cross sections for electrons are about twice those obtained with protons. The experiments of Andersen et al. [12,13] and Hvelplund et al. [14], done with antiproton projectiles, have made clear that at high velocities the mass of the projectile is not important, and the difference in the cross sections obtained by protons and electrons/antiprotons is due to the charge sign.

McGuire [23] has suggested that this dependence can be explained by the interference of the first-order (shake) and second-order (TS2) amplitudes, but he did not perform any quantitative calculations.

Olson [26] have explained the behaviour of the two electrons during the double ionization process on a classical bases. Performing a classical trajectory Monte Carlo (CTMC) calculation, he could follow the positions and momenta of each particle. He have observed that the antiproton preferentially scatters the first electron inward via its repulsive interaction toward the second electron from larger impact parameters than the proton projectile. In contrast, the proton must have a trajectory between one electron and the nucleus in order to attract this electron into a trajectory that will collide with the second electron, leading to a smaller cross section of the double ionization via electron–electron correlation. The more recent dynamical CTMC calculations of Meng et al. [48] are not consistent with these explanations and lead to higher cross sections for protons than for antiprotons.

Végh [27] have introduced in the semiclassical IEA a correction based on a similar argument: because the positive projectile attracts the first electron, making the other through electron–electron interaction to move away, the impact parameter for the second electron is increased. In case of a negative projectile the impact parameter for the second electron is decreased, increasing the double ionization cross section versus that obtained with positive projectiles. This semiempirical calculation takes into account only the second-order amplitude, the first-order amplitude is neglected.

The most elaborate calculations for the double ionization were made by Reading and Ford [24]. Their forced impulse method takes into account the electron–electron correlations several times during the collision. In their recent paper [25] they report results in good agreement with the experimental data.

Marshall et al. [49] have performed an independent-event model calculation for the double ionization of the helium atom by  $\alpha$  particle impact, using correlated wavefunctions. Their results are well above the experimental data.

We have performed perturbational calculations for the double ionization of the helium atom [47] based on the formulas presented in Subsection 2.2. The cross sections obtained taking into account the shake-off and the TS2 mechanisms as a function of the projectile energy, are presented in Fig. 1. These are compared with the experimental data and with the theoretical calculations of Ford and Reading [25].

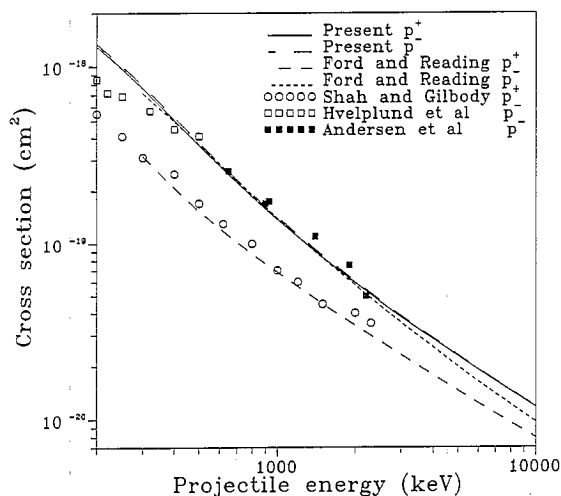


Fig. 1. Cross sections for the double ionization of the helium atom by proton and antiproton impact as a function of the projectile energy. Our results are compared with the theoretical cross sections of Ford and Reading [25], the experimental data of Shah and Gilbody for protons [11] and of Hvelplund et al. [14] and Andersen et al. [13,50] for antiprotons.

Our results reflect only partly the observed difference between cross sections obtained for positive and negative projectile impact. We think, this is mainly because of the poor representation of the final-state correlation. Correlated final-state continuum wave functions may be applied, or, alternatively, the TS1 amplitude may be included. We appreciate the effect of the initial-state correlation to be less important, because a CI wavefunction for the ground state has a neglectable component from the continuum.

However, these calculations allow us to compare the relative importance of the first-order and second-order processes. In Fig. 2 we represent the cross sections due to the different mechanisms. For projectile energies below 1 MeV the TS2 contribution dominates over the shake-off cross section. At 1.5 MeV the two contributions are equal, above this energy the shake-off becomes dominant. We show separately the contribution of the independent-electron approximation (IEA) and the IEA with shifted energies of the intermediate states (IEA-SH), excluding the contribution of the time-ordering effect.

### 3.2. Ionization-excitation of the helium atom

Experimental cross sections for the ionization of the helium atom with the excitation of the other electron to the  $2p$  state were published by Forand et al. [17], Pedersen and Folkmann [18], Schartner et al. [19], Fülling et al. [20] and Bailey et al. [21]. For this transition the situation is similar to the double ionization: for high projectile velocities the cross sections by electron impact are about twice those get by proton impact.

First-order calculations were made by Rudge [51]. His cross sections underestimate the data for medium projectile

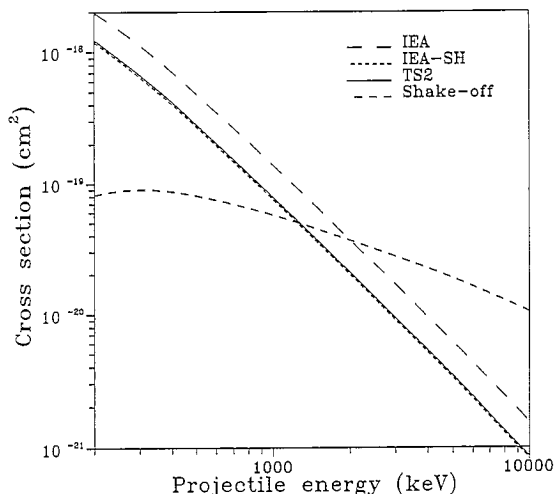


Fig. 2. The contributions of the first-order and second-order amplitudes to the double ionization cross sections of the helium atom. These contributions are independent of the sign of the charge of the projectile. IEA is the independent-electron, frozen-orbital approximation, IEA-SH is obtained by the non-time-ordered amplitude with shifted energies of the intermediate states. TS2 is the time-ordered second-order cross section, and the shake-off is the first-order term.

velocities, and are independent from the sign of the projectile charge. However, for high velocities his results are satisfactory.

We have applied a perturbational method, similar to that for the double ionization, for the calculation of the ionization-excitation cross sections [31].

Our cross sections are below the experimental data [21], and reflect only partly the dependence on the sign of the projectile charge. Our first-order amplitude contains only the shake-off term (excitation of one electron by the projectile, and relaxation of the other to the continuum), the shake-up term (meaning the ejection of the first electron and the relaxation of the second to an excited state) is obtained to be zero because the  $2p$  state is orthogonal to the  $1s$ . In this case the ground-state correlation may be important: taking a CI wavefunction for the initial state, which contains also  $p$  orbitals, the overlap with the final  $2p$  state could be significant.

### 3.3. Double excitation of the helium atom

The doubly excited states of the helium atom are not stationary discrete states. Their energy is above the single ionization threshold, and can be observed as resonances in the energy spectrum of the ejected electron in the single ionization process. Some experimentalists (Pedersen and Hvelplund [15], Giese et al. [16]) have extracted from the obtained spectra the double excitation cross section of the helium atom for the lowest resonances. Others, like Bordenave-Montesqueu et al. [52] argue that this separation cannot be rigorously done, and give only the parameters which char-

acterize directly the resonances in the ionization process.

Giese et al. [16] give double excitation cross sections for electron, proton and other positive ion projectiles at 1.5 MeV/amu impact energy. Like for the other two-electron processes, the cross sections for electron projectiles are higher than for the same velocity protons. At 1.5 MeV/amu the ratio between cross sections obtained with electrons and protons depend on the specific doubly excited state. For the excitation of the  $2s^2(^1S)$  and of the  $2s2p(^1P)$  states this ratio is high (2.5 and 1.9 respectively), but for the  $2p^2(^1D)$  state it is nearly 1. From this result they conclude that for the excitation of the  $2p^2(^1D)$  state the interference term between the first-order and the second-order term in the perturbation expansion is negligible, but it is important for the other two excited states.

Pedersen and Hvelplund [15] did not separate the  $2s2p(^1P)$  and  $2p^2(^1D)$  resonances, and for the sum of these cross sections obtain the opposite: higher cross sections for protons than for electrons.

Coupled-channel calculations for the double excitation of the helium atom were performed by several authors [28,29,33–35].

Fritsch and Lin [28], after pointing out the ambiguity in extracting the double excitation cross sections from the ejected electron spectra, have compared their results with the experimental data. For the sum of the cross sections for the excitation to the  $2s2p(^1P)$  and  $2p^2(^1D)$  states their results agree approximately with the data of Giese et al. [16], but does not reproduce the charge sign dependence. When separating the different doubly excited states, their theoretical calculations disagree with the experiments. The calculated excitation cross section for proton impact to the  $2p^2(^1D)$  state is four times less than the experimental one, and is twice larger for protons than for antiprotons. The cross sections for the transitions to the  $2s2p(^1P)$  and the  $2s^2(^1S)$  are overestimated. It is not clear yet that this discrepancy is because of the theoretical formalism or of the problems in the interpretation of the experimental spectra. However, Fritsch and Lin point out that for the excitation of the  $2s2p(^1P)$  and the  $2s^2(^1S)$  states the first-order processes dominates, but for the  $2p^2(^1D)$  state the second-order term is important, too. Studying the impact parameter dependence for the transition probability to the  $2s2p(^1P)$  state, they obtain for small impact parameters a larger probability for proton impact than for antiprotons, but for large impact parameters the situation is reversed. This is in agreement with the classical analysis of Olson [26].

The calculations of Moribayashi et al. [29] lead to different results. For the excitation of the  $2s2p(^1P)$  they obtain 3 times larger cross sections than Fritsch and Lin [28], and 12 times than Giese et al. [16]. For the other excited states their results are below those of Fritsch and Lin, and for all transitions they obtain higher cross sections for proton impact compared to the antiproton impact.

Winter [33] has made calculations for the excitation of the  $2s^2(^1S)$  state. His results are between those of Frisch and



Lin [28] and of Giese et al., and does not show dependence on the sign of the projectile charge.

Martín and Salin have performed also coupled-channel calculations for the double excitation of the helium atom. In their papers [34,35] they argue, that it is not possible to extract from experiment a double excitation cross section. The experimentalists measure the resonance structure in the doubly differential ionization cross section, which is very sensitive to post-collision interactions. This puts severe constrain on a significant comparison between the theory and experiments. The inclusion of the ionization channel in a theoretical study of the double excitation process is essential. They calculate the Shore and the Fano parameters, which characterize directly the resonance structure of the ionization process. Their results for proton impact are in fair agreement with the experimental data of Bordenave-Montesquieu et al. [52]. Performing also second Born calculations [35], they state that the second Born approximation is valid at 1.5 MeV/amu impact energy for proton and antiproton projectiles, but not for projectiles with  $Z_P > 1$ .

Perturbation expansion methods were also applied for the study of the double excitation of the helium atom. Straton et al. [41] have used CI wavefunctions for the initial and the final states, so electron–electron correlation is included. For the intermediate states in the second-order amplitude they make the closure approximation. This does not influence significantly the absolute value of the cross section for high projectile energies, where the first-order term dominates, but may cause an important error in the interference term, responsible for the  $Z^3$  effect. Their results for the excitation of the  $2s^2(^1S)$  and of the  $2p^2(^1D)$  states lie between the data of Fritsch and Lin [28] and of Giese et al. [16]. As for the excitation of the  $2s2p(^1P)$  state their cross sections are clearly overestimated, and decrease too slow with the increase of the projectile energy. For every double excitation process, cross sections for proton impact are obtained larger than those with antiprotons.

As a first attempt, we have calculated double-excitation cross sections for the helium atom through second order, using simple wavefunctions [42]. The initial state was described by a Hartree–Fock, and the final states by hydrogenic wavefunctions. The intermediate states were taken to be singly excited states. Our results for the excitation of the  $2s2p(^1P)$  states are between the experimental data of Giese et al. [16] and the theoretical cross sections of Fritsch and Lin [28]. We do obtain higher cross sections for antiprotons than for protons in accordance with these data.

In order to make these calculations more reliable, one can use almost exact, correlated wavefunctions from the literature (see for example Ref. [53] for the ground state of the helium atom and Ref. [54] for the doubly excited states). Cross sections obtained with these wavefunctions are presented in a joint paper [43].

### 3.4. Two-electron processes in the hydrogen molecule

Another simple, but less studied system with two electrons is the hydrogen molecule. Edwards et al. [22] have reported cross sections for the double ionization, ionization–excitation and double excitation of the hydrogen molecule by proton and electron impact. Every studied state is dissociative. They are separated by measuring the energies of the two nuclei after the dissociation. The extraction of the double excitation cross section is more direct than for helium. For this target, too, the cross section for electron impact is about two times larger than the cross sections obtained with proton projectiles of the same velocity.

Very recently, ionization–excitation cross sections by fast proton impact have been published by Ben-Itzhak et al. [55].

We have performed perturbation expansion calculations for some of these processes [56]. We have neglected the time-ordering in the second-order amplitude, therefore we have got the same cross sections for proton and electron projectiles. For the double ionization, the second-order process is more important than the first-order one up to 500 keV/amu projectile energies, above 1 MeV/amu the first-order process dominates. For the ionization plus excitation to most of the excited states, the first-order process dominates.

Including the time-ordering in the second-order, and the TS1 process in the first-order amplitude, the results may be improved.

## 4. Conclusions

The perturbational methods for the study of the two-electron transitions are a good alternative beside the coupled-channel and other types of calculations. They have the advantage of relative simplicity and of the interpretation of these processes in terms of some simple mechanisms.

In order to obtain reliable results, one has to take into account the electron correlation. This can be done by using correlated two-electron (CI) wavefunctions for each state. Presently this requirement can be achieved only for discrete states (case of the double excitation), but not for the continuum. In the case of the double ionization and ionization–excitation, by a proper choice of the unperturbed Hamiltonian, the shake contribution to the first-order amplitude can be taken into account to all orders. The remaining final-state correlation (TS1) can be considered by using the many-body perturbation theory. The initial-state correlation can be described by using CI wavefunctions for the ground state.

The presented perturbational method may be suitable for more complex targets, too.

## Acknowledgements

The author would like to thank L. Végh, J.H. McGuire, N. Stolterfoht and B. Sulik for useful discussions.

This paper was supported by the Hungarian OTKA grant under contract No. T014323.

## References

- [1] J.H. McGuire, *Adv. At. Mol. Opt. Phys.* 29 (1992) 217.
- [2] J.H. McGuire and O.L. Weaver, *Phys. Rev. A* 16 (1977) 41.
- [3] H.K. Haugen, L.H. Andersen, P. Hvelplund and H. Knudsen, *Phys. Rev. A* 26 (1982) 1962.
- [4] B. Adamczyk, A.J.H. Boerboom, B.L. Schram and J. Kistenmaker, *J. Chem. Phys.* 44 (1966) 4640.
- [5] S. Wexler, *J. Chem. Phys.* 41 (1964) 1714; 44 (1966) 2221.
- [6] L.J. Puckett and D.W. Martin, *Phys. Rev. A* 1 (1970) 1432.
- [7] V. Schmidt, N. Sander and H. Kuntzenmüller, *Phys. Rev. A* 13 (1976) 1743.
- [8] P. Nagy, A. Skutlartz and V. Schmidt, *J. Phys. B* 13 (1980) 1249.
- [9] K. Stephan, H. Helm. and T.D. Märk, *J. Chem. Phys.* 73 (1980) 3763.
- [10] 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.
- [11] M.B. Shah and H.B. Gilbody, *J. Phys. B* 18 (1985) 899.
- [12] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, A.H. Sørensen, K. Elsner, K-G. Rensfelt and E. Uggerhøj, *Phys. Rev. A* 36 (1987) 3612.
- [13] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, J.O.P. Pedersen, S. Tang-Petersen, E. Uggerhøj, K. Elsner and E. Morenzoni, *Phys. Rev. A* 40 (1989) 7366.
- [14] P. Hvelplund, H. Knudsen, U. Mikkelsen, E. Morenzoni, S.P. Møller, E. Uggerhøj and T. Worm, *J. Phys. B*, 27 (1994) 925.
- [15] J.O.P. Pedersen and P. Hvelplund, *Phys. Rev. Lett.* 62 (1989) 2373.
- [16] J.P. Giese, M. Schultz, J.K. Swenson, H. Schöne, M. Benhenni, S.L. Varghese, C.R. Vane, P.F. Dittner, S.M. Shafrath and S. Datz, *Phys. Rev. A* 42 (1990) 1231.
- [17] J.L. Forand, K. Becker and J.W. McConkey, *J. Phys. B* 18 (1985) 1409.
- [18] J.O.P. Pedersen and F. Folkmann, *J. Phys. B* 23 (1990) 441.
- [19] K.-H. Scharner, B. Lommel and D. Detleffsen, *J. Phys. B* 24 (1991) L13.
- [20] S. Fülling, R. Bruch, E.A. Rauscher, P.A. Neil, E. Träbert, P.H. Heckmann and J.H. McGuire, *Phys. Rev. Lett.* 68 (1992) 3152.
- [21] M. Bailey, R. Bruch, E. Rausher and S. Bliman, *J. Phys. B* 28 (1995) 2655.
- [22] A.K. Edwards, R.M. Wood, J.L. Davies and R.L. Ezell, *Phys. Rev. A* 42 (1990) 1367; *A* 44 (1991) 797; A.K. Edwards, R.M. Wood, M.A. Mangan and R.L. Ezell, *Phys. Rev. A* 46 (1992) 697.
- [23] J.H. McGuire, *Phys. Rev. Lett.* 49 (1982) 1153.
- [24] J.F. Reading and A.L. Ford, *Phys. Rev. Lett.* 58 (1987) 543; *J. Phys. B* 20 (1987) 374.
- [25] A.L. Ford and J.F. Reading, *J. Phys. B* 27 (1994) 4215.
- [26] R.E. Olson, *Phys. Rev. A* 36 (1987) 1519.
- [27] L. Végh, *Phys. Rev. A* 37 (1988) 992.
- [28] W. Fritsch and C.D. Lin, *Phys. Rev. A* 41 (1990) 4776.
- [29] Kengo Moribayashi, Ken-ichi Hino, Michio Matsuzawa and M. Kimura, *Phys. Rev. A* 44 (1991) 7234.
- [30] J.H. McGuire and J.C. Straton, *Phys. Rev. A* 43 (1991) 5184.
- [31] L. Nagy, J. Wang, Jack C. Straton and J.H. McGuire, *Phys. Rev. A*, 52 (1995) R902.
- [32] R.L. Becker, private communication (1983).
- [33] T.G. Winter, *Phys. Rev. A* 43 (1991) 4727.
- [34] F. Martín and A. Salin, *J. Phys. B* 28 (1995) 639.
- [35] F. Martín and A. Salin, *J. Phys. B* 28 (1995) 2159.
- [36] N. Stolterfoht, *Lecture Notes in Physics*, Vol. 376 (1990) p. 139.
- [37] N. Stolterfoht, *Phys. Rev. A* 48 (1993) 2980.
- [38] L. Végh, B. Sulik and N. Stolterfoht, *Phys. Rev. A* 51 (1995) 3017.
- [39] N. Stolterfoht, A. Mattis, D. Schneider, G. Schiwietz, B. Skagwall, B. Sulik and S. Ritz, *Phys. Rev. A* 48 (1993) 2986.
- [40] N. Stolterfoht, A. Mattis, D. Schneider, G. Schiwietz, B. Skagwall, B. Sulik and S. Ritz, *Phys. Rev. A* 51 (1995) 350.
- [41] J.C. Straton, J.H. McGuire and Zheng Chen, *Phys. Rev. A* 46 (1992) 5514.
- [42] L. Nagy and D. Bodea, *Studia UBB Ser. Physica*, in press.
- [43] L. Nagy and D. Bodea, these Proceedings (FIAC-6), *Nucl. Instr. and Meth. B* 124 (1997) 401.
- [44] A.L. Godunov and V.A. Schipakov, *J. Phys. B* 26 (1993) L811.
- [45] Ken-ichi Hino, Takeshi Ishihara, Futoshi Shimizu, Nobuyuki Toshiba and J.H. McGuire, *Phys. Rev. A* 48 (1993) 1271.
- [46] J.H. McGuire, N. Berrah, R.J. Bartlett, J.A.R. Samson, J.A. Tanis, C.L. Cocke and A.S. Schlachter, *J. Phys. B* 28 (1995) 913.
- [47] L. Nagy, J.H. McGuire, L. Végh, B. Sulik and N. Stolterfoht, unpublished.
- [48] L. Meng, R.E. Olson, R. Dörner, J. Ullrich and H. Schmidt-Bocking, *J. Phys. B* 26 (1993) 3387.
- [49] D.P. Marshall, C. Le Sech and D.S.F. Crothers, *J. Phys. B* 26 (1993) L219.
- [50] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, J.O.P. Pedersen, S. Tang-Petersen, E. Uggerhøj, K. Elsner and E. Morenzoni, *Phys. Rev. A* 41 (1990) 6536.
- [51] M.R.H. Rudge, *J. Phys. B* 21 (1988) 1887.
- [52] A. Bordenave-Montesqueu, P. Moretto-Capelle, A. Gleizes, S. Andriamonje, F. Martín and A. Salin, *J. Phys. B* 28 (1995) 653.
- [53] R.K. Nesbet and R.E. Watson, *Phys. Rev.* 110 (1958) 1073.
- [54] Lester Lipsky and M.J. Conneely, *Phys. Rev. A* 14 (1976) 2193.
- [55] I. Ben-Itzak, Vidhya Krishnamurthi, K.D. Carnes, H. Aliabadi, H. Knudsen, U. Mikkelsen and B.D. Esry, *J. Phys. B* 29 (1996) L21.
- [56] L. Nagy and L. Végh, *Phys. Rev. A* 50 (1994) 3984.