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Nuclear Instruments and Methods in Physics Research B 154 (1999) 131–141

NIM B
Beam Interactions with Materials & Atoms

www.elsevier.nl/locate/nimb

Advances and challenges in collisions of fast ions with few-electron atoms

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Abstract

This report reviews the recent theoretical results on the fast ion-few-electron atom collisions obtained in the framework of an approach using the perturbation theory expansion in the scattering potential and the diagonalization approximation for CI-wavefunction of the target atom. The uniform consideration of the electron transitions to states of discrete and continuous spectra is set forth. The results of investigations of the two-electron transitions in helium induced by fast charged projectiles, such as, the total and differential cross sections, mechanisms of electron transitions, interference problem and charge asymmetry of the cross sections, normalization of CI-wavefunctions of the discrete and continuous spectrum states, obtained on the basis of the present approach, are discussed.

PACS: 34.50.-s; 34.50.Fa
Keywords: Few-electron atom; Multielectron transition; Scattering amplitude; Double-electron excitation; Simultaneous ionization–excitation of helium

1. Introduction

The collisions of charged particles with few-electron atoms have attracted much interest of both experimentalists and theorists in the last years. The increase of activity in the theoretical investigations of multi-electron processes like double excitation, double ionization, ionization–excitation, transfer excitation and double capture was due to the pioneer measurements of the double-ionization cross sections of helium by protons and antiprotons performed by Andersen and co-workers [1,2]. Their measurements showed a two-fold exceeding of the cross sections for antiprotons over the proton ones at ion energies from 2 to 5 MeV/u and stimulated an active study of the problem of correlations in atomic collisions.

The single-electron transitions, such as ionization or excitation, are relatively well understood, especially at high collision energies where the description of the single-electron processes on the basis of the first Born approximation is really simple. However, the use of the first Born approximation is not always correct, even for high

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0168-583X/99/$ – see front matter
PII: S0168-583X(99)00012-9

enough collision energies. The first Born approximation implies that the cross sections do not depend on the sign of the projectile charge. At the same time, the more complete calculations of the single-electron excitation cross sections of helium by protons and antiprotons, performed by Balashov and co-workers [3] in the framework of the multichannel diffraction approximation, showed a strong charge asymmetry for the optically-forbidden transitions in the collision energy interval from 0.05 to 1.0 MeV/u, owing to the significant contribution of two-step processes in such transitions.

The two-electron processes in fast ion-atom collisions were investigated theoretically by many authors (see, e.g., Refs. [4–31]). In contrast to the single-electron processes, the situation in the case of the multi-electron ones is not so clear. The double-excitation cross sections of helium calculated by different authors [4–10] do not conform with each other and are in a rather bad agreement with the available experimental data [32]. The analysis of such a situation has been done in Refs. [11,12]. Calculations using the different modifications of the close-coupling method have been performed in the works [4–6,9,10]. The main shortcoming of almost all close-coupling calculations of the double-excitation processes is the lack of the continuum states in the expansion of the electron wavefunction of the target atom. Later Martin and Salin [33] suggested to include the continuum states with help of a discretization procedure [34,35]. However, at such an approach one cannot be sure in advance that the included continuum states are exactly those which give the dominant contribution to the scattering process. Recently new measurements and theoretical estimations of excitation cross sections of the helium $2s^{21}S$, $2s2p^{1}P$ and $2p^{21}D$ autoionizing states produced in collisions of 100 keV protons with helium have been performed in the work [36].

Elaborate theoretical investigations of the double ionization of helium by protons and antiprotons have been done by Reading and Ford using the forced impulse method [13,14]. In this method the system is in a definite correlated state at the beginning of the collision. The whole collision process is divided into a set of short enough time intervals. During the short time step the system evolves without correlations. At the end of every time interval the system is allowed to collapse back into a linear superposition of all possible correlated states. The new set of states is then used as a basis set to define a correlated wavefunction at the new time step, and so on. Reading and Ford have obtained a pronounced difference in the double-ionization cross sections for positively and negatively charged particles. In a more later work [17] they have presented double-ionization cross sections of helium by fast charged projectiles which are in a very good agreement with the experimental data [37–40].

Another theoretical model used for the consideration of the inelastic transitions in ion-atom collisions is that developed by Presnyakov and Uskov [26]. This is a natural generalization of the Keldysh method treating the ionization of an atom in the electromagnetic field [41] to the case of ion-atom collisions. The idea of this method consists in replacement of the time-dependent Schrödinger equation of the collision problem with the non-stationary equation for the electron moving in the Coulomb field of the target core and in the dipole field of the projectile. The latter equation can be solved exactly which warrants the necessity of such a replacement. Since this method is not a perturbative one, it can be very useful when examining collisions with taking part of multicharged ions [27–29].

The methods based on the perturbation expansions in the scattering potential and the correlation interaction potential are often used for the investigation of multi-electron processes [7–9,18,21,23,24,30,31]. The study of the mechanisms of two-electron transitions in fast collisions of charged projectiles with helium atoms has been carried out exactly in the framework of the perturbation theory in Refs. [1,2,7,8,11,12,24,31].

In the present report the recent results on fast ion-helium atom collisions obtained in the framework of the perturbation expansion in the scattering potential and the diagonalization approximation for the electron wavefunction of the target atom are reviewed.

2. The basic points of the theoretical approach

2.1. Description of the scattering process

The scattering of a fast charged projectile on a few-electron atom is considered in the impact parameter method. During the collision the projectile moves along a straight line $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t$ (where $\mathbf{b}$ is the impact parameter and $\mathbf{v}$ is the ion velocity relative to the nucleus of the target atom), and the electron wavefunction Ψ of the target atom is determined by the non-relativistic Schrödinger equation, which in the interaction picture has the form

$$\mathrm{i}\frac{\partial}{\partial t}\Psi^{\mathrm{int}}(t) = \tilde{V}(t)\Psi^{\mathrm{int}}(t)$$
$$\text{with} \qquad \Psi^{\mathrm{int}}(t)\mid_{t\to\pm\infty} = \Psi_{\mathrm{I,F}}(\mathbf{r}), \tag{1}$$

where

$$\tilde{V}(t) = \exp(\mathrm{i}\hat{H}_0 t)\left(-\sum_{j=1}^{n}\frac{Z_{\mathrm{p}}}{\mid \mathbf{R}(t)-\mathbf{r}_j\mid}\right)\exp(-\mathrm{i}\hat{H}_0 t) \tag{2}$$

is the operator of the interaction of the fast ion with the target atom in the interaction picture; $\hat{H}_0 = \hat{H}_{\mathrm{a}} + \hat{K}$ is the free-motion Hamiltonian; $\hat{H}_{\mathrm{a}}$ is the atomic system Hamiltonian and $\hat{K} = \hat{\mathbf{P}}^2/2M$ is the kinetic-energy operator; $\hat{\mathbf{P}}$ is the relative-motion momentum operator and M is the reduced mass of the colliding particles; $\mathbf{r}$ denotes a set of all electron coordinates of the atomic system, determined relative to the atomic nucleus; $\mathbf{r}_j$ is the radial vector of the jth atomic electron; Z_{p} is the ion charge.

The amplitude of the transition from the state I to the state F as a function of the impact parameter $\mathbf{b}$ is given by the expression

$$A(\mathrm{F}\leftarrow\mathrm{I};\mathbf{b}) = \langle\Psi_{\mathrm{F}}\mid S(+\infty,-\infty)\mid\Psi_{\mathrm{I}}\rangle, \tag{3}$$

where Ψ_{I} and Ψ_{F} are the orthonormalized wavefunctions for the initial and final states, respectively; the scattering S-matrix is of the form

$$S(+\infty,-\infty) = T\exp\left(-\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\,\tilde{V}(t)\right). \tag{4}$$

2.2. Electron wavefunction of a multi-electron atom

The wavefunction $\Psi_{\mathrm{I,F}}(\mathbf{r})$ is an eigenfunction of the atomic Hamiltonian $\hat{H}_{\mathrm{a}}$ with an eigenvalue $E_{\mathrm{I,F}}$

$$\hat{H}_{\mathrm{a}}\Psi_{\mathrm{I,F}}(\mathbf{r}) = E_{\mathrm{I,F}}\Psi_{\mathrm{I,F}}(\mathbf{r}). \tag{5}$$

The non-relativistic atomic Hamiltonian for the few-electron atomic system has the form

$$\hat{H}_{\mathrm{a}} = \sum_{j=1}^{n}\left(\frac{\hat{\mathbf{p}}_j^2}{2m} - \frac{Z_{\mathrm{t}}}{r_j}\right) + V_{\mathrm{ee}}, \tag{6}$$

where V_{ee} is the electron–electron interaction potential; $\hat{\mathbf{p}}_j$ is the momentum operator of the jth atomic electron; $r_j = \mid \mathbf{r}_j \mid$; m is the electron mass; Z_{t} is the target atom nuclear charge. As a solution of Eq. (5) we can take the normalized CI-wavefunctions determined in the form

$$\mid\{\tilde{\gamma}^{(\mathrm{I})}\}^{(\pm)}\rangle \equiv \frac{1}{N}\mid\{\gamma^{(\mathrm{I})}\}^{(\pm)}\rangle$$
$$= \frac{\pm\mathrm{i}}{N}\left(\mid\gamma\rangle + \sum_{\nu}{}'\mid\nu\rangle\frac{\langle\nu\mid U\mid\gamma\rangle}{E_\gamma - E_\nu \pm \mathrm{i}\epsilon}\right). \tag{7}$$

Here N is the normalizing factor; $\mid\mu\rangle$ is the IPM wavefunction of the considered atomic system and represents by itself an antisymmetrical product of the single-electron wavefunctions; $E_\mu = E_\mu^0 + \langle\mu\mid U\mid\mu\rangle$; E_μ^0 is the energy of the μ-state of the atomic system determined without including the electron-electron interaction; U is the correlation potential [42]; the imaginary portion $\pm\mathrm{i}\epsilon$ in the energy denominator has the effect of moving the pole off the real axis. The sign $\sum_\nu'$ denotes the summation over all discrete states (except the state that can lead to self-mixing) and integration over all continuous states. The wavefunction Eq. (7) is the first order term of power series expansion of the exact CI-wavefunction $\mid\{\tilde{\gamma}\}^{(\pm)}\rangle$ in terms of correlation potential U [42] and up to a phase multiplier this wavefunction coincides with that [11,12], determined in the diagonalization approximation. It may be shown that any two functions from the set $\{\mid\{\tilde{\gamma}_j^{(\mathrm{I})}\}^{(\pm)}\rangle\}$ corresponding to different values of energy E and E', respectively, are orthogonal accurate up to the first order in the potential U.

In accordance with the definitions introduced in Ref. [43], the first term ($|\ \gamma\rangle$) in the right-hand side of Eq. (7) we shall call the basic state. All states entering in the last term in the right-hand side of Eq. (7) we shall call the included states. As

$$\frac{1}{E_\gamma - E_v \pm \mathrm{i}\epsilon} = \mathrm{i}\pi\delta(E_\gamma - E_v) \mp \frac{P}{E_\gamma - E_v}, \tag{8}$$

then in the sum over the different electron states in Eq. (7) there are states which possess the same energy as the basic state. Such states are called the resonant included states; the rest of the included states are the nonresonant included states. The appropriate reaction channel corresponds to each state on the right-hand side of Eq. (7). We shall call them, respectively: basic channel, resonant included channels, and nonresonant included channels. Accordingly, the coupling of the basic channel with the resonant or nonresonant included channels is called, respectively, the resonant or nonresonant channel coupling.

3. The theory of double-electron processes in collisions of charged particles with helium atoms

3.1. Mechanisms of the double-electron transitions

Examining the two-electron transitions in helium we can restrict ourselves by taking into account the terms of the perturbation theory series up to the second order in the potential $\tilde{V}(t)$ and the diagonalization approximation for CI-wavefunction. Since the orthogonality of the CI-wavefunctions obtained by the diagonalization approximation breaks down for the terms of second- (or higher-) order in the potential U, therefore evaluating the transition amplitude we do not need to take into account the matrix elements containing the potential U in power higher than unity. At such restrictions we can represent the scattering amplitude of the double-electron transition as a superposition of the amplitudes for transitions described in the framework of two kind of mechanisms [11,12]: (i) correlation mechanism, $c1$ (or $c2$), describes the transitions occurring as a result of a single (or double) scattering of a projectile by the helium atom and the correlation interaction of atomic electrons; (ii) mechanism of the independent electron transitions, I2, describes the transition of two helium electrons as a result of a single interaction of each of them with the projectile. When the correlations are taken into account in the final state wavefunction only the correlation mechanism $c1$ coincides with the well-known TS-1 mechanism [2]. The amplitude a^{I2} coincides with the amplitude called the TS-2 one [2] which, usually, is determined for the IPM wavefunctions.

So for the helium double excitation scattering amplitude and for the amplitude of the double-electron transition to the continuous state of helium (e.g., simultaneous ionization-excitation or double ionization) we, respectively, have

$$\begin{aligned} A^{(d)}\big(\,|\, n_1 l_1 n_2 l_2\ {}^1LM\rangle \leftarrow |\ 1\mathrm{s}^2\ {}^1\mathrm{S}\rangle; b\big) \\ = \sum_{m_1,m_2} C^{LM}_{l_1 m_1 l_2 m_2}\big(a^{c1}(\gamma_1\gamma_2; b) \\ + a^{c2}(\gamma_1\gamma_2; b) + a^{I2}(\gamma_1\gamma_2; b)\big) \end{aligned} \tag{9}$$

and

$$\begin{aligned} A^{(c)}\big(\,|\,\gamma_1\gamma_2\rangle \leftarrow |\ 1\mathrm{s}^2\ {}^1\mathrm{S}\rangle; b\big) \\ = a^{c1}(\gamma_1\gamma_2; b) + a^{c2}(\gamma_1\gamma_2; b) + a^{I2}(\gamma_1\gamma_2; b) \end{aligned} \tag{10}$$

where $b = |\ \mathbf{b}\ |$; $C^{LM}_{l_1 m_1 l_2 m_2}$ are the Clebsch–Gordan coefficients. In Eq. (9) γ_1 and γ_2 denote‘ the quantum numbers of the single-electron discrete states; in Eq. (10) only one of the quantities γ_1 and γ_2 may denote the quantum numbers of the single-electron discrete state. The allowance for the terms up to the second order in the potential $\tilde{V}(t)$, when calculating the transition amplitudes, gives us a possibility to investigate the charge asymmetry in the total cross sections of the examined double-electron processes. Namely these terms are responsible for the charge asymmetry, because only they can contribute to the term proportional to Z_p^3 in the scattering cross sections.

3.2. Uniform consideration of electron transitions to the states of discrete and continuum spectra

For uniform consideration of electron transitions into discrete and continuum states we shall represent the single-electron wavefunction of the continuous spectrum state with the Coulomb as-

ymptotic at infinity over the superposition of the wavefunctions of continuous spectrum states with specified energy ε and different values of orbital angular momentum l and its projection on the quantization axis m [44]

$$|\,\vec{\kappa}\rangle = \frac{1}{\kappa}\sum_{l,m} \mathrm{i}^l \exp(\mathrm{i}\delta_l) R_{\kappa l}(r) Y^*_{lm}(\Omega_{\vec{\kappa}}) Y_{lm}(\Omega_{\mathbf{r}}). \quad (11)$$

Here $Y_{lm}(\Omega)$ is the spherical harmonic; $\Omega_{\mathbf{t}}$ is the spherical angle of vector $\mathbf{t}$; δ_l is the phase shift; $\vec{\kappa}$ is the electron momentum in the continuum; $\kappa = |\,\vec{\kappa}\,|$; $R_{\kappa l}(r)$ is the Coulomb wavefunction determined in the field of charge Z_t.

Now we can represent any of amplitudes a^{c1}, a^{c2} and a^{I2} as a superposition of the corresponding amplitudes $\tilde{a}$ for the transitions to the states, characterized by the specific energy and different possible values of the orbital angular momentum and its projection on the quantization axis [11,12] for each atomic electrons

$$a^q(\gamma_1\gamma_2; b) = \sum_{l'_1,m'_1,l'_2,m'_2} U^*_{l'_1m'_1}(\tilde{n}_1) U^*_{l'_2m'_2}(\tilde{n}_2) \tilde{a}^q(\tilde{n}_1 l'_1 m'_1 \tilde{n}_2 l'_2 m'_2; b) \quad (12)$$

where

$$U_{l'm'}(\tilde{n}) = \begin{cases} \delta_{ll'}\ \delta_{mm'}, & \tilde{n} = n, \\ \frac{1}{\kappa}\ \mathrm{i}^{l'} \exp(-\mathrm{i}\delta_{l'}) Y^*_{l'm'}(\Omega_{\vec{\kappa}}), & \tilde{n} = |\,\vec{\kappa}\,|\,. \end{cases} \quad (13)$$

The introduction of the functions $\tilde{a}^q$ is very convenient because the problem of calculating the amplitudes $\tilde{a}^q$ for transitions to the states of continuous spectrum is not distinguished from that for transitions to the states of discrete spectrum. In the case of transitions to the states of discrete spectrum the amplitude $\tilde{a}^q$ coincides with the corresponding amplitude a^q.

Any of the amplitudes $\tilde{a}^q$ may be expressed with help of two functions $D^{(1)}_j$ and $D^{(2)}$ [11,12]: the first of them, up to a multiplier depending on the projectile velocity $\mathbf{v}$, is the conventional semiclassical amplitude of single-electron transition, and the second is the matrix element from the interconfiguration interaction potential U. For the transition between two arbitrary states characterized by the values of quantum numbers of every atomic electrons the functions $D^{(1)}_j$ and $D^{(2)}$ have the form

$$\begin{aligned} &D^{(1)}_j\Big(\,|\,\tilde{n}'_j l'_j m'_j \tilde{n}'_k l'_k m'_k(\mathrm{F})\rangle \overset{j}{\leftarrow} \tilde{n}_j l_j m_j \tilde{n}_k l_k m_k(\mathrm{I})\rangle\,|\,q_\parallel; \mathbf{b}\Big) \\ &\equiv \int \frac{\mathrm{d}^2 q_\perp}{q^2} \exp(-\mathrm{i}\mathbf{q}_\perp \mathbf{b}) \\ &\quad \times \langle \tilde{n}'_j l'_j m'_j \tilde{n}'_k l'_k m'_k(\mathrm{F})\,|\,\exp(\mathrm{i}\mathbf{q}\mathbf{r}_\mathbf{j})\,|\,\tilde{n}_j l_j m_j \tilde{n}_k l_k m_k(\mathrm{I})\rangle \\ &= 2\pi i^{l_j - l'_j} \sum_{l'',m''} i^{m''} (2l''+1) \left[\frac{(2l_j+1)(l''-|\,m''\,|)!}{(2l'_j+1)(l''+|\,m''\,|)!}\right]^{1/2} \\ &\quad \times C^{l'_j 0}_{l_j 0 l'' 0}\, C^{l'_j m'_j}_{l_j m_j l'' m''} \int \frac{q_\perp \mathrm{d}q_\perp}{q^2} J_{|m''|}(q_\perp b) P^{|m''|}_{l''}(\cos\theta_q) \\ &\quad \times \int r_j^2\, \mathrm{d}r_j R^*_{\tilde{n}'_j l'_j}(r_j)\, R_{\tilde{n}_j l_j}(r_j)\, j_{l''}(qr_j)\, \delta_{\tilde{n}'_k \tilde{n}_k}\, \delta_{l'_k l_k}\, \delta_{m'_k m_k}, \end{aligned} \quad (14)$$

and

$$\begin{aligned} &D^{(2)}\Big(\,|\,\tilde{n}'_j l'_j m'_j \tilde{n}'_k l'_k m'_k(\mathrm{F})\rangle \Leftarrow |\,\tilde{n}_j l_j m_j \tilde{n}_k l_k m_k(\mathrm{I})\rangle\Big) \\ &\quad \equiv \langle \tilde{n}'_j l'_j m'_j \tilde{n}'_k l'_k m'_k(\mathrm{F})\,|\,U\,|\,\tilde{n}_j l_j m_j \tilde{n}_k l_k m_k(\mathrm{I})\rangle \\ &\quad = i^{l'_j + l_k - l'_k - l_j} \sum_{l'',m''} (-1)^{l''} \left[\frac{(2l'_j+1)(2l_k+1)}{(2l_j+1)(2l'_k+1)}\right]^{1/2} \\ &\qquad \times C^{l_j 0}_{l'_j 0 l'' 0}\, C^{l_j m_j}_{l'_j m'_j l'' m''}\, C^{l'_k 0}_{l_k 0 l'' 0}\, C^{l'_k m'_k}_{l_k m_k l'' m''} \\ &\qquad \times \int r_j^2\, \mathrm{d}r_j \int r_k^2\, \mathrm{d}r_k\, \frac{r^{l''}_<}{r^{l''+1}_>} R^*_{\tilde{n}'_j l'_j}(r_j)\, R_{\tilde{n}_j l_j}(r_j) \\ &\qquad \times R^*_{\tilde{n}'_k l'_k}(r_k)\, R_{\tilde{n}_k l_k}(r_k). \end{aligned} \quad (15)$$

where $J_m(q_\perp b)$ is a Bessel function of order m; $P^m_l(\cos\theta)$ is an associated Legendre polynomial; $j_l(qr)$ is a spherical Bessel function of order l.

3.3. Interference in collision processes

McGuire [45] was the first who suggested that the difference in cross sections of the double ionization of helium by protons and electrons is due to the interference between the first-order (shake-off) and the second order (TS-2) processes which gives rise to a Z_p^3 term in the cross section. The problem of interference in the process of the double ionization from the ground state of helium at some simplifying assumptions has been rigorously solved in the work [46]. It was shown that

the on-energy shell transitions, described by the amplitude a^{c1}, must interfere with the transitions described by the amplitude a^{I2}, determined in the independent particle model. The qualitative reasoning about the difference between the helium double ionization cross sections for protons and antiprotons, adduced in the work [2], is in agreement with the result of Ref. [46].

As one can see easily from Eqs. (14) and (15), each single scattering act of the projectile with the jth helium electron brings about an imaginary unit to the sth power, where $s = l'_j + l'_k - l_j - l_k + m_j + m_k - m'_j - m'_k$. Here the quantum numbers with and without primes are, respectively, related to the electrons in states before and after the scattering. The value of s for two sequential scatterings is determined by the same expression, only the quantum numbers marked by primes are related to the state before the first scattering and the corresponding numbers without primes, to the state after the second scattering. The rth-order term of the perturbation theory series in the scattering amplitude contains the additional imaginary unit in the rth power; every off-energy shell transition occurring under the influence of the projectile-atom interaction reduces the power of the imaginary unit by one; each on-energy shell transition occurring under the influence of the electron correlation potential gives rise to the addition of the imaginary unit to the amplitude.

Now we introduce the following definition [11,12]. The index of a power of the imaginary unit in some function will be called the index of imaginarity of that function. The indexes of imaginarity of partial amplitudes have an important property: they allow to find the phase differences between different amplitudes $\tilde{a}^q$ and therefore to determine the possibility of the interference of the various transitions with each other. For the total index of imaginarity n of any partial scattering amplitude $\tilde{a}^q$ we may write

$$n = s + r - n_{\mathrm{sc}}^{(\mathrm{off})} + n_{\mathrm{prior}}^{(\mathrm{on})} + n_{\mathrm{post}}^{(\mathrm{on})}, \tag{16}$$

where r is the perturbation theory series order of the partial scattering amplitude; $n_{\mathrm{sc}}^{(\mathrm{off})}$ is the total number of the single off-energy shell transitions occurring under the influence of the projectile–atom interaction; $n_{\mathrm{prior}}^{(\mathrm{on})}$ ($n_{\mathrm{post}}^{(\mathrm{on})}$) is the summed number of the on-energy shell transitions, taking place before (after) the direct collision of the projectile with the atomic electrons, occurring under the influence of the electron correlation potential in all r single scatterings. Only the transition for which the index of imaginarity n is either even or odd can interfere with each other.

We use the formula (16) in the particular case of the double-electron transitions from the ground state of helium. For different partial scattering amplitudes we have: amplitudes $\tilde{a}_{\mathrm{on}}^{c1}$ $(r = 1, n_{\mathrm{sc}}^{(\mathrm{off})} = 0, n_{\mathrm{prior}}^{(\mathrm{on})} + n_{\mathrm{post}}^{(\mathrm{on})} = 1)$ and $\tilde{a}_{on}^{I2} (r = 2, n_{\mathrm{sc}}^{(\mathrm{off})} = n_{\mathrm{prior}}^{(\mathrm{on})} = n_{\mathrm{post}}^{(\mathrm{on})} = 0)$ contain the multiplier $\mathrm{i}^{m_1+m_2-l_1-l_2+2}$; amplitudes $\tilde{a}_{\mathrm{off}}^{c1}$ $(r = 1, n_{\mathrm{sc}}^{(\mathrm{off})} = n_{\mathrm{prior}}^{(\mathrm{on})} = n_{\mathrm{post}}^{(\mathrm{on})} = 0)$ and $\tilde{a}_{off}^{I2}$ $(r = 2, n_{\mathrm{sc}}^{(\mathrm{off})} = 1, n_{\mathrm{prior}}^{(\mathrm{on})} = n_{\mathrm{post}}^{(\mathrm{on})} = 0)$, the multiplier $\mathrm{i}^{m_1+m_2-l_1-l_2+1}$ and $\mathrm{i}^{m_1+m_2-l_1-l_2+3}$, respectively. Here $\tilde{a}_{\mathrm{on}}^{c1}(\tilde{a}_{\mathrm{on}}^{I2})$ and $\tilde{a}_{\mathrm{off}}^{c1}(\tilde{a}_{\mathrm{off}}^{I2})$ are the parts of the amplitudes $\tilde{a}^{c1}(\tilde{a}^{I2})$ describing the on-energy shell and off-energy shell transitions, respectively. So we see that the transitions, described by the amplitudes $\tilde{a}_{\mathrm{on}}^{c1}$ and $\tilde{a}_{\mathrm{on}}^{I2}$, must interfere with each other [2,11,12,46] as well as the transitions, described by the amplitudes $\tilde{a}_{\mathrm{off}}^{c1}$ and $\tilde{a}_{\mathrm{off}}^{I2}$, do.

4. Application of the formalism to the specific problems

Below the results of the investigations of the double-electron excitation and the simultaneous ionization-excitation of helium in fast collisions of protons, antiprotons and multicharged ions with helium atoms, performed in the framework of the presented formalism, will be shown. When performing the calculations the partial amplitude a^{c2} was omitted as it is much less than the other terms of the amplitudes Eqs. (9) and (10) and in the partial amplitude a^{I2} only the on-energy shell transitions were taken into account.

4.1. Normalization of CI-wavefunctions

The wavefunctions for $1s^2\ ^1S$, $2s^2\ ^1S$ and $2s2p\ ^1P$ states of helium were determined with allowance for orbitals $1s^2, 1s2s, 1s2p, 1s\vec{\kappa}, 2s^2, 2s2p, 2p^2, 2s\vec{\kappa}$,

$2p\vec{\kappa}$ only. The calculations gave the values 1.08, 1.312 and 1.561 for the normalizing factors for the CI-wavefunctions of $1s^2\,{}^1S$, $2s^2\,{}^1S$ and $2s2p\,{}^1P$ states, respectively. For the normalizing factor of the $|\{2s\vec{\kappa}'\}^{(\pm)}\rangle$ wavefunction, retaining only the on-energy shell transitions, we obtain the following relation [31,47]

$$\langle\{2s\vec{\kappa}\}^{(\pm)} \mid \{2s\vec{\kappa}'\}^{(\pm)}\rangle = N^2_{2s\vec{\kappa}}(\kappa')\,\delta(\vec{\kappa}-\vec{\kappa}'), \qquad (17)$$

i.e. the continuous spectrum state CI-wavefunction of helium has to be normalized to the δ-function of the momentum. The normalizing factor $N_{2s\vec{\kappa}}(\kappa)$, determined with allowance for only the $ns\vec{\kappa}$ resonant included states in the expansion of $|\{2s\vec{\kappa}\}^{(\pm)}\rangle$ over the atomic orbitals, is presented in Fig. 1. Contributions from states with $n > 4$ were determined as $1/n^3$. Jumps on the curve for $N(\kappa)$ are observed at values of the ejected electron momentum $\vec{\kappa}$ conforming to the relation $\kappa^2/2 = E_{nl\,{}^2L} - E_{2s\,{}^2S}$ (here $E_{nl\,{}^2L}$ is the energy of the $nl\,{}^2L$ state of the He^+ ion; n, l and L are the principal and orbital quantum numbers and the orbital angular momentum for the states of the He^+ ion lying above the $2s^2S$ one), namely, at ejected electron energies corresponding to the threshold ones. At these energies the opening of new ways of transferring the electrons from the basic state to the other ones occurs.

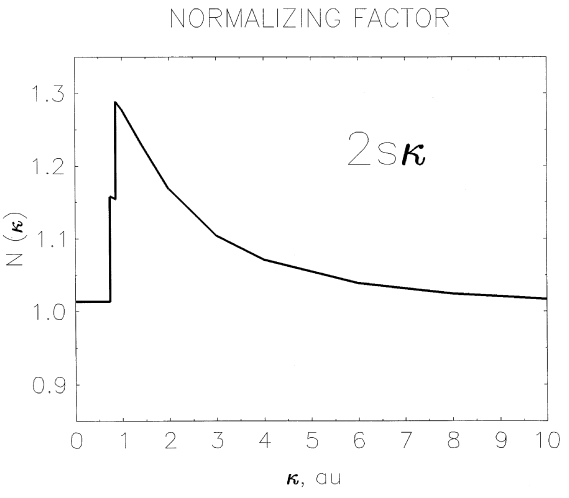

Fig. 1. The normalizing factor $N(\kappa)$ for the wave function of the $2s\vec{\kappa}$ helium state vs the electron momentum κ (Ref. [31]).

4.2. The helium double-electron excitation

The cross sections of the double-electron excitation to the $2s^2\,{}^1S$ autoionizing state in collisions of helium with protons and antiprotons are presented in Fig. 2a. The figure shows that the cross sections for antiprotons significantly exceed those for protons at scattering energies from 0.15 to ~2 MeV. The available experimental data and calcu-

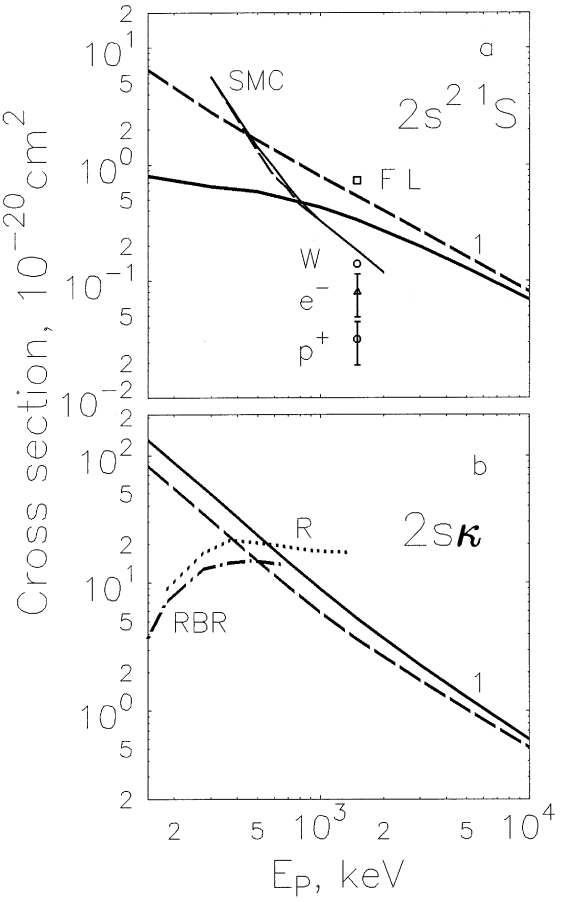

Fig. 2. The cross sections for the double-electron $p^{\pm} + He(1s^2\,{}^1S) \rightarrow p^{\pm} + He(2s^2\,{}^1S)$ (a) and $p^{\pm} + He(1s^2\,{}^1S) \rightarrow p^{\pm} + e^- + He^+(2s^2S)$ (b) transitions vs the projectile energy E_p. Calculated results: 1 – present approach Ref. [24] (a) and Ref. [31] (b); SMC – second Born results Ref. [8]; FL (Ref. [4]) and W (Ref. [6]) – close-coupling results for proton impact; R – first Born results for electron impact Ref. [18]; RBR – R-matrix results for electron impact Ref. [19]. Full curves stand for protons; broken curves, for antiprotons. Experimental data Ref. [32].

lated cross sections received in other theoretical approaches are presented there. Contributions from the different excitation mechanisms to the helium double-electron $1s^2\,{}^1S \rightarrow 2s^2\,{}^1S$ transition for protons are presented in Fig. 3. Almost for all considered collision energies the contribution to the double-electron excitation cross section from the correlation mechanism of excitation exceeds the contribution made from the independent electron transitions. Contribution from the interference term in the cross section is compared with those from the two mentioned excitation mechanisms. The difference between cross sections for protons and antiprotons must be significant as the interference terms for protons and antiprotons have opposite signs.

The helium $1s^2\,{}^1S \rightarrow 2s^2\,{}^1S$ excitation cross sections for particles with charges Z_p from 3 to 9 at projectile energy $E = 1.5$ MeV/u are presented in Fig. 4. The results of the calculations carried out without taking into account the states of continuous spectrum in the amplitude a^{c1} are also presented there. A significant difference between the results performed with and without taking into account the continuum states (see Fig. 4) points out the important role of the transitions through the continuum states in the double excitation of helium. The qualitative reasoning showed that in the case, when absolute values of terms of the 1st- and 2nd-orders in the scattering amplitude are approximately equal to each other, the cross section may be described within the accuracy of ~50% by the terms up to the second order in the scattering potential. In the case of the

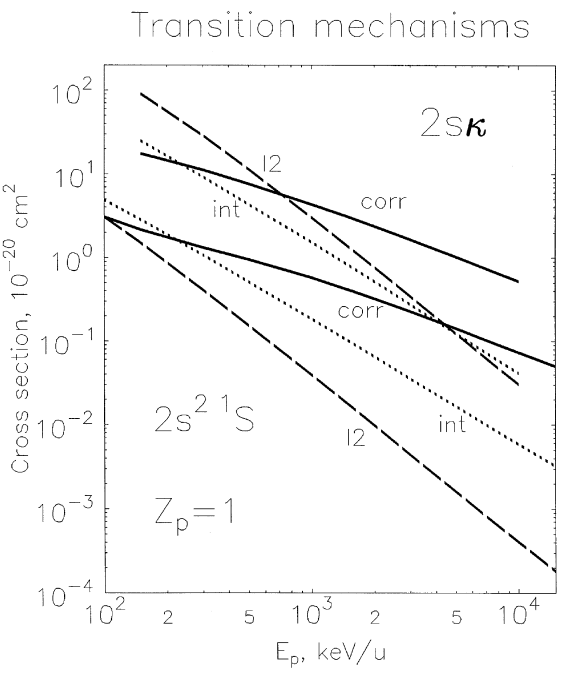

Fig. 3. Contributions from different transition mechanisms to the helium total $1s^2\,{}^1S \rightarrow 2s\vec{\kappa}$ (Ref. [31]) and $1s^2\,{}^1S \rightarrow 2s^2\,{}^1S$ (Ref. [24]) cross sections for proton impact vs. the projectile energy E_p. Full curve stands for the contribution from the correlation mechanism; broken curve, for the contribution from the independent transitions mechanism; dotted curve, for the modulus of the interference term of the cross section.

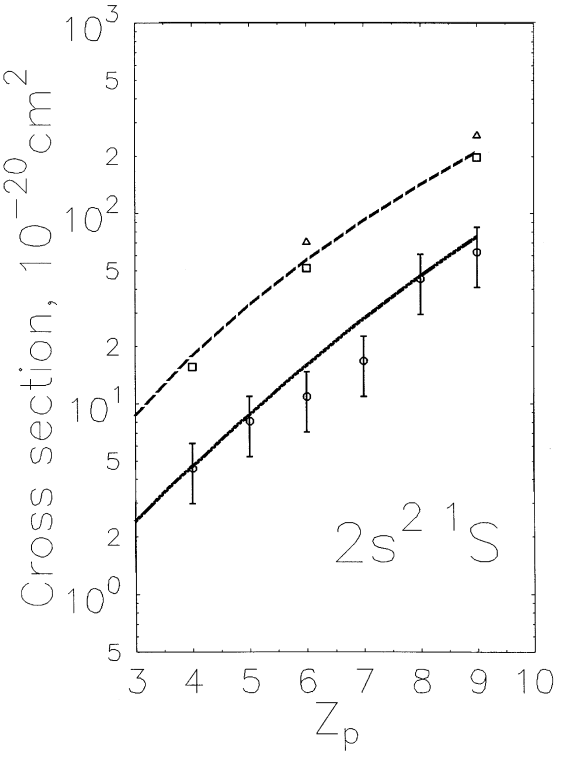

Fig. 4. The helium $1s^2\,{}^1S \rightarrow 2s^2\,{}^1S$ excitation cross section at scattering energy $E = 1.5$ MeV/u as a function of the projectile charge Z_p. Full curve denotes the results received in the present approach Ref. [24]; dashed curve, the results obtained without taking into account of the continuous spectrum states in the amplitude a^{c1}; triangles and squares present the close-coupling results of Refs. [9,10] and Ref. [4], respectively; circles experimental data Ref. [32].

$1s^2\,{}^1S \rightarrow 2s^2\,{}^1S$ excitation of helium by charged particles with energy $E = 1.5$ MeV/u that condition is fulfilled at $Z_p \sim 5$–7 for the impact parameters bringing in the main contribution to the excitation process. The accuracy must be better when $Z_p < 5$, and it must be worse when $Z_p > 7$. The calculated cross sections (full curve) agree with the available experimental data [32] within the measurement errors.

4.3. The simultaneous ionization–excitation of helium

Fig. 2b shows that for the $1s^2\,{}^1S \rightarrow 2s\vec{\kappa}$ helium ionization–excitation process the calculations predict the exceeding of the total cross sections for protons over the antiproton ones at all collision energies considered. This is a very interesting situation because for all previously investigated two-electron transitions in helium the antiproton cross sections were greater than those for protons. Contributions from different mechanisms to the $2s\vec{\kappa}$ ionization-excitation cross section are presented in Fig. 3.

The calculated results of the single differential cross section (SDCS) for the $2s\vec{\kappa}$ simultaneous ionization-excitation, induced in collisions of protons and antiprotons with helium atoms, are presented in Fig. 5 for the projectile energy $E_p = 1.5$ MeV versus the ejected electron energy E_e. The calculation results show that at ejected electron energies $E_e = E_{nl\,{}^2L} - E_{2s\,{}^2S}$ there are sharp drops in SDCS. All these drops in the energy spectrum of electrons, ejected at the $1s^2\,{}^1S \rightarrow 2s\vec{\kappa}$ transition, are located in the range of electron energies $0 < E_e \leqslant -E_{2s\,{}^2S}$. Drops in the electron energy spectrum conform to jumps on the curve for $N_{2s\vec{\kappa}}(\kappa)$ (Fig. 1). The appearance of the drops is due to the opening of new resonant channels. Sharp drops in the energy spectrum of the ejected electrons is the effect of the resonant channel coupling.

To elucidate the charge asymmetry in the helium $2s\vec{\kappa}$ ionization-excitation cross sections at greater length we shall consider here the ionization-excitation probabilities for protons and antiprotons which are presented in Fig. 6 at projectile energy $E_p = 1.5$ MeV. The ejection of high energy electrons is due to the collisions at small impact

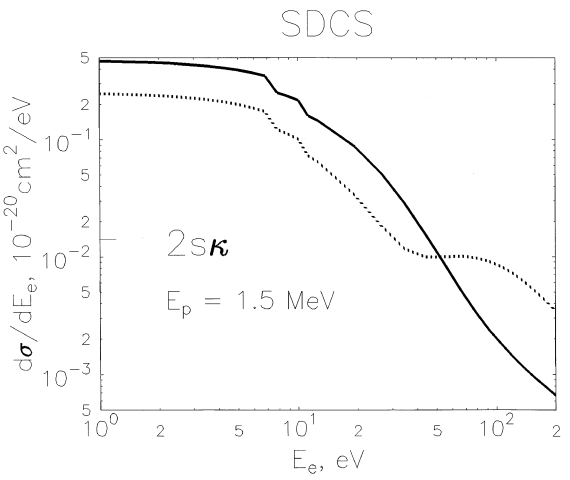

Fig. 5. The value of $d\sigma/dE_e$ as a function of E_e, the ejected electron energy, for the $1s^2\,{}^1S \rightarrow 2s\vec{\kappa}$ transition induced in collisions of protons and antiprotons with helium at projectile energy $E_p = 1.5$ MeV (Ref. [31]). Full curve stands for SDCS for protons; dotted curve, for SDCS for antiprotons.

parameters b, where the screening of the helium nucleus charge by antiprotons promotes SDCS for antiprotons and the antiscreening of the helium nucleus charge by protons reduces SDCS for protons. The ejection of small energy electrons is

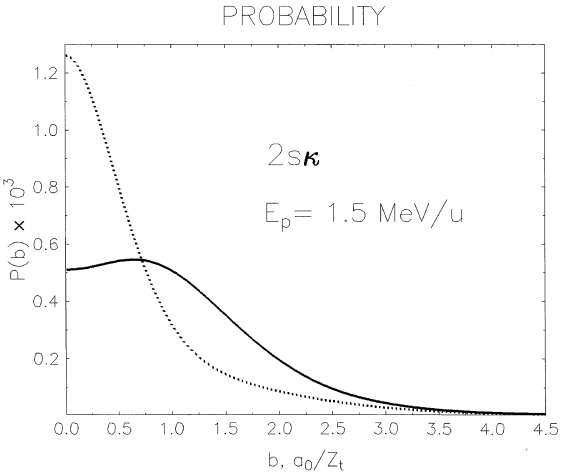

Fig. 6. The ionization–excitation probability $P(b)$ as a function of the impact parameter b for the $1s^2\,{}^1S \rightarrow 2s\vec{\kappa}$ transition induced in collisions of protons and antiprotons with helium at projectile energy $E_p = 1.5$ MeV (Ref. [31]). Full curve stands for the probability for protons; dotted curve, for the probability for antiprotons.

due to the collisions at large impact parameters b, where we have now the exceeding of the proton SDCS over the antiproton ones.

5. Outstanding questions

The top priority problem in physics of collisions of atomic particles is the working out a new concept of electron correlations in few-electron atoms having a clear physical meaning and strict mathematical justification. The present concept of electron correlations as some equivalent to V_{ee} which can be defined as the difference between the exact and Hartree–Fock calculations [25,48] is, to my mind, unsatisfactory. The strict physical definition should not rely on the calculated results.

The solution of this problem enables us to obtain the correct wavefunction of few-electron atom that, in its turn, will allow to achieve a pronounced progress in future investigations of collisions of charged particles with few-electron atoms.

6. Conclusion

In the present report I have reviewed results, mainly, of some of my recent own investigations of the double-electron transitions induced in collisions of protons, antiprotons and multicharged ions with helium atoms performed on the basis of the approach using the perturbation expansions in terms of the scattering potential and the diagonalization approximation for the target atom wavefunction. An important quality of the presented approach is its universality: *to determine the amplitude of any inelastic transition we need to evaluate only two functions* $D_j^{(1)}$ *and* $D^{(2)}$ *for different elementary scattering events*.

References

[1] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, K.G. Rensfelt, E. Uggerhøj, Phys. Rev. Lett 57 (1986) 2147.
[2] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, A.H. Sørensen, K. Elsener, K.G. Rensfelt, E. Uggerhøj, Phys. Rev. A. 36 (1987) 3612.
[3] V.V. Balashov, M.V. Gorelenkova, A.I. Magunov, Yadernaya Fizika 53 (1991) 663.
[4] W. Fritsch, C.D. Lin, Phys. Rev. A. 41 (1990) 4776.
[5] W. Fritsch, C.D. Lin, Phys. Rep. 202 (1991) 1.
[6] T.G. Winter, Phys. Rev. A. 43 (1991) 4727.
[7] J.H. McGuire, J.C. Straton, Phys. Rev. A. 43 (1991) 5184.
[8] J.C. Straton, J.H. McGuire, Z. Chen, Phys. Rev. A. 46 (1992) 5514.
[9] K. Moribayashi, K. Hino, M. Matsuzawa, M. Kimura, Phys. Rev. A. 44 (1991) 7234.
[10] K. Moribayashi, K. Hino, M. Matsuzawa, M. Kimura, Phys. Rev. A. 46 (1992) 1684.
[11] V.A. Sidorovich, Zh. Eksp. Teor. Fiz. 103 (1993) 806.
[12] V.A. Sidorovich, JETP 76 (1993) 396.
[13] J.E. Reading, A.L. Ford, Phys. Rev. Lett. 58 (1987) 543.
[14] J.E. Reading, A.L. Ford, J. Phys. B: At. Mol. Phys. 20 (1987) 3747.
[15] R.E. Olson, Phys. Rev. A. 36 (1987) 1519.
[16] L. Végh, Phys. Rev. A. 37 (1988) 992.
[17] A.L. Ford, J.E. Reading, J. Phys. B: At. Mol. Opt. Phys. 27 (1994) 4215.
[18] M.R.H. Rudge, J. Phys. B: At. Mol. Opt. Phys. 21 (1988) 1887.
[19] A. Raeker, K. Bartschat, R.H.G. Reid, J. Phys. B: At. Mol. Opt. Phys. 27 (1994) 3129.
[20] A. Franz, P.L. Altick, J. Phys. B: At. Mol. Opt. Phys. 28 (1995) 4639.
[21] L. Nagy, J. Wang, J.C. Straton, J.H. McGuire, Phys. Rev. A. 52 (1995) 902.
[22] L. Végh, B. Sulik, N. Stolterfoht, Phys. Rev. A. 51 (1995) 3017.
[23] L. Nagy, J.H. McGuire, L. Vegh, B. Sulik, N. Stolterfoht, J. Phys. B: At. Mol. Opt. Phys. 30 (1997) 1939.
[24] V.A. Sidorovich, Physica Scripta 50 (1994) 119.
[25] J.H. McGuire, Adv. At. Mol. Opt. Phys. 29 (1992) 217.
[26] L.P. Presnyakov, D.B. Uskov, Zh. Eksp. Teor. Fiz. 86 (1984) 882.
[27] L.P. Presnyakov, H. Tawara, I.Yu. Tolstikhina, D.B. Uskov, J. Phys. B: At. Mol. Opt. Phys. 28 (1995) 785.
[28] F. Melchert, M. Benner, S. Krüdener, R. Schulze, S. Meuser, K. Huber, E. Salzborn, D.B. Uskov, L.P. Presnyakov, Phys. Rev. Lett 74 (1995) 888.
[29] L.P. Presnyakov, D.B. Uskov, Pis'ma Zh. Eksp. Teor. Fiz. 66 (1997) 22.
[30] V.A. Sidorovich, Nucl. Instrum. Methods B 98 (1995) 328.
[31] V.A. Sidorovich, J. Phys. B: At. Mol. Opt. Phys. 30 (1997) 2187.
[32] J.P. Giese, M. Schulz, J.K. Swenson, M. Benhenni, S.L. Varghese, C.R. Vane, P.F. Dittner, S.M. Shafroth, S. Datz, Phys. Rev. A. 42 (1990) 1231.
[33] F. Martin, A. Salin, J. Phys. B: At. Mol. Opt. Phys. 28 (1995) 639.
[34] A. Macias, F. Martin, A. Riera, M. Yanez, Eur. Lett. 4 (1987) 799.
[35] A. Macias, F. Martin, A. Riera, M. Yanez, Int. J. Quantum. Chem. 33 (1988) 279.
[36] P. Moretto-Capelle, D. Bordenave-Montesquieu, A. Bordenave-Montesquieu, A.L. Godunov, V.A. Schipakov, Phys. Rev. Lett. 79 (1997) 5230.

[37] M.B. Shah, H.B. Gilbody, J. Phys. B: At. Mol. Opt. Phys. 18 (1985) 899.
[38] P. Hvelplund, H. Knudsen, U. Mikkelsen, E. Morenzoni, S.P. Møller, E. Uggerhøj, T. Worm, J. Phys. B: At. Mol. Opt. Phys. 27 (1994) 925.
[39] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, J.O.P. Pedersen, S. Tang-Petersen, E. Uggerhøj, K. Elsener, E. Morenzoni, Phys. Rev. A 40 (1989) 7366.
[40] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, J.O.P. Pedersen, S. Tang-Petersen, E. Uggerhøj, K. Elsener, E. Morenzoni, Phys. Rev. A41 (1990) 6536.
[41] L.V. Keldysh, Zh. Eksp. Teor. Fiz. 47 (1964) 1945.
[42] V.A. Sidorovich, Phys. Scripta, submitted for publication.
[43] V.A. Sidorovich, Phys. Lett. A. 225 (1997) 92.
[44] L.D. Landau, E.M. Lifshitz, Quantum mechanics. Non-relativistic theory (Nauka, Moscow, 1989).
[45] J.H. McGuire, Phys. Rev. Lett. 49 (1982) 1153.
[46] V.A. Sidorovich, Phys. Lett. A. 159 (1991) 257.
[47] V.A. Sidorovich, to be published.
[48] N. Stolterfoht, in: D. Bereny, G. Hock (Eds.), Lecture Notes in Physics, High-Energy Ion-Atom Collisions, Proceedings of the fourth Workshop on High-Energy Ion-Atom Collisions, Debrecen, Hungary, 17–19 September 1990, Springer, Berlin, 1991 vol. 376, p. 139.