

Mechanisms of the Double-Electron Excitation in Fast Ion-Atom Collisions: The Helium $1s^2S \rightarrow 2s^2S$ Excitation

V. A. Sidorovich

Skobeltzyn Institute of Nuclear Physics, Moscow State University, Moscow 119899, Russia

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Abstract

The probabilities and cross sections of the helium $1s^2S \rightarrow 2s^2S$ excitation in collisions of protons, antiprotons and multicharged ions with helium atoms have been calculated with allowance for the configuration interaction at ion energies ranging from 0.1 to 10 MeV/u. The mechanisms for the helium $2a^2S$ autoionizing state excitation are determined, the role of the continuous spectrum states at the helium double-electron excitation is examined. The criterion of the helium atom nucleus effective charge choice at the description of a collision process is established. The comparison of the present results with the available experimental data and with the results received in different theoretical approaches has been made.

1. Introduction

The investigation of the multielectron transitions induced in ion-atom collisions is one of the most interesting problems in atomic particle collision physics. At present, when the many-body problem in atomic physics is not understood in full, the studying of the double-electron transitions in collisions of structureless charged particles with few-electron atomic systems is especially urgent as in such transitions the physical nature of multielectron transitions is accessible for understanding.

Measurements of the helium double-electron ionization by protons and antiprotons, performed by Andersen and co-workers [1, 2] in a broad energy range around 2–5 MeV, show that the cross sections by antiprotons are about twice as large as those seen with equivelocity protons. To understand this difference, calculations have been carried out [3] and various qualitative interpretations have been made [2, 4–7].

To study the double-electron excitation processes in ion-atom collisions, the cross sections of the helium low-lying autoionizing states excitation in collisions of fast protons, antiprotons and multicharged ions with helium atoms have been calculated [8–13]. The results of the close-coupling calculations using the one-center atomic orbital expansion method including the electron–electron interaction between correlated helium wave functions [8] and the one-electron Sturmian functions [9], of the calculations in the second Born approximation including only off-energy shell transitions to states of the discrete spectrum [10, 11] and also of the calculations carried out in the second Born approximation and in the close-coupling method using hyperspherical wave functions with allowance for only states of the discrete spectrum [12, 13] are in a unsatisfactory agreement with the available experimental data [14, 15]. The cause of a difference between the calculated and experimental results consists in neglecting of the continuous spectrum states in the atomic orbital expansion of the helium electron wave function in the theoretical investigations [8, 10–13]. A

substitution of the pseudostates for the states of the continuous spectrum, as it was done in Ref. [9], does not reproduce the measured results. Only taking into account the relationship between the states of the continuous and discrete spectra at the helium autoionizing states excitation, as the calculations of the cross section for the $1s^2S \rightarrow 2s^2S$ excitation induced in collisions of helium with fast multicharged ions [16] have shown, permits to receive a complete agreement between calculated and experimental results.

It is the purpose of the present work to analyse the cross sections of the $1s^2S \rightarrow 2s^2S$ excitation of helium by protons, antiprotons and multicharged ions obtained from theoretical calculations, to determine the double-electron excitation mechanisms, to study the cause of the charge asymmetry in the helium double-electron excitation cross section, to examine the role of the continuous spectrum states at the helium double-electron excitation and to investigate the double-electron excitation cross section dependence from the value of the helium nucleus effective charge, to determine the choice criterion of the effective charge. Here we shall consider only fast ion-atom collisions when the polarization of the helium electron shell by the projectile and the competing charge–transfer process at the scattering of a positively charged ion by helium can be neglected.

2. Method of calculations

Let us consider the scattering of a fast structureless charged particle by the helium atom in the impact parameter representation. It is assumed that the projectile moves along a straight line $\mathbf{R}(t) = \boldsymbol{\rho} + \mathbf{v} \times t$ (where $\boldsymbol{\rho}$ is the impact vector and \mathbf{v} is the velocity of motion of the projectile relative to the atomic nucleus), while the electron wave function of helium is independent of the relative distance between the colliding particles and is given by the Schrödinger equation which in the interaction representation has the form

$$i \frac{\partial \phi(t)}{\partial t} = \tilde{\mathbf{V}}(t) \times \phi(t); \quad \phi(t) \Big|_{t \rightarrow \pm \infty} = \phi_{i, f}(\mathbf{r}_1, \mathbf{r}_2) \quad (1)$$

where

$$\tilde{\mathbf{V}}(t) = \exp(iH_0 t) \left\{ - \sum_j \frac{Z}{|\mathbf{R}(t) - \mathbf{r}_j|} \right\} \exp(-iH_0 t) \quad (2)$$

is the interaction operator in the interaction representation. The wave function $\phi(\mathbf{r}_1, \mathbf{r}_2)$ is the eigenfunction of the atomic Hamiltonian H_α with the eigenvalue E ,

$$H_\alpha \phi(\mathbf{r}_1, \mathbf{r}_2) = E \phi(\mathbf{r}_1, \mathbf{r}_2). \quad (3)$$

Here, $H_0 = H_\alpha + K$ is the freemotion Hamiltonian; $K = \hat{\mathbf{p}}^2/2M$ and M are the kinetic energy operator and the reduced mass of the colliding particles; $\hat{\mathbf{P}}$ is the relative

motion momentum operator; $R(t)$ and r_j are the radius vectors of the ion and of the j th atomic electron relative to the target atom nucleus; Z is the ion charge.

To determine the wave function $\phi(r_1, r_2)$ it is convenient to express the atomic Hamiltonian H_α as a sum of two terms: the single particle Hamiltonian, H_α^0 , and the term W^c containing the electron-electron correlation potential, $V^c(|r_1 - r_2|) = 1/|r_2 - r_2|$,

$$H_\alpha = H_\alpha^0 + W^c, \quad (4)$$

where

$$H_\alpha^0 = \sum_j^2 \left(\frac{\hat{p}_j^2}{2} - \frac{Z_{\text{He}}}{r_j} + w_j \right); \quad W^c = V^c - \sum_j^2 w_j; \quad (5)$$

Z_{He} is the helium nucleus charge; w_j is the screening potential working on the j th helium electron by the another electron; \hat{p}_j is the momentum operator of the j th electron of the helium atom.

As it follows from Ref. [7], in the case of fast collisions the electron wave function of the helium μ state $\phi_\mu(r_1, r_2)$ is determined by the expression

$$\phi_\mu(r_1, r_2) = \Phi_\mu(r_1, r_2) + \left(\Sigma'_v + \int dv \right) \lambda_v \Phi_v(r_1, r_2) \quad (6)$$

with

$$\lambda_v = \frac{\langle \Phi_v | W^c | \Phi_\mu \rangle}{E_\mu - E_v - i0}, \quad (7)$$

where $\Phi_\Gamma(r_1, r_2)$ is the wave function of the helium atom in the Γ state determined in the independent electron approximation. Last term in the r.h.s. of (6) defines a correction to the wave function of the μ state $\Phi_\mu(r_1, r_2)$ for configuration mixing. The prime on a summation sign denotes elimination from the sum of states that can lead to self-mixing. We choose in the energy denominator the imaginary portion $i0$, which has the effect of moving the pole off the real axis when Φ_v describes a state in the continuous spectrum, with the minus sign. In the case of quasistationary states such a choice corresponds to the negativity of the imaginary part of the quasistationary state energy that, in turn, must secure the decay of the quasistationary state in time.

The wave functions (6), (7) for initial and final states are not orthogonal and normalized. Using the Gram-Schmidt orthogonalization procedure we will receive the orthonormal wave functions of the helium $1s^{21}S$ and $2s^{21}S$ states. The amplitude of the helium double-electron $1s^{21}S \rightarrow 2s^{21}S$ transition determined with allowance for only terms of the perturbation-theory series up to the second order in the interaction potential is determined by the expression [7]

$$A(2s^{21}S \leftarrow 1s^{21}S; \rho) = \alpha^{c1}(2s^2; \rho) + \alpha^{T2}(2s^2; \rho) + \alpha^{c2}(2s^2; \rho), \quad (8)$$

where α^{c1} is the amplitude of the double-electron transition occurring as a result of a single scattering of a projectile by the helium atom and the correlation interaction of atomic electrons; α^{T2} is the amplitude of the transition of two helium electrons as a result of a single interaction of each of them with the projectile ($\alpha^{T2} = (1/N_{1s^2} N_{2s^2}) \times \alpha^{\text{IEA}}$, α^{IEA} is the amplitude of the two electron transition determined in the independent electron approximation, N_{1s^2} and N_{2s^2} are the normalizing factors for $1s^{21}S$ and $2s^{21}S$ states,

respectively); α^{c2} is the amplitude of the two electron transition occurring as a result of the double scattering of the projectile on helium and the correlation interaction of the atomic electrons; $\rho = |\rho|$ is the impact parameter.

3. Results and discussion

(a). The double-electron excitation cross section

In the framework of the present approach the helium $1s^{21}S \rightarrow 2s^{21}S$ excitation cross sections have been calculated in collisions of helium with protons, antiprotons and multi-charged ions at ion energies E changing from 0.1 to 10 MeV/u. Some of these results have been presented earlier in Ref. [16]. At determining of the wave functions for $1s^{21}S$ and $2s^{21}S$ states we restricted ourselves by taking into account only the configurations $1s^2$, $1s2s$, $1s2p$, $1s\kappa$, $2s^2$, $2s2p$, $2p^2$, $2s\kappa$, $2p\kappa$ (where κ is the electron momentum into the continuous spectrum). In the present calculations the helium nucleus effective charge was equal to 2 (concerning the choice of the effective charge, see below). The energies of the different states of helium were taking from Refs [12, 18]. At performing the calculations the term α^{c2} in the double electron excitation amplitude (8) was not taken into account as it is much less than the other terms of the amplitude. The normalizing factors for the wave functions of the $1s^{21}S$ and $2s^{21}S$ states were equal to $N_{1s^2} = 1.095$ and $N_{2s^2} = 1.183$, respectively.

Figure 1 shows that the helium double-electron excitation cross section to the state $2s^{21}S$ for antiprotons significantly exceed the proton one at the scattering energies from 0.1 to

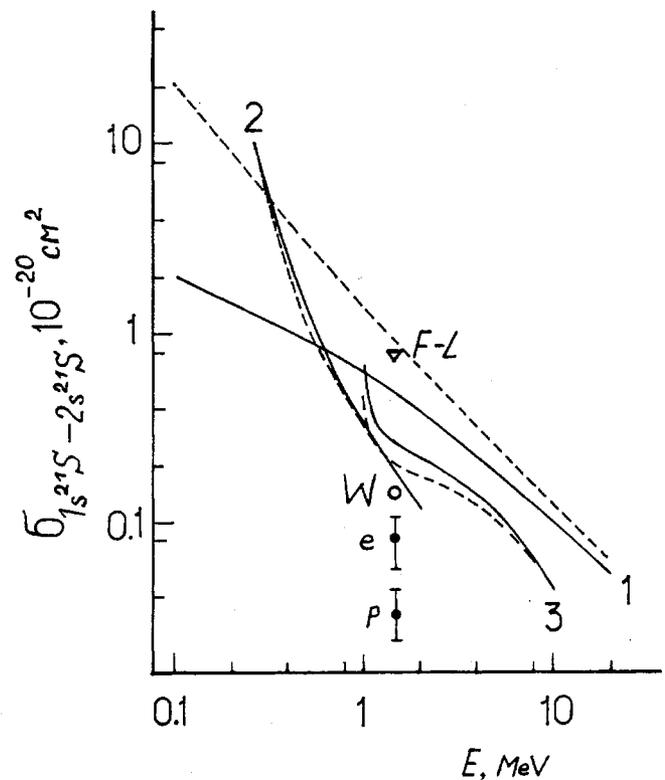


Fig. 1. Proton and antiproton double-electron excitation cross sections for the $1s^{21}S \rightarrow 2s^{21}S$ transition in helium vs. the projectile energy, E . Curves 1 are the present results; curves 2 are the results from Ref. [11]; curves 3 are the results from Ref. [12]. Points F-L and W are the calculated results from Refs [8] and [9], respectively. Experimental data for electrons and protons are taken from Ref. [15]. Solid lines denote the results for protons and dashed lines for antiprotons.

~ 2 MeV. At energies around 100 keV this exceeding may reach 10 times. The calculations performed in the second Born approximation [11] and in the different modifications of the close-coupling method [8, 9, 12] shown insignificant exceeding of the helium double-electron excitation cross sections for protons over the antiproton ones. Contributions from different excitation mechanisms to the helium double-electron $1s^{21}S \rightarrow 2s^{21}S$ transition for protons and antiprotons are presented in Fig. 2. For all considered 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. It is typical of the correlation mechanism that a contribution to the excitation cross section from on-energy shell transitions exceeds a contribution from off-energy shell transitions. Contribution from the interference term in the cross section is compared with contributions from the different excitation mechanisms. The difference between cross sections for protons and antiprotons must be significant as the interference terms for protons and antiprotons have the opposite signs. As it follows from Ref. [7] when we take into account only terms of the perturbation-theory series up to the second order in the interaction potential in the double-electron excitation amplitude the difference between the helium double-electron excitation cross sections for protons and antiprotons must be determined by the interference between the transitions described by the amplitudes α^{T2} and α^{e2} with the transitions described by the amplitude α^{e1} . The main contribution to the difference comes from the term $\alpha^{T2} \times \alpha_{\text{on}}^{e1*}$ (α_{on}^{e1} and α_{off}^{e1} are the on- and off-energy shell parts of the amplitude α^{e1}). The electron transitions to the $2s^{21}S$ state determined by the amplitude α_{on}^{e1} occur through the one-electron continuum states. So, the difference in the helium double-electron excitation cross sec-

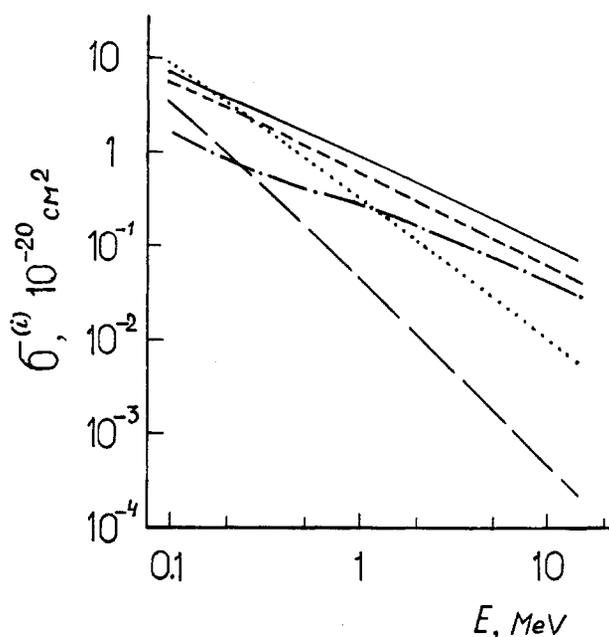


Fig. 2. Contributions of the different double-electron excitation mechanisms for the $1s^{21}S \rightarrow 2s^{21}S$ transition in helium induced by protons and antiprotons vs. the projectile energy, E . Solid curve is the contribution from the correlation mechanism (short-dashed and dash-dotted lines denote the contributions from the on- and off-energy shell transition, respectively); long-dashed curve is the contribution from the independent electron transitions mechanism; dotted curve is the modulus of the interference term.

tions for protons and antiprotons is mainly determined by the interference of the discrete-discrete transitions with the transitions occurring through states of the continuous spectrum.

The helium $1s^{21}S \rightarrow 2s^{21}S$ excitation cross sections induced by particles with charges Z from -9 to $+9$ at the energy of ions $E = 1.5$ MeV/u are presented in Fig. 3. The results show that the double-electron excitation cross section possesses a strong charge asymmetry (solid curves). Figure 3 also presents the results of the calculations carried out without taking into account the states of the continuous spectrum (dashed curves). As it can be seen from Fig. 3 the calculations realized without taking into account continuum states are in agreement with the available calculations performed in different modifications of the close-coupling method [8, 12, 13] with the same restrictions. A significant difference between the results performed with and without taking into account the continuum states (see Fig. 3) points out an important role of the continuum states at the double-electron excitation of helium. The present results with exception of proton and electron ones (solid curves) agree with the available experimental data [15] within the measurement errors. The calculated double-electron cross sections for protons and electrons exceed the corresponding experimental data almost in 10 times. That is very strange and new testing measurements in these two cases are desirable.

(b). The double-electron excitation probabilities

To elucidate the cause of arising the charge asymmetry in the helium $1s^{21}S \rightarrow 2s^{21}S$ excitation cross section at greater length we shall consider here the excitation probabilities. The calculation results for the helium $1s^{21}S \rightarrow 2s^{21}S$ excitation probabilities for protons and antiprotons vs. the impact

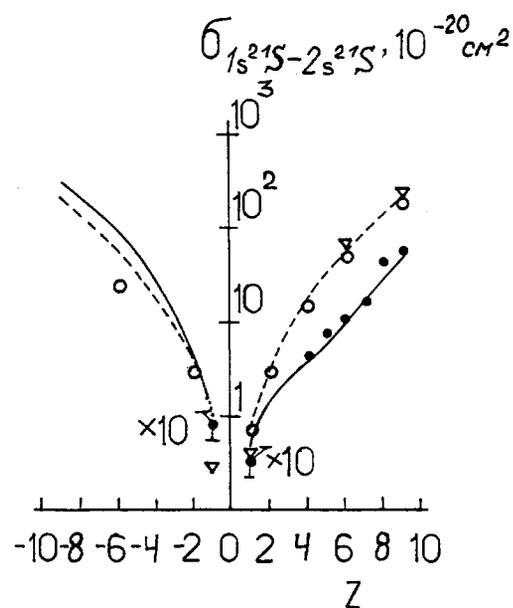


Fig. 3. The helium $1s^{21}S \rightarrow 2s^{21}S$ excitation cross sections as a function of the projectile charge, Z . Solid curves and dashed curves are the results of the calculations performed with and without allowance for the electron-electron correlations, respectively. Open circles are the calculated results from Ref. [8], open triangles are the calculated results from Ref. [12, 13]. Closed circles are the experimental data from Ref. [15]. The experimental data for electrons ($Z = -1$) and for protons ($Z = +1$) are multiplied by 10.

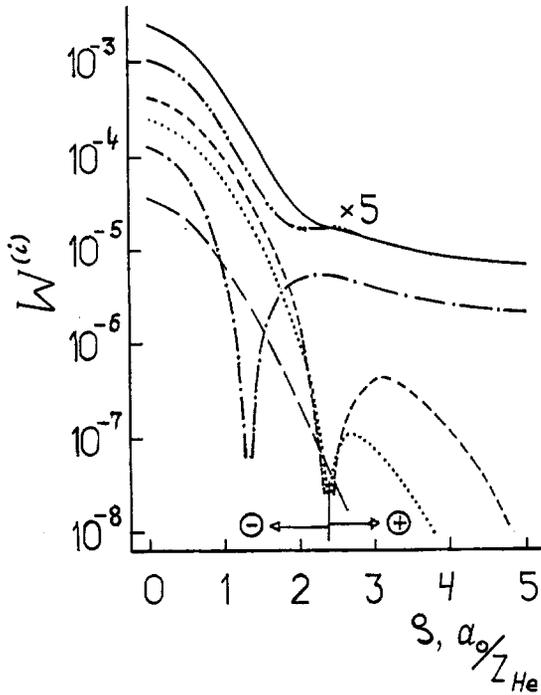


Fig. 4. Excitation probabilities for $1s^2S \rightarrow 2s^2S$ transition in helium induced by 1.5 MeV protons and antiprotons vs. the impact parameter ρ . Solid and dash-double-dotted lines are the total excitation probabilities for antiprotons and protons, respectively (the total excitation probabilities are multiplied by 5); long-dashed line is the probability corresponding to the independent electron excitation mechanism; short-dashed line and dash-dotted line are the probabilities corresponding to the correlation mechanism of excitation, respectively, for on- and off-shell transitions; dotted line is the modulus of the interference term in the excitation probability. The signs plus and minus show the impact parameter values where the interference for protons is constructive and destructive, respectively.

parameter at ion energy $E = 1.5$ MeV are presented in Fig. 4. The probabilities for different excitation mechanisms and the interference term responsible for the charge asymmetry in the double-electron excitation probability are also represented there. In the case of the correlation mechanism of excitation the contributions from transitions occurring on- and off-energy shell are divorced from each other. Calculations show that the probabilities for the correlation excitation mechanism corresponding to the on- and off-energy shell transitions at the impact parameter values $\rho_{01} \approx 2.37\alpha_0/Z_{He}$ and $\rho_{02} \approx 1.3\alpha_0/Z_{He}$ (α_0 is the atomic length unit) are equal to zero. In the present calculations, when we refused the term α^{e2} in the double-electron amplitude, the equality to zero of a part of the correlation probability (or amplitude) corresponding to the on-energy shell transitions leads to the equality to zero of the interference term in the double-electron excitation probability.

As calculations show at the values of the impact parameter ρ , less than ρ_{01} , the interference is destructive for protons and constructive for antiprotons; at $\rho > \rho_{01}$ the interference is constructive for protons and destructive for antiprotons. At $\rho < \rho_{01}$ the interference term brings up an essential contribution into the double-electron excitation probability and so the helium double-electron excitation probabilities for protons and antiprotons are greatly different; at $\rho > \rho_{01}$ the contribution of the interference term is small and the probabilities for protons and antiprotons practically coincide. As the main contribution in the helium double-electron excitation cross section is brought up by the

collisions at small impact parameters ρ , where the probabilities for protons and antiprotons are quite different, then the helium $1s^2S \rightarrow 2s^2S$ excitation cross sections for protons and antiprotons differ one from another. Such a situation is observed at other ion energies considered.

4. Choice of the helium atom nucleus effective charge

The target atom nucleus effective charge, in the field of which the hydrogen-like wave functions entering into the electron target wave function $\phi_{\Gamma}(r_1, r_2)$ are determined, strongly affects upon the cross section value. It can be seen from Figs 5 and 6 where the ratios of the helium $1s^2S \rightarrow 2s^2S$ excitation cross sections, calculated with the effective charges 1.69 and 2, are displayed vs. the ion energy and charge, respectively. So, it is particularly important to choose correctly an effective charge at performing the calculations. Different authors (see, e.g. [8–13]) choose the helium atom nucleus effective charge resulting from various criteria, as a rule, not bearing a direct relation to the scattering problem. As such it may be charge chosen variationally to minimize the ground state energy [10–11], to minimize the energy of states included in the close-coupling expansion [8] and the charge of the helium atom [9]. Here we shall formu-

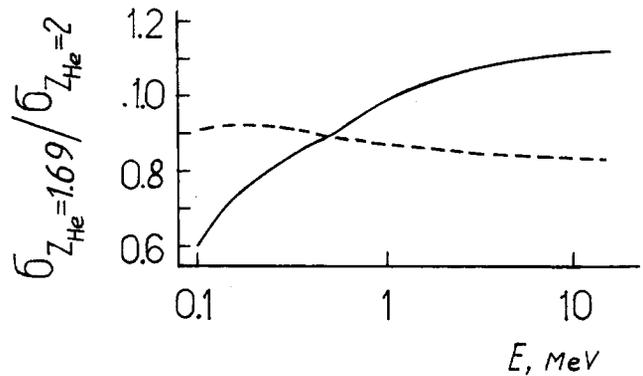


Fig. 5. Ratio of the helium $1s^2S \rightarrow 2s^2S$ excitation cross sections, calculated with the effective charges 1.69 and 2, for protons (solid line) and antiprotons (dashed line) vs. the projectile energy, E .

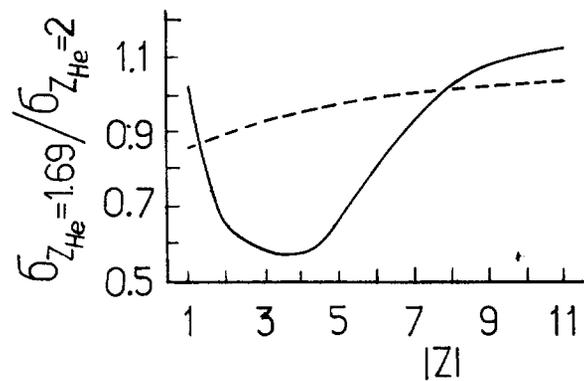


Fig. 6. Ratio of the helium $1s^2S \rightarrow 2s^2S$ excitation cross sections, calculated with the effective charges 1.69 and 2, for different projectiles vs. the modulus of the projectile charge at projectile energy $E = 1.5$ MeV. Solid and dashed lines correspond, respectively, to the positively and negatively charged projectiles.

late and prove the statement which permits to choose an optimum effective charge.

Statement: If the helium electron wave function is determined in the independent electron approximation then, at the describing of a scattering of a charge particle by helium, the atomic nucleus effective charge, in the field of which the Coulomb wave functions for the single helium electrons are defined, must be equal to the value corresponding to the self-consistent field potential; if the helium electron wave function is determined with allowance for the electron-electron correlations then the corresponding effective charge must be equal to the helium nucleus charge itself.

The proof:

According to [7], in the framework of the diagonalization approximation, the wave function (6)–(7) is an exact solution of the Schrödinger equation. Let us introduce the quantity $W^{(k)c} = V^c - \sum_i^2 w_i^{(k)}$, where $w_i^{(k)}$ is the choice of some k th

way centre symmetrical screening potential working on the i th helium electron by the another helium electron. Let us define a limiting value of the screening potential \tilde{w}_i corresponding to the Hartree–Fock potential V_i^{H-F} ,

$$\tilde{w}_i \sim V_i^{H-F}. \quad (9)$$

The helium electron wave function for the k th choice of the screening potential will be determined by the expression

$$|\phi_L\rangle = |\Phi_L^{(k)}\rangle + \sum_P' \frac{|\Phi_P^{(k)}\rangle \langle \Phi_P^{(k)} | W^{(k)c} | \Phi_L^{(k)} \rangle}{E_L - E_P - i0}, \quad (10)$$

where $|\Phi_P^{(k)}\rangle$ is the solution of the equation

$$\sum_i^2 \left(\frac{\hat{p}_i^2}{2} - \frac{Z_{He}}{r_i} + w_i^{(k)} \right) |\Phi_P^{(k)}\rangle = E_P |\Phi_P^{(k)}\rangle; \quad (11)$$

here and below the sign \sum_P' means the summation over all discrete states and the integration over the continuum states.

Let us consider two cases:

1. the helium wave function is determined in the independent electron approximation.

In this case we must in the expression for the exact wave function (10) substitute the Hartree–Fock potential $V^{H-F} = \sum_i^2 V_i^{H-F}$ for the correlation potential V^c . Using the relation (9) we may write the exact solution of the Schrödinger equation in the form

$$|\phi_L\rangle = |\Phi_L^{(k)}\rangle + \sum_P' \frac{|\Phi_P^{(k)}\rangle \langle \Phi_P^{(k)} | \sum_i^2 (\tilde{w}_i - w_i^{(k)}) | \Phi_L^{(k)} \rangle}{E_L - E_P - i0}. \quad (12)$$

When $w_i^{(k)} = \tilde{w}_i$ the exact solution will be determined by the first term in the r.h.s. of (12) and the helium nucleus effective charge should be equal to the value corresponding to the self-consistent field potential. At any other value, of $w_i^{(k)}$ the first term of (12) corresponding to the independent electron approximation will be differed from the exact solution:

2. the helium electron wave function is determined with allowance for the electron correlations.

In this case the exact solution of the Schrödinger equation has the form

$$|\phi_L\rangle = \begin{cases} |\Phi_L^{(k)}\rangle + \sum_P' \frac{|\Phi_P^{(k)}\rangle \langle \Phi_P^{(k)} | V^c | \Phi_L^{(k)} \rangle}{E_L - E_P - i0} \\ - \sum_P' \frac{|\Phi_P^{(k)}\rangle \langle \Phi_P^{(k)} | \sum_i^2 w_i^{(k)} | \Phi_L^{(k)} \rangle}{E_L - E_P - i0}, & \text{at } w_i^{(k)} \neq 0 \\ |\Phi_L^{(0)}\rangle + \sum_P' \frac{|\Phi_P^{(0)}\rangle \langle \Phi_P^{(0)} | V^c | \Phi_L^{(0)} \rangle}{E_L - E_P - i0}, & \text{at } w_i^{(0)} = 0. \end{cases} \quad (13)$$

For simplicity we shall restrict ourselves by the proof of the statement only for the double-electron excitation. We shall also consider the scattering problem in the second order of the perturbation-theory series. In case of need the proof may be given in any order of the perturbation-theory series both for single- and double-electron excitations.

As can be seen (Refs [7, 17]) the terms in the double-electron transition amplitude satisfy the next conditions:

$$\begin{aligned} \alpha^{(k)T2}(W^{(k)c}) &= \alpha^{(k)T2} \left(\sum_i^2 w_i^{(k)} \right); \\ \alpha_{on}^{(k)c1}(W^{(k)c}) &= \alpha_{on}^{(k)c1}(V^c); \\ \alpha_{off}^{(k)c1}(W^{(k)c}) &= \alpha_{off}^{(k)c1}(V^c); \\ \alpha^{(k)c2}(W^{(k)c}) &= \alpha^{(k)c2}(V^c). \end{aligned} \quad (14)$$

That is to say, in the case when $w_i^{(k)} \neq 0$, the helium double-electron excitation amplitude is determined not by the exact electron wave function, but only a part (its first two terms). At $w_i^{(k)} = 0$, when $W^{(k)c} = V^c$, the helium double-electron excitation amplitude will be determined by an exact electron wave function. So, in this case the correct helium nucleus effective charge is the nucleus charge itself.

The statement is proved.

5. Conclusion

The carried out calculations of the $1s^2S \rightarrow 2s^2S$ excitation cross sections in collisions of helium with protons, anti-protons and multicharged ions show that:

(1) the excitation cross section has a strong dependence from the projectile charge sign at ion energies from 0.1 to ~ 2 MeV/u. The exceeding of the excitation cross section for antiprotons over the protons one may reach 10 times;

(2) the charge asymmetry in the excitation cross section is mainly determined by the interference between discrete-discrete transitions and transitions occurring through the continuum states;

(3) the present theory leads to results which coincide with the experimental cross sections (with the exception of the proton and electron results) within the measurement errors;

(4) the excitation cross section depends strongly from the magnitude of the helium atom nucleus effective charge;

(5) the main contribution to the helium double-electron excitation for protons and antiprotons at all considered energies is brought by the correlation mechanism. At energies $E = 0.1 - 2$ MeV the independent electron transitions give an essential contribution as well.

It is shown that at the describing of a scattering of a charge particle by helium on the basis of the independent electron approximation the helium atom nucleus effective charge must be equal to the value corresponding to the self-consistent field potential and in the case of taking into account the electron-electron correlations the corresponding effective charge must be equal to the helium nucleus charge itself.

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