Calculation of charge-changing cross sections in collisions of H^+, He^{2+}, and Li^{3+} with He atoms

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Cross sections for single and double ionization σ^{i1} and σ^{i2}, the single and double electron capture to the ground state σ^{c1} and σ^{c2}, and the ionization with electron capture to the ground state σ^{ic} in collisions of H^+, He^{2+}, and Li^{3+} nuclei with He atoms at nuclei energies from 0.025 to 4 MeV/amu are calculated. The independent-electron approximation is used with probabilities that are unitarized at the lower energies. Two kinds of calculations are performed: (i) The cross sections for all charge-changing processes are calculated including both the ionization and capture channels; (ii) the ionization cross sections σ^{i1} and σ^{i2} are calculated with neglect of the capture channel, the capture cross sections σ^{c1} and σ^{c2} are calculated with neglect of the ionization channel, and the cross sections σ^{ic} for ionization with capture are calculated with the single-electron transition probabilities obtained separately for ionization and capture. The direct-ionization calculations are based on the semiclassical Coulomb approximation, and electron capture is calculated with use of the approximation of Bassel and Gerjuoy [Phys. Rev. **113**, 749 (1960)]. The calculation results show that in single and double ionization the capture to the ground state strongly affects the value of σ^{i1} and σ^{i2} only in collisions of He atoms with the He^{2+} nuclei whereas the ionization channel leads to a marked decrease of the cross sections σ^{c1} and σ^{c2} in collisions with the He^{2+} and Li^{3+} nuclei.

INTRODUCTION

It is sensible to study the few-body problem in atomic physics in a systematic way. The two-body problem in atomic physics is well understood. And in some cases, the three-body problem is fairly well understood. For example, at high collision velocities, ionization and electron capture in a one-electron target, e.g., $p+H$, is fairly well understood. Consequently it is possible to consider single and double ionization and capture, as well as simultaneous ionization and capture in collisions of charged particles with two-electron targets.

In this paper we evaluate cross sections for various charge-changing collisions for protons, alpha particles, and lithium nuclei on helium, a two-electron target that is experimentally accessible. We work at moderately high velocities, 25 to ~ 1000 keV/amu, for systems symmetric and nearly symmetric in the projectile and target charges. In this region it has been established[1–9] that single ionization and capture may be fairly well described, respectively, by first-order perturbation theory and by two-state coupled-channel or Bassel-Gerjuoy (Bates-Born) calculations. Double ionization and capture and ionization with capture in this region are expected to be describable in terms of the independent-electron approximation[10] to the extent that electron correlation may be ignored or approximated. Since the two electrons are opposite spin, we do not expect Pauli exclusion effects[11] to be significant here. It is our purpose to seek the limits of this approach, especially at the lower velocities where the cross sections are largest and where experimental data is readily available. For this purpose a unitarization of ionization and capture probabilities is used. This unitarization is found from coupled equations describing the electron vacancy production into capture and ionization channels.

In the paper we calculate cross sections for all possible five charge-changing processes: the single and double ionization, one- and two-electron capture, and ionization with capture in collisions of the H^+, He^{2+}, and Li^{3+} nuclei with the He atoms at a collision energy of 0.025 to 4 MeV/amu in the independent-electron approximation. The calculations simultaneously take into account the ionization and electron capture to the ground states of fast nuclei. Here we also calculate the cross sections for the single and double ionization with the neglect of capture, for the one- and two-electron capture with the neglect of ionization and, also, the cross sections for ionization with capture to the ground state when the single-electron transition probabilities are determined separately for each process. The comparison of different variants of the calculations enable us to estimate the effect of unitarization of the single-electron transition probabilities upon the total cross section of all five processes in question and also the influence of the capture to the ground state upon the single- and double-ionization cross sections and the ionization influence upon the cross sections for the one- and two-electron capture to the ground state. Our calculations are compared with the available experimental data.

DESCRIPTION OF THE CALCULATIONS

In the collisions of atomic nuclei with the He atoms there are five possible elementary charge-exchange processes: the single and double ionization of helium, the one- and two-electron capture by nuclei and, also, the ionization of He atoms with the simultaneous electron capture by a bombarding nucleus. In the impact-parameter method, the cross section for each of the noted processes is

$$\sigma=2\pi\int P(b)b\,db\ . \tag{1}$$

The probabilities $P(b)$ of the above processes in the independent-electron approximation area determined by the relations[10]

$$P^{i1}(b)=2w_1^i(1-w_2^i-w_2^c)\ , \tag{2}$$

$$P^{i2}(b)=w_1^iw_2^i\ , \tag{3}$$

$$P^{c1}(b)=2w_1^c(1-w_2^i-w_2^c)\ , \tag{4}$$

$$P^{c2}(b)=w_1^cw_2^c\ , \tag{5}$$

$$P^{ic}(b)=2w_1^iw_2^c\ . \tag{6}$$

Here $P^{in}(b)$, $P^{cn}(b)$, and $P^{ic}(b)$ ($n=1$ and 2) are the probabilities of the n-fold ionization, n-fold electron capture, and ionization with the simultaneous electron capture, respectively: w^i and w^c are the transition probabilities of one electron to the continuum of the He atom and to the bound state of an incident nucleus.

Since the Born ionization probabilities can be higher than unity the present calculations employed, along with the Born ionization and capture probabilities W_B^i and W_B^c, the unitarized ionization and capture probabilities W_u^i and W_u^c:

$$W_u^i=\frac{W_B^i}{W_B^i+W_B^c}\{1-\exp[-(W_B^i+W_B^c)]\}\ , \tag{7}$$

$$W_u^c=\frac{W_B^c}{W_B^i+W_B^c}\{1-\exp[-(W_B^i+W_B^c)]\}\ . \tag{8}$$

The expressions (7) and (8) are the solutions of the differential equations of balance for population $g^i(b,t)$ of states of the continuum of He atoms, the population $g^c(b,t)$ of bound states of a bombarding nucleus, and the population $g_0(b,t)$ of the ground state of the He atoms:

$$\frac{d}{dt}g^i(b,t)=\lambda_i(b,t)g_0(b,t)\ , \tag{9a}$$

$$\frac{d}{dt}g^c(b,t)=\lambda_c(b,t)g_0(b,t)\ , \tag{9b}$$

$$\frac{d}{dt}g_0(b,t)=-[\lambda_i(b,t)+\lambda_c(b,t)]g_0(b,t)\ . \tag{9c}$$

As may be seen, this set of equations corresponds to the decay model of the electron initial state over two independent channels: ionization and electron capture. We note that our equations couple probabilities, whereas in more complete quantum coupled state calculations, it is probability amplitudes that are coupled. By ionization channel we mean the complete set of single-electron states of the continuum of the He atom, and by capture channel we mean the bound single-electron states of a bombarding nucleus.

Solving (9) for $g^i(b,t)$ and $g^c(b,t)$ at $t\to\infty$ gives

$$g^i(b,+\infty)=ag(b,+\infty)\ , \tag{10a}$$

$$g^c(b,+\infty)=(1-a)g(b,+\infty)\ , \tag{10b}$$

where

$$g(b,+\infty)=1-\exp\{-[g_B^i(b,+\infty)+g_B^c(b,+\infty)]\}\ . \tag{11}$$

The coefficient a is positive and does not exceed unity. The quantities $g_B^i(b,+\infty)$ and $g_B^c(b,+\infty)$ have the form

$$g_B^i(b,+\infty)=\int_{-\infty}^{+\infty}\lambda_i(b,t)dt\ , \tag{12a}$$

$$g_B^c(b,+\infty)=\int_{-\infty}^{+\infty}\lambda_c(b,t)dt\ , \tag{12b}$$

and are the populations of states of the continuum of the He atom and the bound states of a bombarding nucleus on the assumption that $g_0(b,t)=1$ on the right-hand sides of Eqs. (9a) and (9b) which corresponds to the Born approximation for ionization and electron capture, i.e., $W_B^i=g_B^i(b,+\infty)$ and $W_B^c=g_B^c(b,+\infty)$. The present calculations employ capture probabilities obtained in the Bassel-Gerjuoy approximation.[8] The Bassel and Gerjuoy approximation is the high-velocity limit of the two-state atoms expansion approximation which has been established to be valid for symmetric systems at moderately high velocities. For a we now have

$$a=\frac{W_B^i}{W_B^i+W_B^c}\ . \tag{13}$$

Introducing the symbols $W_u^i=g^i(b,+\infty)$ and $W_u^c=g^c(b,+\infty)$ we arrive at (7) and (8).

In the calculations of the single and double ionization with the neglect of capture and the one- and two-electron capture with the neglect of ionization the corresponding probabilities will have the form

$$\widetilde{P}^{i1}(b)=2\widetilde{W}_1^i(1-\widetilde{W}_2^i)\ , \tag{14}$$

$$\widetilde{P}^{i2}(b)=\widetilde{W}_1^i\widetilde{W}_2^i\ , \tag{15}$$

$$\widetilde{P}^{c1}(b)=2\widetilde{W}_1^c(1-\widetilde{W}_2^c)\ , \tag{16}$$

$$\widetilde{P}^{c2}(b)=\widetilde{W}_1^c\widetilde{W}_2^c\ . \tag{17}$$

Here $\widetilde{W}^i$ and $\widetilde{W}^c$ are the transition probabilities of an electron to the continuum of a He atom and the bound states of an incident nucleus, respectively, that are separately calculated for each of the two reaction channels under consideration here, namely direct Coulomb ionization (simply called ionization in this paper) and electron capture. The unitarization of the single-electron transition probabilities in the analysis of ionization and also capture with the neglect of the second channel leads to the following expressions for the corresponding unitarized probabilities:[1,12]

$$\widetilde{W}_u^i=1-\exp(-W_B^i)\ , \tag{18}$$

$$\widetilde{W}_i^c=1-\exp(-W_B^c)\ . \tag{19}$$

The tilde above the probabilities for ionization and capture processes means that the corresponding processes are calculated with the neglect of the second channel. For the ionization with capture process the tilde above $\widetilde{P}^{ic}(b)$ will mean that this quantity was calculated using the probabilities $\widetilde{W}^i$ and $\widetilde{W}^c$, i.e.,

$$\widetilde{P}^{ic}(b)=2\widetilde{W}^i_1\widetilde{W}^c_2 . \qquad (20)$$

The Born ionization probabilities W^i_B were calculated by the formulas for ionization probabilities of hydrogen-like systems.[13] In this case the effective charges in the Coulomb matrix elements were determined from the binding energy of the removed electrons. Strictly speaking, the formulas (2)—(6) can be obtained only if the effective charge for each of the two electrons of the He atom is the same. However, the choice of the effective nuclear charge of the He atom from the binding energy corresponds to the best agreement of the cross sections calculated by the formulas (1) and (14) with experiment.[14] In the calculations of the double-ionization probabilities $P^{i2}(b)$ the binding energy was assumed to be the same for each of the helium electrons. And so in the matrix elements of the ionization transition probabilities $Z_1^*=1.345$ and $Z_2^*=2$ for $P^{i1}(b)$.

For capture probabilities we have simply used $Z_1^*=Z_2^*=1.6875$ for $P^{i2}(b)$, $Z_2=2$ for $P^{c1}(b)$, and $Z_1^*=1.6875$ for $P^{ic}(b)$. Here we have used the initial potential U_i in our Bassel-Gerjuoy (BG) calculations. This differs by up to 20% from calculations using U_f for the nonsymmetric systems considered here. The capture probabilities were also calculated using the hydrogenic wave functions. The effective nuclear charge Z^* for the atomic nucleus of He was assumed to be 1.6875 and that for the ion produced via the electron capture by a bombarding nucleus, to the nuclear charge.

As it follows from (7) and (8), when W^i_B and W^c_B are much less than unity, the probabilities W^i_u and W^c_u are actually equal to W^i_B and W^c_B and the cross sections calculated with the unitarized and nonunitarized probabilities should be the same. In this case the ionization should not markedly affect the electron capture cross sections and vice versa. Also, if one of the probabilities W^i_B or W^c_B is much greater than the other, the lower-probability process does not exert strong influence over the cross section of the other process. The ionization and electron-capture probabilities W^i_B and W^c_B strongly decrease as the collision energy increases starting from the value corresponding to the maximum cross sections. As the energy decreases starting from the noted value, the ionization probability also strongly decreases. In this connection the collision energy region, when the ionization effect on the capture probabilities and cross sections is essential, should have upper and lower bounds, and the energy region where the capture influence on the ionization probabilities and cross sections is important should have an upper bound. The lower boundary of the collision energy region, where the ionization and excitation processes substantially affect the capture cross section, has previously been given in Ref. 2. Inasmuch as we consider the capture to the ground state only, the collision energies at which the electron capture substantially affects the ionization probabilities and cross sections can have a lower bound as well.

CALCULATION RESULTS AND DISCUSSION

The results of numerical calculations of the single-electron transition probabilities and the cross sections for all five charge-exchange processes as shown in Figs. 1—7 along with the experimental[14—35] data. In Figs. 1 and 2 the probabilities W^i_B, W^i_u, $\widetilde{W}^i_u$, W^c_B, W^c_u, and $\widetilde{W}^c_u$ plotted against the impact parameter b for two nuclei energies $E=50$ and 110 keV/amu. In Figs. 3—7 we present the single-electron ionization cross sections σ^{i1}_B, $\widetilde{\sigma}^{i1}_B$, σ^{i1}_u, and $\widetilde{\sigma}^{i1}_u$, the cross sections for single-electron capture to the ground state σ^{c1}_B, $\widetilde{\sigma}^{c1}_B$, σ^{c1}_u, and $\widetilde{\sigma}^{c1}_u$, the double-electron ionization cross sections σ^{i2}_B, σ^{i2}_u, and $\widetilde{\sigma}^{i2}_u$, the cross sections for two-electron capture to the ground state σ^{c2}_B, σ^{c2}_u, and $\widetilde{\sigma}^{c2}_u$, and the cross sections for the ionization with capture to the ground state σ^{ic}_B, σ^{ic}_u, and $\widetilde{\sigma}^{ic}_u$, for collisions of He atoms with the H^+, He^{2+}, and Li^{3+} nuclei at energies from 0.025 to 4 MeV/amu. The cross sections σ^{i1}_B, σ^{i2}_B, σ^{c1}_B, σ^{c2}_B, and σ^{ic}_B were calculated by formulas (1)—(6), and $\widetilde{\sigma}^{i1}_B$ and $\widetilde{\sigma}^{c1}_B$ by (1), (14), and (16) with the Born ionization probabilities W^i_B and the Bassel-Gerjuoy capture probabilities W^c_B. The cross sections σ^{i1}_u, σ^{i2}_u, σ^{c1}_u, σ^{c2}_u, and σ^{ic}_u were calculated by formulas (1)—(6) with the single-electron transition probabilities (7) and (8), and the cross sections $\widetilde{\sigma}^{i1}_u$, $\widetilde{\sigma}^{i2}_u$, $\widetilde{\sigma}^{c1}_u$, $\widetilde{\sigma}^{c2}_u$, and $\widetilde{\sigma}^{ic}_u$ by (1), (14)—(17), and (20) with the single-electron transition probabilities (18) and (19).

The experimental cross sections for the single and double ionization $\sigma^{i1}=\sigma^{01}_{ZZ}$ and $\sigma^{i2}=\sigma^{02}_{ZZ}$, the one- and two-electron capture $\sigma^{c1}=\sigma^{01}_{Z,Z-1}$ and $\sigma^{c2}=\sigma^{02}_{Z,Z-2}$, and the ionization with capture $\sigma^{ic}=\sigma^{02}_{Z,Z-1}$ obtained in the experiments with the coincidence-mode detection of the charged fast and slow particles are known for the H^+ and He^{2+} nuclei at the energies $E\leq 50$ keV/amu.[15,16] The superscripts in $\sigma^{0t}_{Z,Z-s}$ denote the charges of He atoms and slow ions before and after collisions; the subscripts denote the similar charges of fast nuclei. At higher energies there are experimental data on the cross sections for free-electron production $\sigma_e=\sigma^{01}_{ZZ}+\sigma^{02}_{Z,Z-1}+2\sigma^{02}_{Z,Z}$, the cross sections for production of singly and doubly charged slow He ions $\sigma^{+1}=\sigma^{01}_{ZZ}+\sigma^{01}_{Z,Z-1}$ and $\sigma^{+2}=\sigma^{02}_{ZZ}+\sigma^{02}_{Z,Z-1}+\sigma^{0}_{Z,Z-2}$, the total cross section of ion production $\sigma^+=\sigma^{+1}+\sigma^{+2}$, and the cross sections for single- and double-electron capture $\sigma_{Z,Z-1}=\sigma^{01}_{Z,Z-1}+\sigma^{02}_{Z,Z-1}$ and $\sigma_{Z,Z-2}=\sigma^{02}_{Z,Z-2}$.[13,16—35] At high energies E the values of the single-ionization cross sections σ^{01}_{ZZ} prove to lie within a narrow band between $\sigma_e-(\sigma^{+2}-\sigma_{Z,Z-2})=\sigma^{01}_{ZZ}+\sigma^{02}_{ZZ}$ and $\sigma_e-2(\sigma^{+2}-\sigma_{Z,Z-2})=\sigma^{01}_{ZZ}-\sigma^{02}_{Z,Z-1}$. The experimental values of $\sigma_e-1.5(\sigma^{+2}-\sigma_{1,-1})\pm0.5(\sigma^{+2}-\sigma_{1,-1})$, σ^{+2}, $\sigma_{Z,Z-1}$, $\sigma_{Z,Z-2}$, and $\sigma^{02}_{Z,Z-1}$ are presented in Figs. 3—7.

If we use the calculated cross section σ^{ic} (see Fig. 7) for correction of the experimental data, we substantially decrease the cross section values for the single and double ionization and the single-electron capture. The maximum decreases are observed for He^{2+} nuclei at energies near 100 keV/amu and can reach 10%, 40%, and 20% of the cross-section values for the single and double ionization and single-electron capture, respectively. In the energy region where the electron capture to excited states is essential, the results of the present calculations omitting excited state capture can strongly differ from experiment.

Single-electron probabilities

The results in Figs. 1 and 2 show that in collisions of He atoms with the He^{2+} and Li^{3+} nuclei at $E=50$ and 110 keV/amu the unitarization leads to a substantial decrease of the ionization probability at the impact parameter ranging from 0 to 7×10^{-9} cm where the probabilities

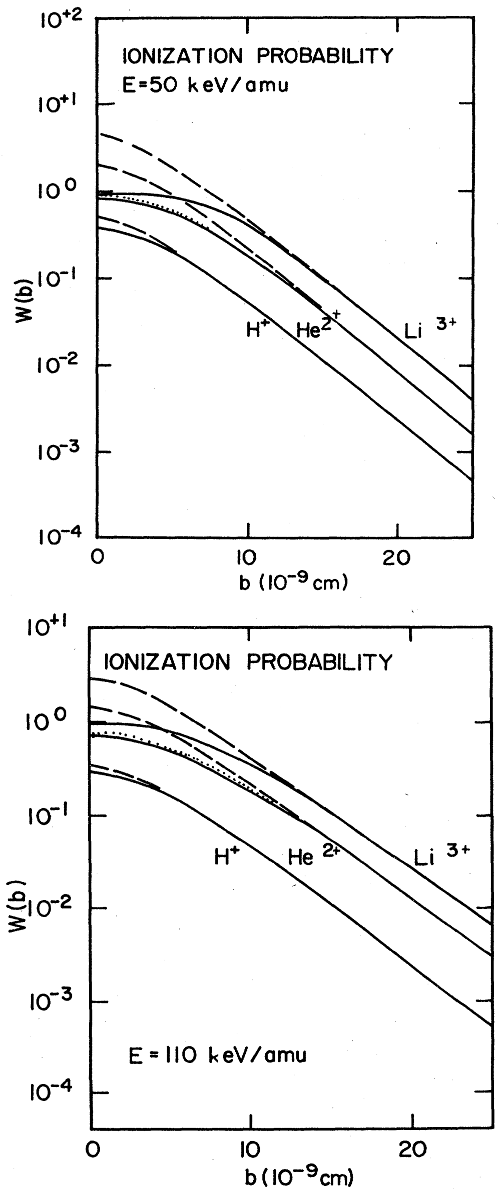

FIG. 1. Single-electron transition probabilities W and $\tilde{W}$ against the impact parameter b. ——, W_u^i and W_u^c; $\cdots$, $\tilde{W}_u^i$ and $\tilde{W}_u^c$; — — —, W_B^i and W_B^c. The effective nuclear charge of the He atom is 1.345 and 1.6875 for ionization and electron capture, respectively.

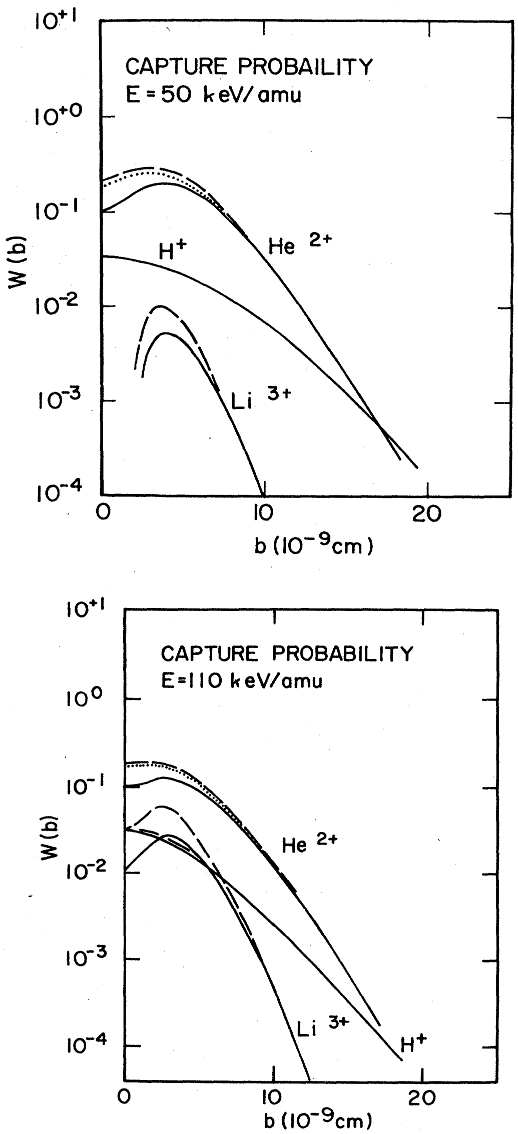

FIG. 2. Same as Fig. 1.

$W_B^i \gtrsim 0.4$ i.e., are still sufficiently high. But in the proton-induced ionization of helium the unitarization produces a weaker effect on W^i because the probabilities W_B^i are a factor of 4 and 9 lower than the corresponding ionization probabilities for He^{2+} and Li^{3+} nuclei.

Taking into account the electron capture to the ground state of a bombarding nucleus in the unitarization of W^i actually has no effect upon the ionization probability $W_u^i \approx \tilde{W}_u^i$ in view of the probabilities W_B^c being much less than W_B^i over the entire region of the impact parameter b. The largest difference between W_u^i and $\tilde{W}_u^i$, of all those shown in Figs. 1 and 2, that is observed in the ionization of He by the He^{2+} nuclei with an energy of 50 keV/amu is not higher than 10% of the probability value. This is due to the fact that electron capture to the ground state is large only in the symmetrical charge-transfer process and so the probabilities W_B^c are in this case closer to W_B^i than in collisions with the protons and Li^{3+} nuclei.

In the case of electron capture the unitarization without ionization reduces the value of W_B^c by less than 20% since the maximum value of W_B^c is not large, being not higher than ~ 0.3 for all cases considered. At the same time, the simultaneous consideration of the two reaction channels leads to a substantial decrease, by a factor of 2 and more, of the probability within the $(0-6)\times 10^{-9}$-cm impact parameters in collisions of He atoms with the He^{2+} and Li^{3+} nuclei for the two nuclei energy values considered. But in collisions of He atoms with the protons the unitarization including both the reaction channels leads to a small reduction in W^c since W_B^c and W_B^i are small as compared with unity.

Single-ionization cross sections

The cross sections for the single-electron ionization of He by the H^+, He^{2+}, and Li^{3+} nuclei as functions of nuclei energy are given in Fig. 3. As seen from Fig. 3, the unitarization leads to a decrease of these cross sections at $E<200$ keV in the proton ionization and $E<500$ keV/amu in the ionization induced by the He^{2+} and Li^{3+} nuclei. So, at $E=25$ keV/amu the Born cross sections σ_B^{i1} are 1.15, 1.3, and 1.4 times as large as the unitarized cross sections σ_u^{i1} in the ionization of He by the protons and He^{2+} and Li^{3+} nuclei, respectively. As follows from the calculations, the electron capture to the ground state of a bombarding nucleus strongly affects the Born ionization cross section σ_B^{i1} only in the ionization of He by the He^{2+} nuclei at $E<500$ keV/amu (Fig. 3). The explanation immediately follows from the consideration of the single-electron transition probabilities. As seen from the results presented in Figs. 1 and 2, in the cases of collisions with protons and Li^{3+} nuclei at all impact parameters we have

$$W_B^i/W_B^c>10 . \tag{21}$$

It follows that

$$P_B^{i1}(b)=2W_{1B}^i(1-W_{2B}^i-W_{2B}^c)$$
$$\approx 2W_{1B}^i(1-W_{2B}^i)=\widetilde{P}_B^{i1}(b) . \tag{22}$$

As a result, in the calculations with the nonunitarized probabilities we have

$$\sigma_B^{i1}\approx\widetilde{\sigma}_B^{i1} \tag{23}$$

for the protons and Li^{3+} nuclei. The calculation results show that the relation (23) is satisfied to within 10%. In collisions of helium with the He^{2+} nuclei the inequality (21), at the impact parameter ranging from 0 to 5×10^{-9} cm, as seen from Figs. 1 and 2, does not hold so strongly ($W_B^i/W_B^c\geq 4.0$) as in collisions of He with the protons and Li^{3+} nuclei. Instead of (22), we shall therefore have in this impact-parameter interval

$$\widetilde{P}_B^{i1}(b)>P_B^{i1}(b) \tag{24}$$

and, hence, in the ionization of He by the He^{2+} nuclei for the noted nuclei energies

$$\widetilde{\sigma}_B^{i1}>\sigma_B^{i1} . \tag{25}$$

Actually, the calculations show that $\widetilde{\sigma}_B^{i1}/\sigma_B^{i1}\approx 1.3$ and 1.2 at energies $E=50$ and 110 keV/amu, respectively.

According to (7), (8), (18), and (19), for the unitarized single-electron transition probabilities W_u for the protons and Li^{3+} nuclei at all impact parameters we have

$$W_u^i\approx\widetilde{W}_u^i \tag{26}$$

and

$$W_u^i/W_u^c>9 . \tag{27}$$

Hence, in the ionization helium by the protons and Li^{3+} nuclei

$$P_u^{i1}(b)\approx\widetilde{P}_u^{i1}(b) \tag{28}$$

and

$$\sigma_u^{i1}\approx\widetilde{\sigma}_u^{i1} , \tag{29}$$

The calculations shown that the relation (29) is valid to within 5—7%. In the ionization of helium by the He^{2+} nuclei at E ranging from 25 to 200 keV/amu W_u^i are not so large as compared with ($W_u^i/W_u^c>3$) in the $0-10^{-8}$-cm impact-parameter region. So, at these impact parame-

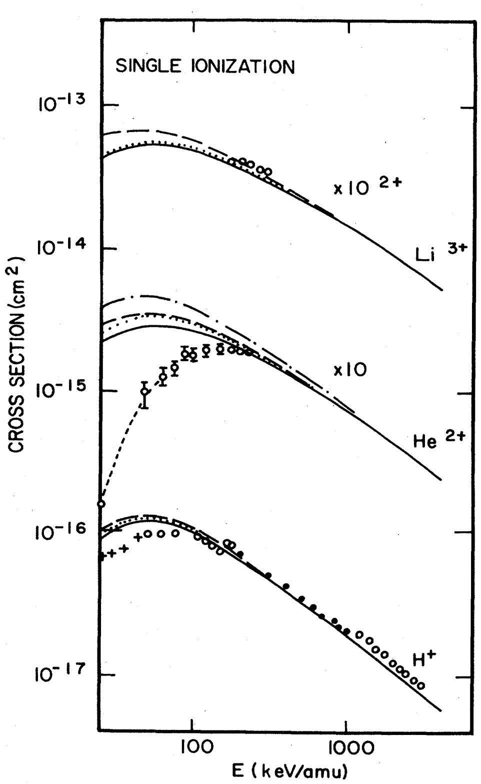

FIG. 3. Cross sections for the single-electron ionization of He by the H^+, He^{2+}, and Li^{3+} nuclei vs nuclei energy. Theoretical curves: ——, σ_u^{i1}; $\cdots$, $\widetilde{\sigma}_u^{i1}$; — — —, σ_B^{i1}; —·—·—·, $\widetilde{\sigma}_B^{i1}$. In the ionization of He atom by the protons and Li^{3+} nuclei the cross sections $\widetilde{\sigma}_B^{i1}$ coincide to within 5% and 10% with σ_B^{i1} and are not given in the figure. Experiment. H^+: + (Ref. 16); ○, at $E<200$ keV (Ref. 17) and at $E>1$ MeV (Ref. 19); ● (Ref. 18). He^{2+}: ϕ (Ref. 35). Li^{3+}: ○ (Ref. 20). Short-dashed curve for He^{2+} is a fit to data.

ters

$$\widetilde{W}^{i}_{u} > W^{i}_{u} \quad (30)$$

and

$$\widetilde{P}^{i1}_{u}(b) \neq P^{i1}_{u}(b) \; . \quad (31)$$

Consequently, in the ionization of helium by the He^{2+} nuclei at an energy of 25 to 200 keV/amu the cross sections σ^{i1}_{u} and $\widetilde{\sigma}^{i1}_{u}$ should differ, as follows from the calculations $\widetilde{\sigma}^{i1}_{u} > \sigma^{i1}_{u}$ (see Fig. 3).

The analysis and the calculations data show that the taking account of the electron capture to the nucleus ground state substantially affects the ionization cross sections σ^{i1} only for collisions of He atoms with the He^{2+} nuclei.

From the comparison of the calculation results with experiment is follows that in the proton ionization of helium at $E > 10$ keV and in the He ionization by the He^{2+} and Li^{3+} nuclei at $E > 200$ keV/amu the calculated cross sections agree to within 15% with experimental data. However, at lower energies shown, there are substantial differences between all of our calculations and observed data. It is at these lower energies[36] where our results based on perturbation theory are expected to breakdown.

Single capture cross sections

In Fig. 4, the cross sections for the one-electron capture to the ground state of a bombarding nucleus in collisions of helium with the H^{+}, He^{2+}, and Li^{3+} nuclei are plotted against the nuclei energy. As follows from the calculations, the unitarization reduces the electron-capture cross sections by a factor of 1.1—1.15 for the He^{2+} nuclei at $E \leq 250$ keV/amu, and by a factor of 1.25—1.5 for Li^{3+} nuclei at $E \leq 500$ keV/amu. The unitarization without taking account of the ionization reduces the cross sections not more than 10%. Taking account of ionization markedly affects the cross section for the electron capture to the ground state σ^{c1}_{B} only in collisions of helium with the Li^{3+} nuclei at $E < 500$ keV/amu. The maximum reduction in the electron-capture cross sections due to the ionization effect at the above noted Li^{3+} nuclei energies is a factor of 1.5. In these cases in the region of the impact parameter b providing the main contribution to the cross section we have $W^{i}_{B} \gg W^{c}_{B}$ and the probabilities W^{i}_{B} are still sufficiently high. For example, at $E = 50$ and 110 keV/amu in collisions of helium with the Li^{3+} nuclei probabilities $W^{i}_{B} > 0.4$ in the $0-10^{-8}$-cm impact-parameter range (see Figs. 1 and 2). In collisions of helium with the protons, in spite of $W^{i}_{B} \gg W^{c}_{B}$, the ionization weakly affects the electron-capture cross section σ^{c1} owing to low probabilities W^{i}_{B} as compared with unity.

From (8) and (19) it follows that the unitarized single-electron transition probabilities are

$$\widetilde{W}^{c}_{u} > W^{c}_{u} \; . \quad (32)$$

The inequality is strictly satisfied at low impact parameters b. As the nuclei energy increases, the impact-parameter region where $\widetilde{W}^{c}_{u}$ is much greater than W^{c}_{u} becomes narrower at energies $E > 80$ keV/amu and $E > 150$ keV/amu in the electron capture by He^{2+} and Li^{3+} nuclei, respectively. Using relations (3), (16), (27), and (32) we obtain

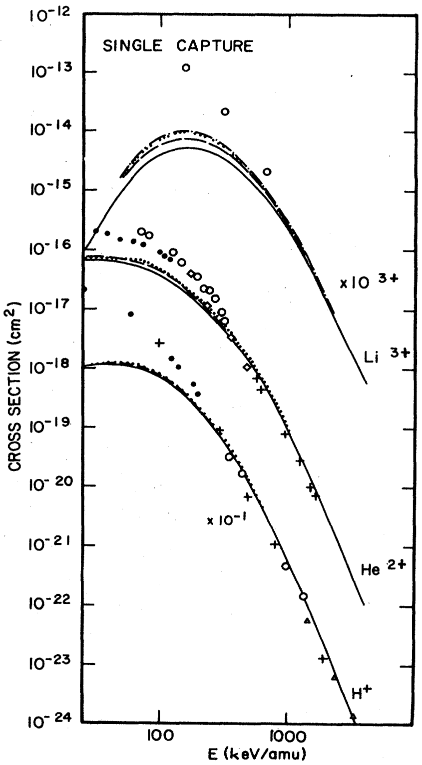

FIG. 4. Cross sections for the single-electron capture to the ground state in the charge transfer of the H^{+}, He^{2+}, and Li^{3+} nuclei in helium vs nuclei energy. Theoretical curves: ——, σ^{c1}_{u}; $\cdots$, $\widetilde{\sigma}^{c1}_{u}$; — — —, σ^{c1}_{B}; —·—·—·, $\widetilde{\sigma}^{c1}_{B}$. The cross sections $\widetilde{\sigma}^{c1}_{B}$ for the electron capture by protons coincide to within 5% with σ^{c1}_{B} and for the electron capture by the He^{2+} nuclei at $E \leq 50$ keV/amu with σ^{c1}_{B} and at $E > 50$ keV/amu with $\widetilde{\sigma}^{c1}_{u}$ and are not given in figure. Experiment. H^{+}: + (Ref. 22); ●, at $E < 50$ keV (Ref. 16) and at $E > 100$ keV (Ref. 21); ○ (Ref. 23); △ (Ref. 24). He^{2+}: ○ (Ref. 26); ◇ (Ref. 27); + (Ref. 28); ● (Ref. 25). Li^{3+}: ○ (Ref. 29).

$$\widetilde{P}^{c1}_{u}(b) \neq P^{c1}_{u}(b) \; . \quad (33)$$

From (33) it follows that

$$\widetilde{\sigma}^{c1}_{u} \neq \sigma^{c1}_{u} \; . \quad (34)$$

The calculations show that in the electron capture by the He^{2+} nuclei at $E < 250$ keV/amu the cross sections $\widetilde{\sigma}^{c1}_{u}$ are no less than 10% higher than σ^{c1}_{u}, the maximum difference between $\widetilde{\sigma}^{c1}_{u}$ and σ^{c1}_{u} being observed at $E \approx 80$ keV/amu. In the electron capture by the Li^{3+} nuclei more than 10% excess of $\widetilde{\sigma}^{c1}_{u}$ over σ^{c1}_{u} is observed within $50 < E < 1000$ keV/amu. In collisions of helium with the protons, in view of W^{i}_{B} being small as compared with unity and

$$\widetilde{W}^{c}_{u} \approx W^{c}_{u} \quad (35)$$

we obtain

$$\widetilde{P}_u^{c1}(b) \approx P_u^{c1}(b) \tag{36}$$

and

$$\widetilde{\sigma}_u^{c1} \approx \sigma_u^{c1} , \tag{37}$$

i.e., the cross sections calculated with the probabilities $\widetilde{W}_u$ and W_u must be close. The calculations have shown that the relation (36) is satisfied to within 10%. In the case of the charge transfer of protons and He^{2+} nuclei in He atoms the discrepancy between the calculated and experimental cross sections at $E > 300$ keV/amu is not more than 25—40 %, as a rule. Higher experimental cross sections at $E < 700$ keV/amu in the electron capture by the Li^{3+} nuclei are likely to be due to the capture of electron to excited states which is neglected in the present calculations.

The analysis of the single-electron ionization cross sections has revealed that the electron capture to the ground state need be taken into account only in the unitarization of the He^{2+}-induced ionization probabilities. Comparison between the calculated σ^{c1} and experiment shows that in all cases in question at $E \leq 100$ keV/amu the experimental values are several times larger than the calculated values. This suggests that the electron capture might also be important in the unitarization of the H^+- and Li^{3+}-induced ionization probabilities. Thus, taking into account the electron capture to excited states should provide better agreement of the calculated single-ionization cross section with experiment.

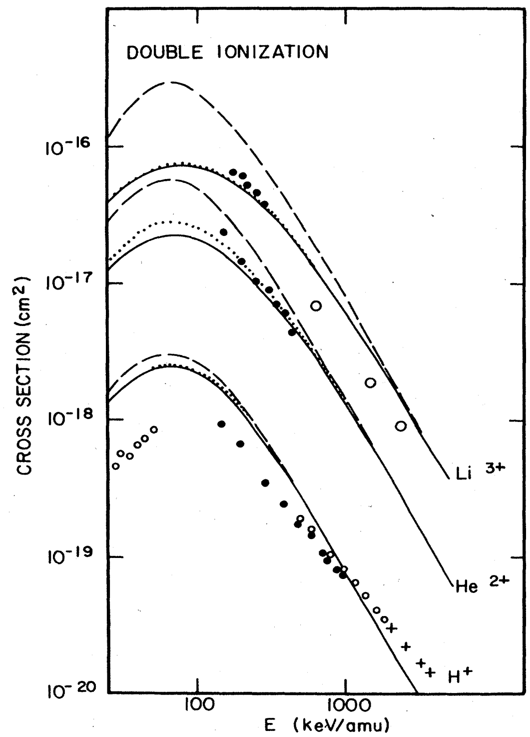

FIG. 5. Cross sections for the two-electron ionization of He atoms by the H^+, He^{2+}, and Li^{3+} nuclei vs nuclei energy. Theoretical curves: ——, σ_u^{i2}; $\cdots$, $\widetilde{\sigma}_u^{i2}$; — — —, σ_B^{i2}. Experiment. H^+: ○ (Ref. 16); ● (Ref. 18); ○ (Ref. 30); + (Ref. 31). He^{2+}: ● (Ref. 30). Li^{3+}: ● (Ref. 30); ○ (Ref. 32).

Double-ionization and capture cross sections

Figures 5—7 present the calculated cross sections for two-electron transitions in collisions of helium with H^+, He^{2+}, and Li^{3+}. As seen from the figures the unitarization leads to a substantial decrease of the double-ionization cross sections for the He^{2+} and Li^{3+} nuclei at $E < 1000$ and 2000 keV/amu, respectively. For example, at $E \approx 60$ keV/amu the unitarization decreases the cross sections for He^{2+} and Li^{3+} by a factor of 2.5 and 4, respectively. With protons the unitarization is not so effective, the peak of cross sections is decreased no more than 20% of the cross section's value. A more than 15% decreasing of the cross sections, due to the unitarization, for two-electron capture to the ground state is observed for He^{2+} and Li^{3+} nuclei at $E < 600$ and 1700 keV/amu, respectively, and that for ionization with electron capture is observed at energies 1.5 times higher.

This influence of unitarization upon the cross sections for two-electron transitions induced by the He^{2+} and Li^{3+} nuclei can be accounted for by the ionization probabilities W_B^i being sufficiently high at nuclei energies of He^{2+} and Li^{3+} $E < 500$ and 2000 keV/amu, respectively, in the impact-parameter region providing the main contribution to the cross section. As a result, the probabilities W_u^i and W_u^c determined by the formulas (7) and (8) strongly differ from W_B^i and W_B^c in the above-noted impact-parameter region (Figs. 1 and 2) and, so, $P_u^{i2}(b)$, $P_u^{c2}(b)$, and $P_u^{ic}(b)$ differ from $P_B^{i2}(b)$, $P_B^{c2}(b)$, and $P_B^{ic}(b)$.

Since the probabilities $P^{i2}(b)$, $P^{c2}(b)$, and $P^{ic}(b)$ are proportional to the product of the single-electron transition probabilities W^i and W^c, and $P^{i1}(b)$ and $P^{c1}(b)$ to W^i and W^c, the unitarization should exert a stronger influence upon the two-electron transition cross sections than on the single-electron ones.

Consideration of the two charge-exchange channels—ionization and electron capture to the ground state—in the case of collisions of helium with the H^+, He^{2+}, and Li^{3+} nuclei markedly affects the double-ionization cross sections only in collisions of helium with He^{2+} and the two-electron capture cross sections and the ionization with electron-capture cross sections in collisions of helium with the He^{2+} and Li^{3+} nuclei. So at $E \approx 60$ keV/amu the ratios $\widetilde{\sigma}_u^{i2}/\sigma_u^{i2}$, $\widetilde{\sigma}_u^{c2}/\sigma_u^{c2}$, and $\widetilde{\sigma}_u^{ic}/\sigma_u^{ic}$ for the He^{2+} nuclei are 1.25, 1.60, and 1.32, respectively. From the results obtained in the discussion of the single-electron transition probabilities, it follows that at the impact parameters b providing the main contribution to the cross section, the probabilities $\widetilde{P}_u^{i2}(b)$ and $P_u^{i2}(b)$ should markedly differ only in collisions of helium with the He^{2+} nuclei, and the probabilities $\widetilde{P}_u^{c2}(b)$ and $P_u^{c2}(b)$ and $\widetilde{P}_u^{ic}(b)$ and $P_u^{ic}(b)$ in collisions of helium with He^{2+} and Li^{3+}.

The comparison of the calculated double-ionization cross sections with experiment shows that at $E < 100$ keV/amu the calculated values are much higher. At $E > 150$ keV/amu the relation between the calculations and experiment is much better. At these energies the

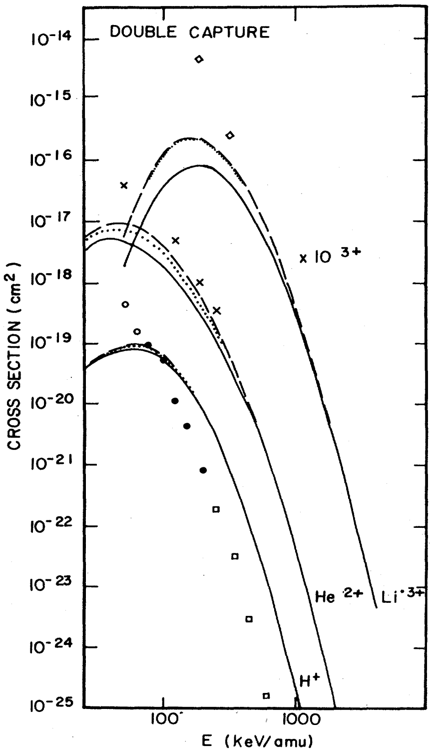

FIG. 6. Cross sections for the two-electron capture to the ground state in the charge transfer of the H^+, He^{2+}, and Li^{3+} nuclei in helium vs nuclei energy. Theoretical curves: ——, σ_u^{c2}; · · · , $\tilde{\sigma}_u^{c2}$; — — —, σ_B^{c2}. Experiment. H^+: ○ (Ref. 33); ● (Ref. 22); □ (Ref. 24). He^{2+}: × (Ref. 8). Li^{3+}: ◊ (Ref. 34).

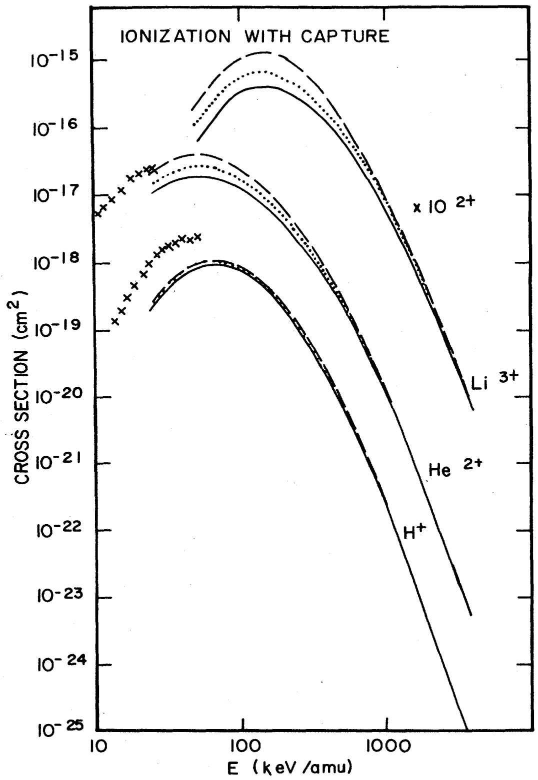

FIG. 7. Cross sections for the ionization of helium with the simultaneous electron capture to the ground state of nuclei in collisions of He atoms with the H^+, He^{2+}, and Li^{3+} nuclei vs nuclei energy. Theoretical curves; ——, σ_u^{ic}; · · · , $\tilde{\sigma}_u^{ic}$; — — —, σ_u^{ic}. Experiment. H^+: + (Ref. 16). He^{2+}: (Ref. 15).

cross sections calculated with the unitarized single-electron transition probabilities are in a little closer agreement with experiment than the ones calculated with the Born probabilities. The deviation of the calculated σ^{i2} from experiment at $E > 500$—600 keV/amu is, seemingly, due to the neglect of the correlation effects (cf. Refs. 1 and 37).

At present the experimental data on the two-electron capture in collisions of He atoms with the He^{2+} and Li^{3+} are available only for $E \leq 300$ keV/amu (see Fig. 6). As already noted, the electron capture is excited states is essential in this energy region and therefore the present calculations of the two-electron capture cross sections cannot be expected to agree quantitatively with the available experimental data. For collisions of helium with the protons at proton energies $E > 100$ keV there is only qualitative agreement between the calculations and experiment. The calculated values are much higher than the experimental ones which may be due to an inadequate choice of the electron wave functions for the negative hydrogen ion.

Simultaneous ionization and capture cross sections

Figure 7 illustrates the calculations of the cross sections for ionization of He atoms with the simultaneous capture of the second electron to the ground state of a bombarding nucleus. Also given here are the available experimental data in collisions of helium with the H^+ and He^{2+} nuclei at nuclei energies $E \leq 50$ keV/amu.[15,16] The comparison shows good qualitative agreement of the calculated results and experiment and also quantitative agreement in collisions of helium with the He^{2+} nuclei. However, the quantitative agreement in this case can be explained only by mutual cancellation of the errors arising in the present study of ionization and electron capture.

CONCLUSION

In the present work the cross sections for single and double ionization, single- and two-electron capture to the ground state, and the cross sections for ionization with the simultaneous capture of the other electron to the ground state in collisions of helium with the H^+, He^{2+}, and Li^{3+} nuclei are calculated in the independent-electron approximation.

The results show that the unitarization decreases the values of σ^{i1} and σ^{i2} for varying nuclei, the difference between the unitarized and Born cross sections being larger the greater the nuclear charge. In collisions of helium atoms with the protons, the cross sections of all five processes calculated with the unitarized probabilities W^{u^i} and

W_u^c agree, to within 15—20%, with the corresponding cross sections calculated with nonunitarized probabilities W_B^i and W_B^c over the entire energy region involved. In collisions of helium with the He^{2+} and Li^{3+} nuclei not more than the 15% discrepancy between the cross sections calculated with unitarized and nonunitarized probabilities is observed only at $E > 900$ and 2500 keV/amu for He^{2+} and Li^{3+} nuclei, respectively.

In the energy ranges within 30—250 keV/amu and 25—150 keV/amu for He^{2+} and Li^{3+} nuclei, respectively, including ionization and electron capture leads to a substantial decreasing of all processes examined. The single- and two-electron transition cross sections decrease, at most, by a factor of 1.3—2 and 2.5—4, respectively, at energies corresponding to the maximum cross-sectional value.

At higher energies the calculated cross sections agree with experiment within 15% for single-electron ionization of helium by the H^+, He^2, and Li^{3+} nuclei for $E > 200$ keV/amu, and within 40% for single-electron capture from helium to H^+ and He^{2+} nuclei for $E > 300$ keV/amu. At these higher energies double-ionization and capture calculations are about twice as far from observation as single ionization and capture, as expected from the independent-electron approximation. At lower energies, while unitarization helps, agreement between our first-order calculations and observed data is not as good, with the exception of simultaneous ionization and capture where the agreement is surprisingly good.

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