Angular and energy dependences of the profiles of autoionization resonances in the cross sections of ionization of the helium atom by fast protons

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An investigation is made of the angular and energy dependences of the profiles of autoionization resonances in the spectra of electrons formed as a result of the ionization of helium atoms by fast protons. A self-consistent quantitative and qualitative explanation is provided of all the available experimental results. The total amplitude of the ionization of an atom in the region of autoionization resonances is obtained in the diagonalization approximation allowing for the three-particle Coulomb dynamics in the final state. The number of resonances is not restricted. A study is made of the influence of the interaction in the final state on the nature of the interference of autoionization resonances with a continuous spectrum. An analysis is made of the possibility of parametrization of the electron ejection spectra under conditions of a strong interaction between charged particles. The results of the calculations, made allowing for the interaction in the final state influencing the amplitudes of the direct and resonant ionization, are used to interpret the available experimental data on the interference effects observed in the electron spectra in the region of autoionization resonances below the $n = 2$ threshold of the He^+ ion when the helium atom is ionized by 100–500 keV protons.

1. INTRODUCTION

In the early seventies experimental investigations of doubly differential cross sections for the ionization of helium atoms by fast protons revealed complex angular and energy dependences of the intensity and asymmetry of autoionization resonances.[1,2] There were striking changes in the profile of the autoionization spectrum, which was of quasiperiodic nature, at low angles of ejection and at a velocity of the ejected electrons which was close—in respect of the magnitude and direction—of the velocity of the scattered protons.[3,4] These theoretical treatments failed to give a complete explanation of the observed effects.[5,8,10]

Considerable attention to fast changes in the resonance profiles, considered as a function of the energy and angle of observation, was given in theoretical treatments reported in Refs. 5–8. At high electron ejection angles the first Born approximation and allowance for the interference of the amplitudes of direct ionization transitions and transitions to the continuous spectrum via autoionizing levels ensured a fully satisfactory reconstruction of the intensities and profiles of the resonances. However, it was found,[5,6] that the adopted approximation cannot account for the nature of the observed changes in the autoionization spectra observed at low electron ejection angles. The use of equations from three-particle-scattering theory and allowance for the influence of the scattered proton on the states of an electron in the continuum when the electron travels at a velocity close to that of the proton has made it possible to determine the nature of the effect of the scattered particle on the profile of the autoionization spectrum and to describe qualitatively the observed behavior at low ejection angles. It has been shown that allowance for the interaction of an electron with a scattered particle in the expression for the amplitude of the direct ionization alters considerably the profile of autoionization resonances.[7,8] Quantum-mechanical calculations[9,10] of the parameters of autoionization resonances in the electron injection spectra obtained for the case of ionization collisions of fast protons with helium atoms, allowing for the influence of the interaction in the final state on the amplitude of direct ionization transitions, account for the quasiperiodic changes in the resonance profiles, but a quantitative agreement between the calculations and experimental data has not been achieved.[1–4] Moreover, there are still some qualitative differences between the calculated and observed dependences of the resonance profiles on the kinematics of collisions.

Later[11,12] it has been shown that a more comprehensive allowance for the interaction of an ejected electron with a scattered ion can alter qualitatively the nature of the quasiperiodic dependence. Fundamental differences were observed between the behavior of the paths of zeros of the asymmetry parameter, corresponding to symmetric resonances and separating asymmetry zones of different signs, considered as a function of the proton energy and the electron ejection angle. If we allow for the interaction of an electron with a scattered proton only in the amplitude of direct ionization and we reduce the relative momentum, we find that the paths of zeros are concentrated at a point corresponding to the equality of the electron and proton velocities, whereas if we allow for the interaction between the amplitudes of the direct and resonant ionization, the paths become branched at this point because the relative phase between these amplitudes remains finite. The positions of the paths depend on the electron energy.

New experimental investigations of autoionization resonances in the cross sections representing the ionization of helium atoms by heavy charged particles have demonstrated[13,14] that, in the case of a strong influence of the field of the scattered particle on the motion of an electron represented by the continuous spectrum, the profiles of autoionization resonances differ from the Fano curve. The profiles of the observed resonances can then be described if we allow not only for the influence of the scattered particle on the electrons ejected as a result of decay of autoionization reson-

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ances, but also for the interference of these resonances with the background of direct transitions.[13,15] A characteristic splitting of a resonance profile appears also as a result of additional scattering of an autoionization electron in the final state by a scattered heavy charged particle.[16]

Our aim will be to provide a theoretical description of the complex angular and energy dependences of the profiles of autoionization resonances exhibited by the cross sections for the ionization of helium atoms by fast protons subject to allowance for the three-particle Coulomb dynamics in the final state, which affects not only the amplitude of the direct transitions but also the amplitude of the resonance transitions which interfere with one another. In the diagonalization approximation, using the results of a three-particle scattering theory, we shall obtain the amplitude of the ionization of an atom on the assumption that the distance between this atom and the scattered particle at the moment of decay of an autoionizing state is large. We shall assume an arbitrary number of resonances interfering with one another and that each of them interacts with a specific partial wave against the background of the rest of the continuum. We shall ignore the influence of a proton on the wave functions, energies, and widths of autoionizing states. These assumptions will be used to study the influence of the interaction of an electron and a scattered proton on the intensity and profile of resonance lines as a function of the kinematic experimental conditions such as the proton energy and the electron ejection angle. We shall consider the influence of the interaction in the final state on the nature of the interference of autoionization resonances with the continuous spectrum. We shall analyze the possibility of parametrization of the electron ejection spectra under conditions of a strong interaction with charged particles. We shall compare the results obtained with the experimental data. A preliminary account of theoretical results obtained below was given at the Tenth All-Union Conference on the Physics of Electron and Atomic Collisions.[17]

2. PRINCIPAL EQUATIONS

The total amplitude of the ionization of an atom by a fast particle in the region of autoionization resonances can be found by dividing the space of possible states of our system into a sum of orthogonal Q and P subspaces and by consigning to the Q subspace the states with two-electron excitation of the target atom which are close on the energy scale to the observed autoionization resonances. The subspace P is then complementary to Q. We shall introduce the operators of the projection of Q and P on the appropriate subspaces, so that the total amplitude of the ionization of an atom is described by

$$t_{fi}^{(-)} = t_{dir}^{(-)} + t_{res}^{(-)}, \tag{1}$$

where

$$t_{dir}^{(-)} = \langle \Psi_f^{(-)} | \hat{V}_i | \Psi_i \rangle \tag{2}$$

is the amplitude of the direct transitions of an electron to a continuous spectrum,

$$t_{res}^{(-)} = \langle \Psi_f^{(-)} | P\hat{H}QG_a^{(+)} \left(1 + \frac{Q\hat{H}P}{E^{(+)} - P\hat{H}P}\right) \hat{V}_i | \Psi_i \rangle \tag{3}$$

is the amplitude of electron transitions to a continuous spectrum via autoionizing levels. Here, Ψ_i is the wave function of the initial state of the colliding particles; $\hat{V}_i$ is the operator representing the interaction of the incident particle with an atom; $\hat{H}$ is the total Hamiltonian; E is the total energy of the system.

The wave function $\Psi_f^{(-)}$ of the final state of three charged asymptotically free particles is found from the equation

$$(E - P\hat{H}P)\Psi_f^{(-)} = 0, \tag{4}$$

the approximate solution of which can be represented—as demonstrated by the results of the three-particle scattering theory—in the following form[18]:

$$\Psi_f^{(-)} = \frac{1}{(2\pi)^{3/2}} \hat{A}[\varphi_f \exp(i\mathbf{k}_f\mathbf{R}) \psi_{\mathbf{k}_{23}}^{(-)}(\mathbf{r}_{23}) \Phi_{\mathbf{k}_{12}}^{(-)} \times (\nu_{12}, \mathbf{r}_{12}) \Phi_{\mathbf{k}_{13}}^{(-)}(\nu_{13}, \mathbf{r}_{13})], \tag{5}$$

where the indices 1, 2, and 3 denote the scattered ion, the ejected electron, and the ion formed as the residue of the target atom, respectively; φ_f is the wave function of the residual ion; $\hat{A}$ is the antisymmetrization operator acting on the electron coordinates; $\mathbf{R}$ is the position of the scattered ion relative to the target atom; $\psi_{k_{23}}^{(-)}(\mathbf{r}_{23})$ is the two-particle Coulomb wave function representing the scattering of the subsystem formed by the ejected electron and the residual ion (formed from the target atom) in the final state:

$$\Phi_{\mathbf{k}_{ij}}^{(-)}(\nu_{ij}, \mathbf{r}_{ij}) = f_c^{(-)}(\nu_{ij})\, {}_1F_1[i\nu_{ij}, 1, -i(k_{ij}r_{ij} + \mathbf{k}_{ij}\mathbf{r}_{ij})],$$
$$f_c^{(-)}(\nu_{ij}) = \exp(-\pi\nu_{ij}/2)\Gamma(1 - i\nu_{ij}), \quad \nu_{ij} = Z_iZ_jm_{ij}/k_{ij}, \tag{6}$$

where $\mathbf{k}_{ij}$ is the momentum of the relative motion of the particles i and j in the final state; Z_i is the charge of the ith particle; m_{ij} is the reduced mass of the particles i and j.

The Green function of the relative motion of the scattered ion of the atom in an autoionizing state can be described by

$$G_a^{(+)} = \left(E^{(+)} - Q\hat{H}Q - Q\hat{H}P \frac{1}{E^{(+)} - P\hat{H}P} Q\hat{H}P\right)^{-1} \tag{7}$$

In the diagonalization approximation[19] the Green function $G_a^{(+)}$ is diagonal in the basis of the functions in the Q subspace. Let us assume that l_a is the effective size of the region of localization of electrons in autoionizing states; then, apart from terms of the order of l_a/R, we have

$$G_a^{(+)} = \sum_{\mu} \int \frac{d\mathbf{k}_a}{(2\pi)^3} \frac{|\Phi_\mu \chi_{\mathbf{k}_a}^{(+)}\rangle \langle \Phi_\mu \chi_{\mathbf{k}_a}^{(+)}|}{E^{(+)} - \varepsilon_\mu - k_a^2/2\mu_a - \langle \Phi_\mu | V \frac{1}{E^{(+)} - k_a^2/2\mu_a - P\hat{H}_aP} V | \Phi_\mu \rangle}, \tag{8}$$

where $\hat{V}$ is the electron–electron interaction operator and μ_a is the reduced mass of the incident particle and of the atom. The wave function Φ_μ and the energy ε_μ are, respectively, the eigenfunction and the eigenenergy of the Hamiltonian $\hat{H}_a$ of the target atom. The function $\chi^{(+)}_{\mathbf{k}_a}(\mathbf{R})$ satisfies the equation

$$\left(K - W_{\mu\mu} - \frac{k_a^2}{2\mu_a}\right)\chi^{(+)}_{\mathbf{k}_a}(\mathbf{R}) = 0, \tag{9}$$

where $W_{\mu\mu} = \langle \Phi_\mu | W | \Phi_\mu \rangle$ is the effective potential representing the interaction of the scattered ion with the atom in an autoionizing state and $\hat{K}$ is the operator of the kinetic energy of the relative motion of the incident particle and the target atom. The spectral representation (8) is approximated satisfactorily by the Green function (7) if $R \gg l_a$. Since the decay of an autoionizing state occurs at distances $R \sim v_i/\Gamma_\mu \gg 1$ (v_i is the velocity of the incident particle and Γ_μ is the width of the μth autoionization resonance), it follows that the representation (8) is completely appropriate for the task in hand.

Substituting the spectral representation (8) in Eq. (3), we obtain the resonance ionization amplitude

$$t^{(-)}_{res} = \sum_\mu \int \frac{d\mathbf{k}_a}{(2\pi)^3} \times \frac{\tau_{dec}(\mu, \mathbf{k}_a \to \mathbf{k}_f)\,\tau_{ex}(i \to \mu, \mathbf{k}_a)}{E^{(+)} - \varepsilon_\mu - k_a^2/2\mu_a - \langle \Phi_\mu | V \dfrac{1}{E^{(+)} - k_a^2/2\mu_a - P\hat{H}_a P} V | \Phi_\mu \rangle}, \tag{10}$$

where

$$\tau_{ex}(i \to \mu, \mathbf{k}_a) = \left\langle \Phi_\mu \chi^{(+)}_{\mathbf{k}_a} \middle| \left(1 + (V+W)\frac{1}{E^{(+)} - P\hat{H}P}\right) V_i \middle| \Psi_i \right\rangle \tag{11}$$

is the amplitude of the excitation of the μth autoionizing state deduced allowing for the coupling with the continuous spectrum,

$$\tau_{dec}(\mu, \mathbf{k}_a \to k_f) = \langle \Psi^{(-)}_f | V + \tilde{W} | \Phi_\mu \chi^{(+)}_{\mathbf{k}_a} \rangle \tag{12}$$

is the amplitude of the decay of the μth autoionizing state, and $\tilde{W}$ is the interaction between colliding particles after subtraction of the effective potential $W_{\mu\mu}$.

Bearing in mind that the decay of autoionizing states occurs at distances $R \gg l_a$ apart, we can (to within terms of the order of l_a/R in the operator of the transition represented by the matrix element τ_{dec}) ignore the interaction of the atom with the scattered particle compared with the electron–electron interaction. Let us assume that $\mathbf{k}_f$ is the momentum of relative motion of the scattered ion and the subsystem formed by the ejected electron and the residual ion in the final state; then $\tau_{\text{dec}} \sim \delta(\mathbf{k}_f - \mathbf{k}_a)$ and the smoothly varying amplitude τ_{ex} can be taken outside the integral at the point $\mathbf{k}_a = \mathbf{k}_f$, whereas the matrix element in the denominator of Eq. (10) can be assumed to be equal to

$$\left\langle \Phi_\mu | \hat{V} \frac{1}{E^{(+)} - k_a^2/2\mu_a - P\hat{H}_a P} \hat{V} | \Phi_\mu \right\rangle \approx \Delta_\mu - \frac{i}{2}\Gamma_\mu, \tag{13}$$

where Δ_μ is the shift of the μth autoionizing level. If we allow for the approximations already made, we find that the amplitude (10) becomes

$$t^{(-)}_{res} = \sum_\mu \tau_{ex}(i \to \mu, \mathbf{k}_f) \int \frac{d\mathbf{k}_a}{(2\pi)^3} \frac{\tau_{dec}(\mu, \mathbf{k}_a \to \mathbf{k}_f)}{E^{(+)} - E_\mu - k_a^2/2\mu_a + i\Gamma_\mu/2}, \tag{14}$$

where $E_\mu = \varepsilon_\mu + \Delta_\mu$.

If in accordance with the approximation $R \gg l_a$ we substitute $r_{12} \approx R$ and $r_{13} \approx R$ in the wave function of the final state, we find that the resonance ionization amplitude of Eq. (14) becomes

$$t^{(-)}_{res} = \sum_\mu \tau_{ex}(i \to \mu, \mathbf{k}_f)\,\tau^0_{dec}\Lambda_{res,\mu}(\nu_{12}, \nu_{13}), \tag{15}$$

where

$$\tau^0_{dec} = \langle \hat{A}[\varphi_f \psi^{(-)}_{\mathbf{k}_{23}}] | V | \Phi_\mu \rangle \tag{16}$$

is the amplitude of decay of an autoionizing level of an isolated atom, and

$$\Lambda_{res,\mu} = \int \frac{d\mathbf{k}_a}{(2\pi)^3} \frac{\langle \exp(i\mathbf{k}_f \mathbf{R}) \Phi^{(-)}_{\mathbf{k}_{12}}(\nu_{12}, \mathbf{R})\, \Phi^{(-)}_{\mathbf{k}_{13}}(\nu_{13}, \mathbf{R}) | \chi^{(+)}_{\mathbf{k}_a}(\mathbf{R}) \rangle}{E^{(+)} - E_\mu - k_a^2/2\mu_a + i\Gamma_\mu/2}. \tag{17}$$

In an analysis of the ionization of an atom by a fast particle we can assume with good accuracy that $\chi^{(+)}_{\mathbf{k}_a}(\mathbf{R}) = \exp(i\mathbf{k}_a \mathbf{R})$. In this case we find that integration with respect to $\mathbf{k}_a$ in Eq. (17) gives

$$\Lambda_{res,\mu} = \frac{K_{res,\mu}(\nu_{12}, \nu_{13})}{E_e - E_\mu + i\Gamma_\mu/2}, \tag{18}$$

where E_e is the energy of an electron relative to the residue ion of the target atom, and

$$K_{res,\mu}(\nu_{12}\nu_{13}) = -\frac{2\mu_a}{4\pi} \int \frac{d\mathbf{R}}{R} \exp(-i\mathbf{k}_f \mathbf{R} + iK_r R)\, \Phi^{(-)*}_{\mathbf{k}_{12}} \times (\nu_{12}, \mathbf{R})\, \Phi^{(-)*}_{\mathbf{k}_{13}}(\nu_{13}, \mathbf{R}). \tag{19}$$

Here,

$$K_r = [k_f^2 + 2\mu_a(E_e - E_\mu + i\Gamma_\mu/2)]^{1/2}, \quad \operatorname{Im} K_r > 0.$$

Calculating the integral in Eq. (19) by the contour method, we obtain

$$K_{res,\mu}(\nu_{12}\nu_{13}) = f^{(+)}_c(\nu_{12}) f^{(+)}_c(\nu_{13}) \times (1+a_{12})^{i\nu_{12}} (1+a_{13})^{i\nu_{13}} {}_2F_1(-i\nu_{12}, -i\nu_{13}, 1, Z),$$

$$a_{ij} = \frac{\mathbf{v}_f \mathbf{k}_{ij} + K_r k_{ij}/\mu_a}{E_e - E_r + i\Gamma_\mu/2}, \tag{20}$$

$$Z = \frac{a_{12}a_{13} + (\mathbf{k}_{12}\mathbf{k}_{13} - k_{12}k_{13})\,\mu_a/(E_e - E_r + i\Gamma_\mu/2)}{(1+a_{12})(1+a_{13})}.$$

The kinematic factor $K_{\text{res},\mu}$ allows for the interaction between an autoionizing electron and a scattered proton, and also between heavy charged particles. Its value varies for different autoionizing states and depends on the electron energy and the resonance width. As the momentum of the rela-

tive motion of an electron and a scattered particle decreases, the influence of $K_{res,\mu}$ on the decay of autoionizing states increases and this is manifested most strongly at low ejection angles. If $\nu_{12},\nu_{13}\to 0$, we find that $K_{res,\mu}\to 1$. If $\mu_a \gg 1$ and $v_f^2 \gg \Gamma_\mu$, then

$$K_r/\mu_a \approx v_f + (E_e - E_r + i\Gamma_\mu/2)/k_f, \quad \mathbf{v}_f = \mathbf{k}_f/\mu_a.$$

This results in redefinition of the quantity a_{ij} in Eq. (20) so that it becomes

$$\tilde{a}_{ij} = (\mathbf{v}_f \mathbf{k}_{ij} + v_f k_{ij})/(E_e - E_r + i\Gamma_\mu/2) + k_{ij}/k_f.$$

The expressions for $K_{res,\mu}$ obtained in this way are more general than the result obtained in the eikonal approximation,[15,20] which becomes invalid at low electron ejection angles.[21]

The excitation amplitude $\tau_{ex}(i\to\mu,\mathbf{k}_f)$ of the μth autoionizing state, found allowing for its coupling to continuous spectrum, is calculated in Ref. 22:

$$\tau_{ex}(i\to\mu,\mathbf{k}_f) = \{t_{ex}(i\to\mu,\mathbf{k}_f) - i\pi\langle\Phi_\mu|V|\hat{A}[\varphi_f\psi^{L_\mu}]\rangle t_{dir}^{L_\mu}\}, \quad (21)$$

where $t_{ex}(i\to\mu,\mathbf{k}_f)$ is the amplitude of excitation of an autoionizing state deduced ignoring its coupling to the continuous spectrum; $t_{\text{dir}}^{L_\mu}$ is the partial component of the direct ionization amplitude; ψ_μ^L is the part of the wave function in the continuous spectrum coupled by the electron–electron interaction to the autoionizing state in question.

The amplitude of direct ionization transitions is calculated in Ref. 18 allowing for the interaction in the final state:

$$t_{dir}^{(-)} = t_{dir}^{B} K_{dir}. \quad (22)$$

Here, t_{dir}^{B} is the direct ionization amplitude obtained in the Born approximation,

$$K_{dir} = f_c^{(-)*}(\nu_{12})\, f_c^{(-)*}(\nu_{13})\,(1+2\mathbf{k}_{12}\mathbf{Q}/Q^2)^{i\nu_{12}}(1+2\mathbf{k}_{13}\mathbf{Q}/Q^2)^{i\nu_{13}} \times {}_2F_1(-i\nu_{12}, -i\nu_{13}, 1, X),$$

where $\mathbf{Q}$ is the transferred momentum, and

$$X = 2\frac{2(\mathbf{k}_{12}\mathbf{Q})(\mathbf{k}_{13}\mathbf{Q}) - Q^2(\mathbf{k}_{12}\mathbf{k}_{13} - k_{12}k_{13})}{(Q^2+2\mathbf{k}_{12}\mathbf{Q})(Q^2+2\mathbf{k}_{13}\mathbf{Q})}.$$

Substituting into Eq. (1) the values of $t_{\text{res}}^{(-)}$ and $t_{\text{dir}}^{(-)}$ obtained allowing for the interaction in the final state, we obtain the total ionization amplitude

$$t_{fi}^{(-)} = t_{dir}^{B} K_{dir} + \sum_\mu K_{res,\mu}(\nu_{12}\nu_{13})\frac{\tau_{dec}^{0}\tau_{ex}(i\to\mu,\mathbf{k}_f)}{E_e - E_\mu + i\Gamma_\mu/2}, \quad (23)$$

which governs the cross sections for the ionization of an atom in the region of excitation of autoionization resonances that are differential with respect to the energy and angle of the ejected electron.

A comparison of the experimental data with theoretical calculations can usually be made conveniently by representing the ionization cross section of an atom in the region of the autoionization resonances in terms of the resonance asymmetry $A_\mu(E_i,\theta_e)$ and yield $B_\mu(E_i,\theta_e)$ parameters[23] which are functions of the energy of the incident particle and of the electron ejection angle. However, allowance for the interaction in the final state, which affects the amplitude of the resonance ionization, has the effect that $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$ become functions of the electron energy and can change significantly in an energy interval of the order of the resonance width. Therefore, the most consistent approach which can be used in this case is a direct comparison of the calculated and experimental electron ejection spectra. However, this is not always convenient and sometimes very cumbersome. If $K_{res,\mu}$ depends weakly on the electron energy, we can adopt a different approach and introduce parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$, which include the bulk of the information on the interaction in the final state. We can obtain these parameters by, for example, using the values of $K_{res,\mu}$ at a resonance point $E_e = E_\mu$. Then, we find that

$$\frac{d^2\sigma}{dE_e\, d\Omega_e} = F(E_i,\theta_e) + \sum_\mu \frac{A_\mu(E_i,\theta_e)\,\varepsilon_\mu + B_\mu(E_i,\theta_e)}{\varepsilon_\mu^2 + 1}, \quad (24)$$

where $\varepsilon_\mu = (E_e - E_\mu)/\frac{1}{2}\Gamma_\mu$ is the relative detuning from a resonance,

$$F(E_i,\theta_e) = 4\frac{k_f}{k_i}\int d\Omega_{\mathbf{k}_f} |t_{dir}^{B} K_{dir}|^2 \quad (25)$$

describes the angular and energy distributions of electrons knocked out from an atom as a result of direct ionization,

$$A_\mu(E_i,\theta_e) = 8\frac{k_f}{k_i}\int d\Omega_{\mathbf{k}_f} \operatorname{Re}(t_{dir}^{B*} K_{dir}^{*} t_{res,\mu}) \quad (26)$$

represents the asymmetry of a resonance, and

$$B_\mu(E_i,\theta_e) = 4\frac{k_f}{k_i}\int d\Omega_{\mathbf{k}_f}[\,|t_{res,\mu}|^2 + 2\operatorname{Im}(t_{dir}^{B*} K_{dir}^{*} t_{res,\mu})\,] \quad (27)$$

determines the yield of a resonance which is proportional to the algebraic area under the resonance curve after subtraction of the contribution made by the direct transitions. Here,

$$t_{res,\mu} = K_{res,\mu}(\nu_{12}\nu_{13})\, t_{dir}^{L_\mu}[q_\mu(Q) - i], \quad (28)$$

$$q_\mu(Q) = t_{ex}(i\to\mu,\mathbf{k}_f)/(\pi\langle\Phi_\mu|V|\hat{A}[\varphi_f\psi^{L\mu}]\rangle t_{dir}^{L\mu}) \quad (29)$$

is the profile index of a resonance, and $d\Omega_{\mathbf{k}_f}$ is an element of a solid angle in the direction of ejection of the scattered particle. It should be pointed out that Eq. (28) is obtained in an approximation which is linear in respect of $K_{res,\mu}(\nu_{12},\nu_{13})$.

Parametrization of Eq. (24) allows for the interactions in the final state, which affect not only the direct ionization amplitude, but partly also the amplitude of decay of an autoionization resonance. Its validity is limited at low ejection angles, when the influence of the interaction in the final state increases and the changes in the parameters (considered as a function of the electron energy) become considerable. If the interaction in the final state is ignored, the parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$ become identical with the values obtained in the plane-wave Born approximation. The process of parametrization represented by Eq. (24) makes it possible to describe also the interference between autoionization resonances. Its allowance results in a redefinition of the parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$, without modification of the general nature of the equation (24) describing the ionization cross section.

We can reduce Eq. (24) to the familiar Fano expression[24] in which the asymmetry of autoionization resonances is described by a profile index $\tilde{q}_\mu(E_i,\theta_e)$ representing a combination of the parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$ (Ref. 23).

3. DISCUSSION OF CALCULATED RESULTS

We shall now consider the results of calculations of the asymmetry parameter $A_\mu(E_i,\theta_e)$, the yield parameter $B_\mu(E_i,\theta_e)$, and profile indices $\tilde{q}_\mu(E_i,\theta_e)$ of autoionization resonances in the spectra of electrons ejected from helium atoms as a result of bombardment with protons. We shall give the helium atom ejection spectra in the region of autoionization $(2s^2)\,^1S$, $(2s2p)\,^1P$, and $(2p^2)\,^1D$ resonances using kinematic variables for which the resonance parameters depend on the electron energy. All the approximations for the atomic wave functions are the same as those used in Ref. 23 and the profile indices of the resonances used in the calculations and dependent on the transferred momentum are taken from Ref. 25.

Figures 1 and 2 give the results of calculations carried out allowing for the interaction in the final state which affects the direct and resonance ionization amplitudes also in the Born approximation, together with the experimental angular dependences of the asymmetry and yield parameters and of the profile indices of the $(2s^2)\,^1S$ resonance of the helium atom determined[26–28] at three proton energies: 100, 300, and 500 keV ($v_1 = 2$–4.5 a.u.). In the case of 100-keV protons the asymmetry and yield parameters depend strongly on the electron ejection angle. At low ejection angles the dependence is quasiperiodic. An allowance for the interaction in the final state in the expression for the resonance amplitude of the ionization by protons of this energy reproduces qualitatively the experimentally observed behavior of the resonance parameters and refinement of the direct ionization amplitude improves quantitatively the agreement between the calculations and the experimental data. Therefore, in the front hemisphere the change in the resonance profile is determined practically completely by the kinematics of the collisions, the correct determination of which is possible (as shown by a comparison with the calculations made using the plane-wave Born approximation) only if we allow for the interaction in the final state influencing the direct and resonance ionization amplitudes.

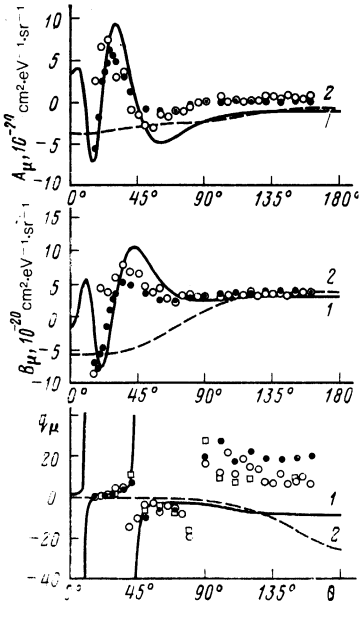

FIG. 1. Angular dependences of the asymmetry parameter $A_\mu(E_i,\theta_e)$, of the yield parameter $B_\mu(E_i,\theta_e)$, and of the profile index $\tilde{q}_\mu(E_i,\theta_e)$ of a $(2s^2)\,^1S$ resonance in the spectrum of electrons ejected as a result of ionization of helium atoms by 100-keV protons: 1) calculation in the $E_e = E_\mu$ approximation for the factor $K_{res,\mu}$; 2) calculation in the Born approximation. Experimental points: ●) Ref. 27; ○) Ref. 26; □) Ref. 28.

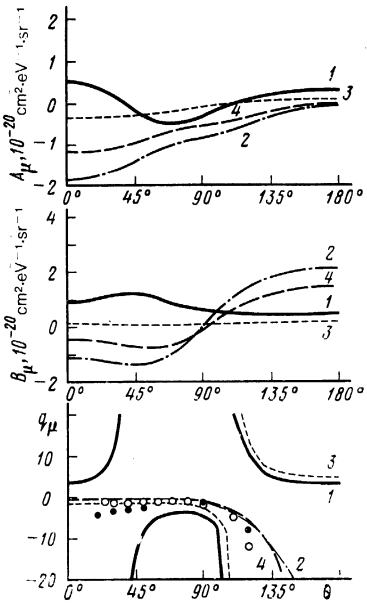

FIG. 2. Angular dependences of the asymmetry parameter $A_\mu(E_i,\theta_e)$, of the yield parameter $B_\mu(E_i,\theta_e)$, and of the profile index $\tilde{q}_\mu(E_i,\theta_e)$ of a $(2s^2)\,^1S$ resonance in the spectrum of electrons emitted as a result of ionization of helium atoms by protons: 1), 3) calculation in the approximation based on $E_e = E_\mu$ for the $K_{res,\mu}$ factor; 2), 4) calculation in the Born approximation for energies 300 and 500 keV, respectively; experimental data from Ref. 28: ●) 300 KeV; ○) 500 keV.

In the rear hemisphere the parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$ depend weakly on the electron ejection angle, which can be explained by a reduction in the influence of the interaction in the amplitudes of the forward and resonance ionizations in the final state on the profiles of autoionization resonances. This approach is confirmed by the results showing that the relative phase of the direct and resonance ionization amplitudes, which determines the resonance parameters, becomes a slowly varying function of the ejection angle, whereas the interaction in the final state determines the rapidly varying part of the same phase.[8]

In the case of protons of energies 300 and 500 keV the oscillations of the resonance parameters become smoother in the front hemisphere, again owing to a reduction of the influence of the interaction in the final state on the nature of the interference of an autoionization resonance with a continuous spectrum. It is clear from Figs. 1 and 2 that the resonance yield $B_\mu(E_i,\theta_e)$ becomes weakly dependent on the electron ejection angle and practically symmetric relative to the angle of 90° and relative to the direction of motion of the incident proton as the energy of this proton increases (see, for example, the results obtained for $E_i = 500$ keV). This means that at high proton energies the $(2s^2)\,^1S$ autoionizing level decays practically isotropically under conditions of a weak interference with the continuous spectrum.

The resonance profile index $\tilde{q}_\mu(E_i,\theta_e)$ is a complex function of the ejection angle. Calculations allowing for the interaction in the final state within the front hemisphere of the ejection angles reproduce all the characteristics of the

behavior of this complex function that are observed experimentally and cannot be explained by the plane-wave Born approximation. It should be pointed that there is an asymptote $[\tilde{q}_\mu(E_i,\theta_e) = \infty]$ at proton energies 300 and 500 keV in the rear hemisphere and at 100 keV at an angle $\theta_e \approx 80°$. This is the only singularity which is reproduced by the Born approximation in the range of high proton energies, and if allowance is made for the interaction in the final state, the singularity in question simply shifts toward lower ejection angles. The singularity appears because of an interference between the $(2s^2)\,^1S$ resonance and an S-wave in the continuous spectrum, which in turn interferes with other partial waves. However, when the proton energy is reduced ($E_i = 100$ keV), the experimentally observed asymptote is not reproduced by the results of the Born approximation or by calculations which allow for the interaction in the final state affecting the direct and resonance ionization amplitudes, although calculations allowing for the interaction of the scattered proton just with the electron emitted as a result of decay of an autoionization resonance do predict such a singularity. Its behavior can be observed also when the effective charge of the residual ion formed from the target atom is altered slightly (the field of this ion determines the wave function of the ejected electron in the continuous spectrum). This is the evidence of a high degree of sensitivity of the interference pattern of a resonance with the continuous spectrum at high ejection angles to the selection of the atomic wave functions.

It is shown above that the doubly differential ionization cross section obtained allowing for the interaction in the final state in the expressions for the amplitude of decay of photoionization resonances can generally be expressed in terms of the asymmetry and the yield parameters, which become functions of the electron energy and can change significantly within one resonance width. Consequently, it would be interesting to compare the spectra of electron emitted at different ejection angles (relative to the primary proton beam) by calculation using an expression similar to Eq. (2), but allowing for the dependence of $K_{\text{res},\mu}$ on the electron energy and assuming $E_e = E_\mu$ for the factor $K_{\text{res},\mu}$.

Figures 3 and 4 give the electron spectra obtained in the region of $(2s^2)\,^1S$, $(2s2p)\,^1P$, and $(2p^2)\,^1D$ resonances of the helium atom bombarded with $E_i = 100$ keV protons calculated for the electron ejection angles $\theta_e = 0$, 16, and 60° either allowing for the dependence of $K_{\text{res},\mu}$ on the electron energy or including the parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$ in accordance with Eq. (24). A strong interaction in the final stae for zero ejection angle (Fig. 3) resulted in qualitative changes in the spectrum of autoionization resonances. For example, the nature of the resonance asymmetry changes and oscillations appear in the wing of a $(2s2p)\,^1P$ resonance; the nature of these resonances is related to the interference between the direct and resonance ionization amplitudes when there is an interaction in the final state. Convolution of the theoretical spectrum with the Gaussian distribution characterized by an average energy scatter of 0.13 eV (which is typical of experimental investigations) suppresses the effect, which is then manifested only by a general shift of a resonance. Experimental observation of these oscillations of the resonance profile are possible if the spectrometer resolution (under the assumed kinematic conditions) is at least 0.04 eV. When the parameters $A_\mu(E_i,\theta_e)$ and $B_\mu(E_i,\theta_e)$ are calculated assuming that $E_e = E_\mu$, the effect in question is not observed. An increase in the electron ejection angle (Fig. 4) reduces the difference between these two calculation variants and in the range of angles $\theta_e \geqslant 60°$ the difference becomes negligible. For all the ejection angles a calculation allowing for the dependence of $K_{\text{res},\mu}$ on the electron energy reproduces well the observed resonance profile. Then, in the range of low ejection angles, when the interaction in the final state becomes considerable, the process of parametrization described by Eq. (24) becomes unsuitable for the analysis of the experimental data. It is then necessary to carry out systematic calculations of the spectra of electrons in the region of autoionization resonances.

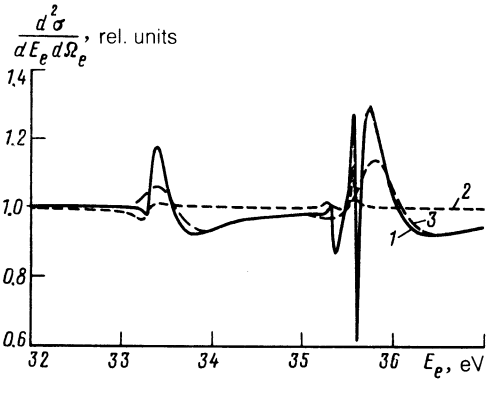

FIG. 3. Spectrum of electrons ejected at an angle of 0° as a result of ionization of helium atoms by 100-keV protons: 1) calculated allowing for the dependence of $K_{\text{res},\mu}$ on the electron energy; 2) calculation in the $E_e = E_\mu$ approximation for the $K_{\text{res},\mu}$ factor; 3) convolution of a calculated spectrum 1 with a Gaussian distribution characterized by an average energy scatter of 0.13 eV.

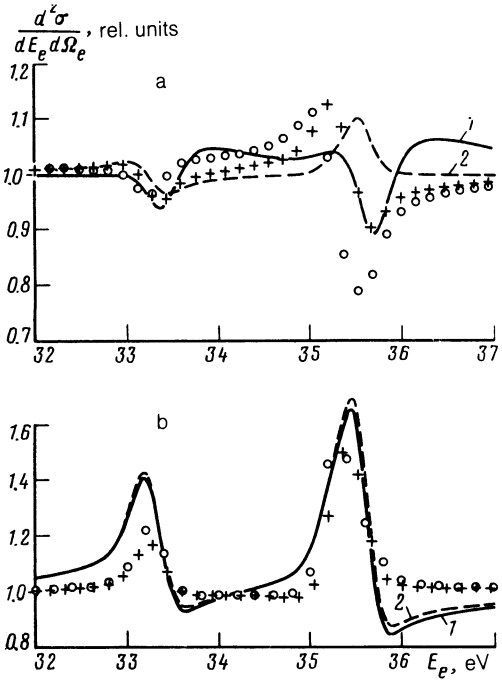

FIG. 4. Spectrum of electrons ejected at an angle of 16° (a) and 60° (b) as a result of the ionization of helium atoms by 100-keV protons: 1) calculation allowing for the dependence of $K_{\text{res},\mu}$ on the electron energy; 2) calculation in the $E_e = E_\mu$ approximation for the $K_{\text{res},\mu}$ factor. In both calculations a convolution is formed with the Gaussian distribution characterized by an average energy scatter of 0.13 eV. Experimental points: +) Ref. 27; ○) Ref. 26.

It is interesting to allow for the interference between the $(2s2p)^1P$ and $(2p^2)^1D$ resonances in the helium atom. These resonances appear as one combined structure in the electron ejection spectra, because the energy resolution in the available experiments is close to the separation between these resonances, which is known to amount to 0.237 eV and this is considerably greater than the combined half-width 0.056 eV of these resonances.[29] Calculations of the parameters allowing for and ignoring the interference between the resonances differ only slightly for the kinematic conditions under consideration here and are practically identical if $\theta_e = 90°$.

Therefore, the proposed model of the ionization of an atom by a fast charged particle in the region of excitation of autoionization resonances can be used to make real progress in the understanding of the mechanism of these resonances in the electron ejection spectra. We have been able not only to account for the influence of the interaction in the final state on the angular and energy dependences of the profiles of autoionization resonances in the cross sections of the ionization of helium atoms by protons, but also to ensure a good agreement with the experimental data.[26–28] An allowance for the interaction in the final state affecting the amplitudes of the direct and resonance ionizations makes it possible to provide a practically complete description of the experimental data on the interference phenomena observed in the spectra of the ejected electrons in the region of autoionization $(2s^2)^1S$, $(2s2p)^1P$, and $(2p^2)^1D$ resonances when atoms of helium are ionized by 100–500 keV protons. It is shown that the majority of the singularities in the angular and energy dependences of the profile indices of the resonances are due to the interaction of an electron and a scattered proton in the final state. The exception is a singularity of the $(2s^2)^1S$ resonance at large ejection angles, the appearance of which is unrelated to the interaction in the final state. One should stress particularly the approximate nature of the parametrization described by Eq. (24), which is frequently used to find doubly differential ionization cross sections when the interaction in the final state has a considerable influence on the ionization spectrum. Calculations show that the use of this parametrization in the case described above can lead to serious errors.

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