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ON THE INTERPRETATION OF THE ENERGY SPECTRA OF ELECTRONS PRODUCED IN ATOMIC COLLISIONS

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The effect of the kinematics of atomic collisions on the character of the energy spectrum of the emitted electrons is studied. It is shown that the effect of the Doppler shift and broadening of the spectral lines of the electrons produced as a result of inelastic processes accompanied by considerable scattering of the atomic particles leads to a significant distortion of the shape of the observed spectrum. The location and width of the spectral lines turn out to be dependent not only on the energy and lifetimes of the autoionization levels, but also on the energy and scattering-angle distributions of the colliding particles. A computation is carried out of the energy spectrum of electrons connected with the excitation of autoionization states of argon and helium in Ar^+–Ar and He^+–He collisions. The results of the computation are qualitatively in good agreement with the available experimental data.

THE study of the energy spectra of electrons is of late becoming an important method in the study of inelastic processes occurring in atomic collisions. In principle, the study of electron spectra permits us to obtain information about the energy and lifetimes of autoionization levels, which are excited in collision processes, and also about the probability of their excitation. Such information is extremely important for the analysis of one of the most difficult problems of the physics of atomic collisions—the mechanism of inelastic transitions. However, the extraction of the necessary information from the spectra of electrons produced in collisions of atomic particles is more difficult a problem than, say, the analysis of the spectra of electrons produced in photoabsorption or in the ionization of atoms by electron impact.

One of the causes making the interpretation of electron spectra difficult is the scattering of the atomic particles in collisions. This circumstance has never been properly taken into consideration in the investigations carried out up to the present time. It has usually been assumed in analyses of electron energy spectra that the electrons are emitted either by a stationary target particle or by a fast moving atomic particle whose momentum does not practically change after the collision. Under these assumptions the energy of an electron emitted by a target particle will be equal to the difference between the energies of the initial and final states of the particle, whereas the spectral lines for electrons connected with transitions in a fast incident particle will undergo a Doppler shift which can easily be taken into account.[1]

In many cases electrons are produced as a result of collisions in which the scattering angle of the fast particle and the kinetic energy imparted to the target particle are indeed small. In that case the indicated simple approach turns out to be sufficiently accurate. However, a very typical situation is the one in which the emitted electrons are produced as a result of violent collisions, which occur at small impact parameters and are accompanied by a strong scattering of the incident particle and a considerable kinetic energy transfer to the target particle. Under these conditions the analysis of the electron energy spectra can be carried out only after the proper allowance has been made for the kinematics of the collision.

Let us consider the effect of scattering on the location and shape of an electron spectral line. Let the electrons be emitted by an atomic particle of mass M which is scattered, as a result of the collision, through an angle ϑ and which has a finite kinetic energy E_i. The analyzer of the energy of the electrons is placed at an angle α to the direction of the incident beam. If E_{e0} is the energy of an electron in the system of coordinates rigidly attached to the emitting atomic particle, then it can be shown that the energy of such an electron in the laboratory system will be determined by the expression

$$E_e = E_{e0} + A + B\cos(\varphi_e - \varphi_i), \tag{1}$$

where

$$A = 2\sqrt{\frac{m_e}{M}E_{e0}E_i}\cos\alpha\cos\vartheta,$$

$$B = 2\sqrt{\frac{m_e}{M}E_{e0}E_i}\sin\alpha\sin\vartheta, \tag{2}$$

m_e is the electron mass, φ_e the azimuthal angle of emission of the electron, and φ_i the azimuthal scattering angle of the ion. It is natural to suppose that the distribution of the emitted electrons with respect to the azimuthal angle φ_e is isotropic, i.e.,

$$dN / d\varphi_e = N_0 = \text{const}, \tag{3}$$

where N is the number of electrons. As follows from (1),

$$dE_e / d\varphi_e = -B\sin(\varphi_e - \varphi_i) = -\sqrt{B^2 - (E_e - E_{e0} - A)^2}. \tag{4}$$

Combining (3) and (4), we obtain the electron distribution function with respect to energy in the laboratory system of coordinates

$$\Phi(E_e) = \frac{1}{N_0}\frac{dN}{dE_e} = -\frac{1}{\sqrt{B^2 - (E_e - E_{e0} - A)^2}}. \tag{5}$$

As can be seen from (1) and (5), the spectral line of electrons with energy E_{e_0} will undergo a Doppler shift A and a broadening ±B relative to the mean position $E_{e_0} + A$. The shape of the resulting distribution will be symmetric with a minimum at $E_{e_0} + A$ and sharp maxima at the edges. As an illustration we show in Fig. 1 contours which are obtained as a result of the convolution of a Gaussian contour of width γ, and of a Doppler distribution (5) for different values of the ratio B/γ. It can be seen that at sufficiently large values of the broadening B the shape of the resulting distribution has nothing in common with the shape of the initial Gaussian contour.

In a real situation electrons with energy E_{e_0} may be emitted by particles which have been scattered through different angles ϑ and have different kinetic energies. Therefore, the electron distribution f(E) observed in experiments will be the convolution of four functions: the function $f_0(E_{e0})$ describing the contour of the line in the system of coordinates attached to the emitting atomic particle, the Doppler distribution (5) $\Phi(E - E', E_i, \vartheta)$, the energy and scattering angle distribution function $\Psi(E_i, \vartheta)$ for the atomic particles, and the apparatus function of the analyzer $a(E' - E_{e0})$:

$$f(E)=\iiiint f_0(E_{e0})\,a(E'-E_{e0})\,\Phi(E-E',E_i,\vartheta)\times\Psi(E_i,\vartheta)\,dE_{e0}\,dE'\,dE_i\sin\vartheta\,d\vartheta. \qquad (6)$$

The examples cited below can serve as an illustration of the influence of collision kinematics on the character of the energy spectra of electrons.

ANALYSIS OF THE ENERGY SPECTRA OF ELECTRONS CONNECTED WITH THE EXCITATION OF INNER SHELLS

The energy spectra of electrons produced in collisions of atomic particles in the kiloelectron-volt energy range have been investigated in papers by Rudd, Jorgensen and Volz[1] and by one of the present authors, Flaks and Avakyan.[2] It was shown that the energy spectrum of electrons consists of a continuous distribution, which monotonically decreases with increase of electron energy, and discrete lines superimposed on the continuous part of the spectrum. It may be assumed[3] that the discrete lines of the electron spectrum are connected with autoionization transitions in atomic particles after their separation, whereas the continuous part of the spectrum corresponds to transitions in quasimolecules formed at the instant of collision. The determination of the relative probability of transitions leading to the appearance of the discrete and continuous parts of the spectrum may yield information about the lifetimes of the autoionization state. Of great interest, in particular, is the study of Auger transitions with occupation of a vacancy in the $L_{2,3}$-subshell of argon. The results of the analysis of this part of the spectrum can be compared with the results of investigations into inelastic energy losses in atomic collisions.

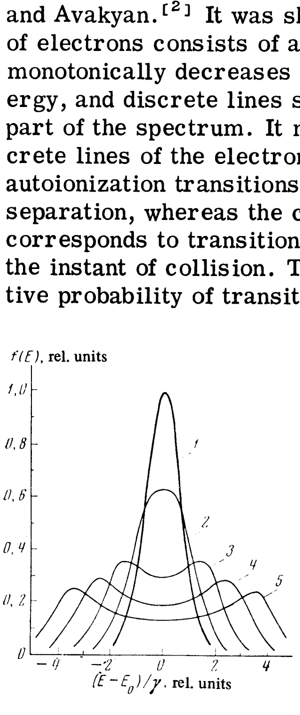

FIG. 1. Deformation of a Gaussian contour under the action of Doppler broadening. 1—A = 0, B = 0 (Gaussian contour); 2—A = 0, B = γ; 3—A = 0, B = 2γ; 4—A = 0, B = 3γ; 5—A = 0, B = 4γ (explanation in the text).

Inelastic energy losses in Ar^+–Ar collisions were studied in [4,5]. It was discovered that the spectrum of inelastic losses consists of three discrete lines. The first one is connected with the excitation of the M shells, and the second and third with the excitation of the L shells of argon. A possible mechanism of excitation of the L shells is the formation of vacancies as a result of the crossing of terms as the atomic particles approach each other.[6] Since the most probable decay channel discovered in [4,5] for the excited levels is autoionization, the study of electron energy spectra can help elucidate the question of the mechanism of excitation of the lines of inelastic energy losses.

Let us discuss as an example the electron spectra obtained in [2] for the Ar^+–Ar pair for an ion energy of 15 keV. The electron spectrum in the range E_e = 100–240 eV, corresponding to Auger transitions with the occupation of $L_{2,3}$-vacancies, has a very complex shape and consists of three components: a continuous "backing," a broad peak, and a fine structure superimposed on these components of the spectrum. The presence of the broad peak makes the analysis of this part of the spectrum difficult, but such a character of the energy distribution can be explained when the kinematics of the atomic collision are taken into account.

In interpreting the electron spectrum, we shall suppose that the lines of inelastic energy losses corresponding to the excitation of inner shells, which were discovered in [4], lead to the formation of $L_{2,3}$-vacancies and, in the final analysis, to the emission of Auger electrons. Using this supposition, we can determine the complete apparatus function in investigations of the energy spectra of the electrons. We shall assume that for the investigated symmetric Ar^+–Ar pair the Auger electrons are emitted with equal probability from both colliding particles. The dependence of the probability of excitation of the inner shells on the scattering angles was investigated in [4]. Using these data, we can determine the dependence of the probability of formation of $L_{2,3}$-vacancies on the scattering angle of the fast particle (we assume then that the second line of the inelastic losses leads to the formation of a single L vacancy while the third line leads to the formation of two L vacancies). Since the scattering angle determines the collision kinematics practically uniquely, the obtained dependence allows the determination of the distribution function with respect to the angle ϑ and energy E_i of the fast particles and the recoil particles emitting Auger electrons. The convolution of these distributions, the distribution (5) and the apparatus function of the analyzer of the electron energy (see (6)) will yield the complete apparatus function in the study of an electron spectrum, i.e., a spectrum corresponding to a narrow discrete line in the system attached to the emitting particle. The following characteristics of the analyzer used in [2] were used in the computation: angle of aperture of the analyzer $\alpha = 54.5°$, resolution $\Delta E_e/E_e = 0.007$. The shape of the apparatus function of the analyzer was assumed to be Gaussian.

As an example we show in Fig. 2 the complete apparatus function corresponding to the line of Auger electrons of energy $E_{e0} = 200$ eV. For comparison we show in the same figure the instrumental function obtained with no allowance for the collision kinematics, under the assumption that the electrons are ejected from a stationary target particle and from a fast particle moving in the initial direction.

To obtain the spectrum of electrons connected with Auger transitions to $L_{2,3}$-vacancies, we used the data in [7] on the locations of the spectral lines in the interval $E_e = 100-240$ eV which are excited in H^+-Ar collisions. It was assumed that the energy E_{e0} of the Auger electrons in the case of Ar^+-Ar collisions was the same as in Auger transitions observed in the case of H^+-Ar collisions. Taking into consideration the absence of accurate information about the relative intensity of the spectral lines and the qualitative nature of the comparison of the results of the computation with experimental data,[2] we assumed the intensities of the lines corresponding to the transitions $L_{2,3}$–MM and $L_{2,3}$M–MMM to be the same and conditionally set them equal to unity. The intensity of the lines due to the less probable three-electron transitions of the type $2p^5 3s^2 3p^6 - 2p^6 3s^2 3p^3 nl$ was set equal to 0.3. Apparatus functions similar to the functions shown in Fig. 2 were calculated for each of the lines discovered in [2] and then summed with the corresponding statistical weights.

The obtained electron spectrum is shown in Fig. 3. The lines at the upper part of the figure indicate the positions of the discrete lines which served as the basis of the computation of the spectrum. Shown also in the figure is the corresponding part of the spectrum obtained in [2] minus the continuous "backing."

There is a very good qualitative agreement between the experimental and theoretical spectra. It goes without saying that the decisive factor leading to the conversion of the discrete lines into the distribution observed in experiments is the collision kinematics. The discrepancies between the theoretical and experimental spectra are connected, apparently, with the crudeness of the initial assumptions about the equality of the probabilities of excitation of the various lines and the sameness of the nature of the lines excited in Ar^+-Ar and H^+-Ar collisions. The good agreement between the experimental and theoretical spectra indicates that there is indeed an interrelationship between the energy spectrum of electrons resulting from the excitation of $L_{2,3}$-shells and the corresponding discrete lines observed in the spectrum of inelastic energy losses.

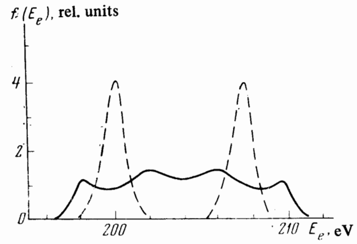

FIG. 2. The effect of collision kinematics on the shape of the lines of the energy spectrum of electrons. The dashed lines are the initial contours; the continuous line is the distribution obtained when the collision kinematics are taken into account.

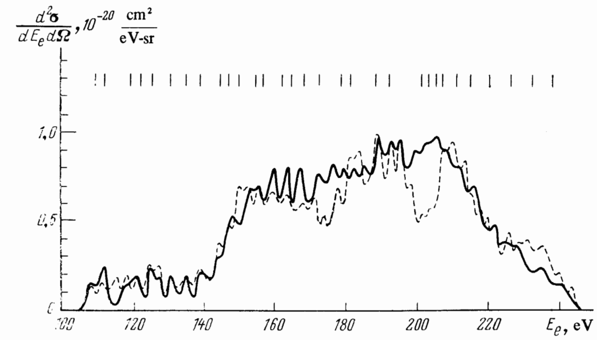

FIG. 3. The discrete part of the energy spectrum of electrons produced in Ar^+-Ar collisions in an ion energy of 15 keV in the 100–240 eV electron energy range. The continuous curve is the result of experiment[2], the dashed curve–of the calculation. The positions of the initial lines are indicated at the upper part of the figure.

The need for taking the collision kinematics into account leads to serious difficulties in the identification of the lines of the spectrum of electrons produced in collisions between complex atomic particles. Investigations carried out in the ion energy region ~ 10 keV[2] can, apparently, yield sufficiently reliable information about the energies of the autoionization transitions in the outer shells of the atoms. The identification of the spectral lines, corresponding to Auger transitions and Koster-Kronig transitions to vacancies in the inner shells, is impossible if the proper allowance is not made for the collision kinematics. Therefore, the graphical comparison made in [2] of the positions of the observed spectral lines with the energies of the above-mentioned transitions in isolated atoms is unnecessary.

In investigations carried out at ion energies ~ 100 keV and an angle of emission of the electrons of 160°,[1] the effect of the collision kinematics is manifested mainly in a Doppler shift of the spectral lines and this can be taken into account in a simple way.

In the case of H^+-Ar collisions at a proton energy of 20 keV[7] the effect of the collision kinematics on the character of the energy spectrum of the electrons can be neglected in view of the small ratio of the mass of the impinging ion to that of the target atom.

PECULIARITIES OF THE ENERGY SPECTRA OF ELECTRONS PRODUCED IN SLOW COLLISIONS BETWEEN IONS AND ATOMS

The effect of the kinematics of collisions between atomic particles on the character of the energy spectrum of electrons may turn out to be important in the case of the excitation of autoionization states of an outer shell of an atom if the velocity of the relative motion is not high. The degree of this influence may be illustrated on the example of the excitation of the autoionization states of helium in He^+-He collisions in the ion energy range 1600–4300 eV.[8] A characteristic feature of the electron energy spectra measured in [8] is the well-defined shift of the positions of the experimental peaks towards lower energies, the shift being inversely proportional to the velocity of the impinging ions. At the same time, the width of the peaks increases in inverse proportion to the velocity.

This effect, discovered and named by Barker and Berry as the "Stark shift" of spectral lines, was explained by them as due to the influence of the Coulomb field of the scattered ion on the decay process of the autoionization state of the atom. Since autoionization in this case is accompanied by Coulomb repulsion of the ions in the final state, the energy corresponding to the continuum limit and, consequently, the energy of the emitted electrons turn out to be dependent upon the distance between the nuclei at which the disintegration takes place. In the case when this distance is sufficiently large, so that the atomic particles participating in the collision can be considered as isolated, the energy distribution of the electrons has the form[8]

$$f(E_e)=\frac{w_\infty}{v(E_{e\infty}-E_e)^2}\exp\left[-\frac{w_\infty}{v(E_{e\infty}-E_e)}\right], \qquad (7)$$

where E_e is the energy of the emitted electron, $E_{e\infty}$ the energy of an autoionization transition in an isolated atom, w_∞ the transition probability for the case of an isolated atom, and v the relative velocity (all quantities are given in atomic units).

The energy distribution function of the electrons (7) has a maximum at an electron energy equal to

$$E_{em}=E_{e\infty}-w_\infty/2v. \qquad (8)$$

The width of the peak at a height equal to half the height of the maximum is then

$$\gamma=1.07w_\infty/v. \qquad (9)$$

It can be seen that the relations (8) and (9) explain the experimentally[8] observed dependence of the shift and width of a line on velocity. Furthermore, the relation (8) makes it possible for us to determine the transition probability w_∞ or the lifetime $\tau_\infty = 1/w_\infty$ of an autoionization state in an isolated atom directly in terms of the value of the shift of the corresponding spectral lines. However, an estimate of the lifetime of the autoionization state 2s2p of He, made in this way in [8], yielded the very strange and unexpected result $\tau_\infty = 2.4 \times 10^{-15}$ sec, which is roughly an order of magnitude less than the value found from experiments on photoabsorption[9] (1.7×10^{-14} sec) and from theoretical calculations[10] (1.5×10^{-14} sec). The question as to the nature of the autoionization state whose lifetime was determined in [8] has up to now remained unexplained.

The availability of data on the spectrum of inelastic energy losses in He^+–He collisions (see [11]) allowed us to carry out an analysis of the kinematics of inelastic processes connected with the excitation of the autoionization states of helium. This analysis showed that the effect of "Doppler" broadening of spectral lines may significantly influence the character of the energy distribution of electrons observed in [8]. In particular, it is not difficult to show on the basis of the relation $E_0\vartheta_0 = 10^4$ eV-deg[11] (E_0 and ϑ_0 are the energy and scattering angle of the impinging ions), determining the position of the peak of an inelastic energy loss line, that at energies E_0 in the interval 1600–4300 eV the broadening of a spectral line as a result of the Doppler effect[1] is ~ 1 eV which, by order of magnitude, corresponds to the width and shift of the lines observed in [8]. The convolution of the three functions (the "Stark" distribution (7), the Gaussian apparatus, and the "Doppler" contour (5) (Fig. 4)) has an asymmetric shape with a strongly pronounced rise in the low-energy part of the distribution. The magnitude of the shift of this low-energy "peak" relative to the position of the initial line E_∞ will be determined by the "Stark" shift[8] as well as by the Doppler broadening.[1] Since the shift of the edges of the Doppler distribution (5) $\Delta E \sim \sqrt{E_0}\,\vartheta_0 \sim \sqrt{E_0}/E_0 \sim 1/v$, the latter effect leads to the same dependence of the shift and width of a line on velocity as the "Stark" shift effect.

The results of the calculation of the complete energy distribution function of the electrons (6) carried out for an incident ion energy E_0 = 1600 eV are shown in Fig. 5. As initial data, we took the values of the lifetime $\tau_\infty = 1.7 \times 10^{-14}$ sec,[9] the resolution of the analyzer $\Delta E_e/E_e$ = 1.33%,[8] and the distribution function $\Psi(E_i, \vartheta)$ found in [11]. Since the width of the function (6) for a separate isolated line is $\gtrsim 1$ eV, it is evident that the peak observed in [8] is the result of the overlapping of the distributions corresponding to several neighboring lines of the spectrum. On the basis of the results of investigations into the energy spectra of electrons produced in H^+–He collisions (E_{H^+} = 75 keV),[12] we can assume that the main contribution to the shaping of the experimental peak is made by transitions from the autoionization states $2s2p(^3P)$ ($E_{e\infty}$ = 33.8 eV), $2p^2(^1D)$ ($E_{e\infty}$ = 35.4 eV) and $2s2p(^1P)$ ($E_{e\infty}$ = 35.5 eV). It is also necessary to take into account the fact that each of the lines corresponding to the indicated transitions has a Doppler twin which, on account of the characteristics of the experiment[8] (α = 90°) will be shifted from the principal line towards lower energies by an amount $\Delta E = m_e v^2/2 \simeq 0.2$ eV (m_e is the electron mass, v the velocity of the impinging ion). In view of the lack of data on the relative intensity of the initial spectral lines, we assumed that they were the same.

For comparison, the data of [8], obtained for the same energy of the impinging ions, are shown in Fig. 5. It can be seen that the distribution calculated by us reproduces sufficiently accurately the main parameters

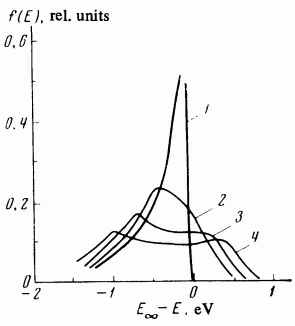

FIG. 4

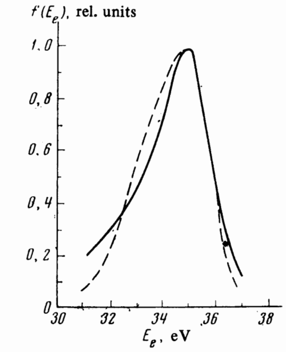

FIG. 5

FIG. 4. Deformation of the "Stark" contour under the action of Doppler broadening. 1–A = 0, B = 0, $\gamma = 1.07\,w_\infty/v = 0.3$ eV ("Stark" contour); 2–A = 0, B = γ; 3–A = 0, B = 2γ; 4–A = 0, B = 3γ (explanation in the text).

FIG. 5. Discrete part of the energy spectrum of electrons produced in He^+–He collisions at an ion energy of 1600 eV, in the electron energy range 30–38 eV. The continuous curve is the result of experiment[8], the dashed curve–of the calculation.

of the experimentally observed contour, in particular, the line width and the position of the maximum. The disagreement in the region of the "wings" of the contour may be explained by the influence of the more distant lines at $E_{e\infty} = 33.2$ and 37.6 eV which we did not take into account.

Thus, it is evident that the shift and broadening of the lines of the electron spectrum observed in [8] owe their origin mainly to the peculiarities of the kinematics of the collisions between the atomic particles and not to the influence of the Coulomb interaction between the ions on the process of the disintegration of the autoionization state, as was previously assumed.

We see from the above analysis that in those cases when the atomic collision is accompanied by appreciable scattering of the particles, the kinematics of the collision may exert a decisive influence on the character of the energy spectrum of the electrons produced. The positions and shapes of the discrete lines observed in the spectra turn out to be dependent not only on the energies and lifetimes of the initial levels, but also on the relative intensities of the lines and the velocity and scattering angle distribution of the ions. In order to accurately take these factors into account, we require such a large amount of additional information that it is practically impossible to establish the connection between the observed spectral lines and the true transition energy. In the cases when the effect of the collision kinematics is considerable and it is not possible to make an accurate allowance for it, the aim of investigations into electron energy spectra should, apparently, not be the study of the fine structure but the extraction of more general integrated characteristics, such as the excitation cross sections for the various shells of the atom and the cross sections corresponding to the continuous part of the spectrum.

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