

THE INNER SHELL IONIZATION OF THE ATOM BY ELECTRONS

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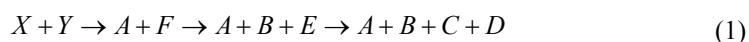
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Abstract. *In this paper, the resonant processes of inner-shell ionization of some atoms, followed by the Auger decay of the created vacancy was considered. The analytical expression for the line profiles in the Auger-electron spectra was analyzed. The line shift in the Auger spectra of the rare gas atom inner-shells was also considered.*

Key words: *Auger decay, line shift, inner-shell ionization.*

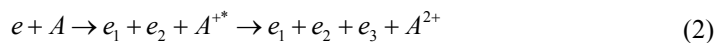
1. INTRODUCTION

The inelastic scattering of atomic particles X , Y has been considered. In this reaction other atomic particles A , F may be obtained. The last of them is in a quasi-stationare state. The process which we considered has the form:



where X , Y , A , B , C , E , F are atomic particles and we assumed that the particles A , B , C , D , E have been charged. After the decay of the autoionization state F , the final state has four interacted particles.

The process of the atomic inner-shell ionization by electron impact in the framework of a quantum mechanical model was investigated. After the vacancy Auger decay, the final state consists of the double ionized atom A^{2+} and three electrons: the scattered e_1 , ejected e_2 and the Auger electron e_3 . The corresponding process is:



where A denotes the atom in the ground state, and A^{+*} is the excited ion.

The phenomenon of particles interactions in the final state is called the post collision interaction (PCI) process. The PCI was first discovered in the process of the electron ex-

citation of an autoionized state [1]. The theoretical description of the PCI effect was given by the quasi-classical description [2], the quasi-molecular adiabatic consideration [3], the shake-down model [4], and the quantum mechanical treatment [5, 6, 7].

The interaction of four particles in the final state of the resonant processes (1) was investigated. The interest in the theoretical description of these processes is based on two reasons: first, the PCI effect in these processes is very important in the large energetic area of the incident electron, and, second, to explain the experimental investigation [8]. Electron-electron coincidence experiments following electron impact on atoms may be divided into two major groups. The first is the $(e, 2e)$ type of experiments [9]. It fully determines the kinematics of the ionization process by measuring values of both the scattered and ejected electrons. The residual target ion is not observed. The second type involves angular correlations with decay products of the atomic target, i.e., autoionization electrons in the case of excitation, and **Auger electrons in the case of the inner-shell ionization**, respectively. Contrary to $(e, 2e)$ experiments, this technique is sensitive to the polarization of the intermediate target state created by the electron impact.

The exact solution of the interaction of all particles in the final state of the reaction (1) was presented, and it is proposed that the width Γ of the auto-ionization state A^{**} is small (which means that the electrons e_1 and e_2 are at large distances from the atom at the moment of the Auger decay).

As a result, the resonant character of the intermediate state A^{**} in the process (1) has the line form in the energetic spectra of the Auger electrons. In the cases when PCI effect is not present, the spectrum takes the form of Lorentz distribution. We have demonstrated that the influence of the PCI effect is very significant in the processes (1). We improved the recently obtained results [10,11,12] by using the many-body theory (the RPAE method).

In this paper we use atomic units $|e| = \hbar = m_e = 1$.

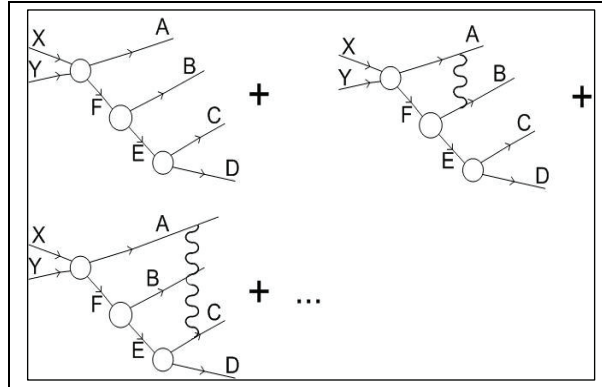


Fig. 1. The diagram describes the interaction of the four particles in the final state in the resonant reactions (1).

2. THEORY

The amplitude of the process that is investigated may be presented in the series of the Feynman's diagrams. These diagrams describe the interaction of four particles in the final state in the resonant reaction (1). Some of the first diagrams in this series are presented in Fig.1.

The propagations of the particles A, B, C, D, E, F are presented by the continual lines, the wavy lines correspond to the their Coulomb interaction; the circles present the vertex (M_i)

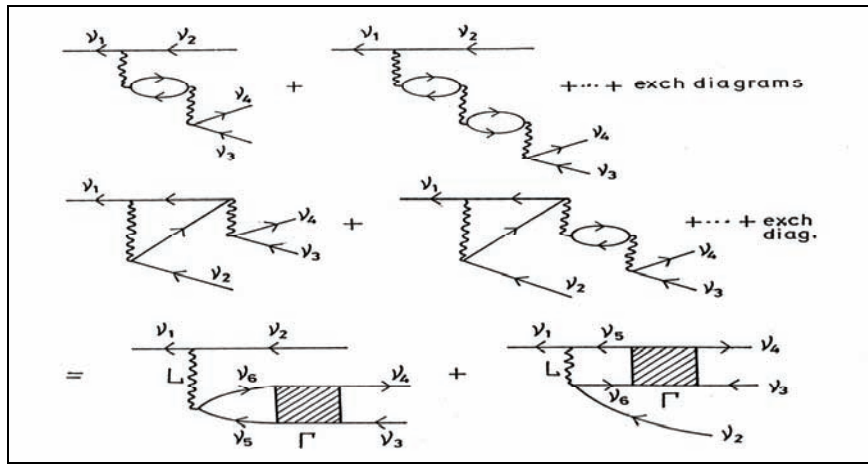


Fig. 2. The diagrammatic presentation of the amplitude of the Auger decay (here Γ and ν denotes the effective interaction and the complete set of quantum numbers, respectively).

which describes the inelastic scattering $X + Y \rightarrow A + F$ and decays $E \rightarrow C + D$ (i.e., excited ion $\rightarrow e + A^{2+}$).

The results of generalization of method [11] which is used for the processes with three particles in the final state (where the PCI is calculated in the eikonal approximation) are presented [12]. The non-resonance processes are ignored because the electrons energies E_1, E_2, E_3 are close to the resonant energies. At first, the amplitude of the process (1) in the infinity series of the Feynman's diagrams is presented and all of the partial amplitudes in the eikonal approximation [6, 12] were calculated. The total amplitude A of the presented process is the function of some quantities (the details of the expression are presented in [6]):

$$A = f(M_1, M_2, M_3, \varepsilon, \Gamma, \int_0^T U(t, \tau) d\tau) \quad (3)$$

where M_i presents the matrix elements of the inelastic scattering and corresponding decays; Γ is the width of the autoionization state of A^{+*} ; $\varepsilon = E_A + E_F - E_X - E_Y$; U is the

potential interaction energy in the final state between the particle A and other particles. The term $\int U(t, \vec{r}) d\tau$ is the classical action. The expression (3) describes the Breit-Wigner resonant amplitude without this term. In our calculations we assumed the following :

The electrons e_1, e_2 (with velocities $v_i, i = 1, 2$) are at large distances from the atom: $r_i = v_i / \Gamma \gg 1, (i = 1, 2)$, and also $\Gamma(A^{*+}) \leq 1 eV = 1 / 27 au$. (Γ is small parameter).

The distances between the ion and e_1, e_2 electrons (r_1, r_2) are large: $r_1, r_2, r_{12}, r_{13}, r_{23} \gg 1$ (where r_{12}, r_{13}, r_{23} are the distances between three electrons). That means that the potential energy interactions between the electrons e_1, e_2 and the products of the Auger decay (e_3, A^{2+}) are small. This kind of interactions is very small compared to the kinetic energy $\varepsilon_1, \varepsilon_2$ of the electrons e_1, e_2 and the kinetic energies of the electron pairs $\varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23}$ (i.e. $e_1, e_2; e_1, e_3; e_2, e_3$, respectively).

The differential cross-sections are [5, 10]:

$$\sigma(E_1, E_3, \Omega_1, \Omega_2, \Omega_3) = \sigma_0(E_1, \Omega_1, \Omega_2) \frac{\Gamma_{Auger}}{2\pi(\varepsilon^2 + \Gamma^2/4)} q(\varepsilon, \xi), \quad (4)$$

where:

$$q(\varepsilon, \eta) = \frac{\pi\eta}{sh(\pi\eta)} \exp(2\eta \operatorname{arccotg} \frac{2\varepsilon}{\Gamma}); \quad \eta = (v_{13}^{-1} - v_1^{-1} + v_{23}^{-1} - v_2^{-1})e^2 / \hbar,$$

$v_{ij} = |\vec{v}_i - \vec{v}_j|$ and $\varepsilon = E_3^0 - E_3$ is the energy of the Auger electron. Γ_{Auger} is the partial width of the Auger decay $A^{*+} \rightarrow e_3 + A^{2+}$; σ_0 is the cross-section of the electron excitation of the autoionization state of A^{*+} . The method recently investigated by Kuchiev and Sheinerman [6,12] is improved and the Γ_{Auger} in the Random Phase Approximation with Exchange (RPAE) is calculated. In atomic units the Auger width is equal to the probability of the Auger decay (Fig.2) [7,11].

The first two terms in (4) describe the simple Breit-Wigner resonance. The term $q(\varepsilon, \eta)$ takes into account the particle interactions in the final state. This quantity depends on ε by the term ε / Γ and consequently $q(\varepsilon, \eta)$ drastically changes when the line spreads. The expression (4) describes the line form of the Auger spectra. The shift of maximum is defined by relation:

$$\Delta\varepsilon = \eta\Gamma / 2 \quad (5)$$

If the velocities of the Auger electrons are large ($v_3 \gg v_1, v_2$) the quantities $\eta, \Delta\varepsilon$ are independent of the direction of the ejected electrons. In this case the shift of the line maximum is defined by:

$$\Delta\varepsilon_M = (-\Gamma/2)(v_1^{-1} + v_2^{-1}) \quad (6)$$

In the case when $v_1 \sim v_2 \sim v_3$, the parameter η very much depends on the ejected electrons' directions.

When the directions of the ejection and scattering electrons, as well as the energies of the Auger, scattering, and ejected electrons are fixed, the cross section is

$$\sigma(E_1, E_3, \Omega_1, \Omega_3) = \int d\Omega_2 [eq.(4)] \quad (7)$$

or, when $v_2 \ll 1$, $v_2 \leq v_3$ the cross section is:

$$\sigma(E_1, E_3, \Omega_1, \Omega_3) \cong \sigma_0(E_1, \Omega_1) \frac{2\Gamma_{Auger}}{(\varepsilon^2 + \Gamma^2 / 4)} \frac{\pi\eta}{sh(\pi\bar{\eta})} \exp(2\bar{\eta} \operatorname{arccotg} \frac{2\varepsilon}{\Gamma}) \quad (8)$$

where is $\bar{\eta} = (1/4\pi) \int \eta d\Omega_2$.

Exactly speaking, after the connection of our cross-section with the detector function (we chose the Gauss normal distribution), the real cross section which we compare with experiments has the form:

$$\sigma_\varepsilon = \int_{-\infty}^{+\infty} \sigma(E_1, E_3, \Omega_1, \Omega_3; \varepsilon') \exp[-(\varepsilon - \varepsilon')^2 / 2\sigma^2] d\varepsilon' \quad (9)$$

3. RESULTS

As an example, we compare the theoretical calculations with the experimental results [8] of the $L_2 - M_{23}M_{23}(^3P)$ Auger line in argon (Fig.3).

The energies of the incident, scattered, ejected and non-perturbed Auger electrons are $E_0 = 1keV$, $E_1 = 744.5eV$, $E_2 = 5eV$, $E_3^0 = 207,2eV$ [6], respectively. The angle between the Auger and scattered electrons is $\theta = 76^\circ$; the parameter $\eta = -1.420$ and $\Gamma = 0.17eV$. In this case, the basic contribution in the PCI comes from the interaction of the ejected electron and the ion field in the following velocity areas $v_2 \ll v_3 < v_1$. In cases when the velocities are $v_1 \sim v_2 \sim v_3 > 1$ the form of the Auger line changes depending on the registries scattered and Auger electrons.

In the double coincidence experiments the velocities v_1 , v_3 are fixed and cross sections are given by the expression (8) (the velocity of the ejected electron is small, $v_2 \ll 1$). The shift of the maximum is then defined by the expression $\overline{\Delta\varepsilon} = (\Gamma/2)\bar{\eta}$.

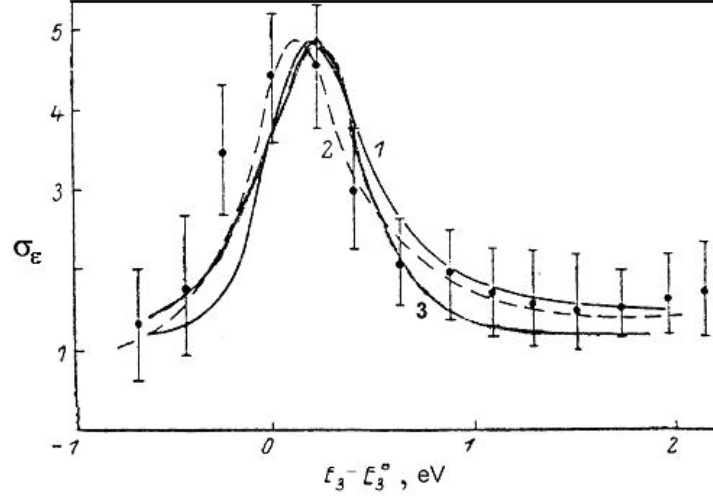


Fig. 3. The line form of the Auger spectra (the line $L_2 - M_{23}M_{23}(^3P)$) in the coincidence measurement techniques for the scattered and Auger electrons. Theoretical results: 1-[6]; 2-[2] (quasi-classical results); 3- our improved many-body results. Experimental results:[8].

Integrating the cross section (4) over the angles of the ejected and scattered electrons, and over the energies of the scattered electron, the distribution of the Auger electrons was obtained:

$$\sigma(E_3, \Omega_3) = \int_0^{E_0-I} dE_1 \int d\Omega_1 d\Omega_2 [eq.(4)] \quad (10)$$

The shift of the Auger line is defined by the position of the maximum (10) at some energy $\bar{\varepsilon} \cong f(\sigma_0, \Gamma, \eta, q(\bar{\varepsilon}, \eta))$. The values $\bar{\varepsilon}$ were obtained by using some approximations. We change η and σ_0 : a) $\eta \rightarrow \langle \eta \rangle =$ average value (on the angles Ω_1, Ω_2) and, b) $\sigma_0 \rightarrow \sigma_0^{bin}$ - from the classical binary theory.

The line shift $\Delta\varepsilon \equiv \Delta\bar{\varepsilon}$ in Ar (Fig.4), Kr (Fig.5) and Xe (Fig.6) was calculated as a function of the electron energy below the ionization threshold $\Delta E = E_0 - I$ (I is the ionization energy of the corresponding sub shell). The parameters which were used in calculations are: $\Gamma_{l_3}(Ar) = 0.17eV$, $\Gamma_{M_{23}}(Kr) = 2.2eV$, $\Gamma_{N_5}(Xe) = 0.11eV$ [6].

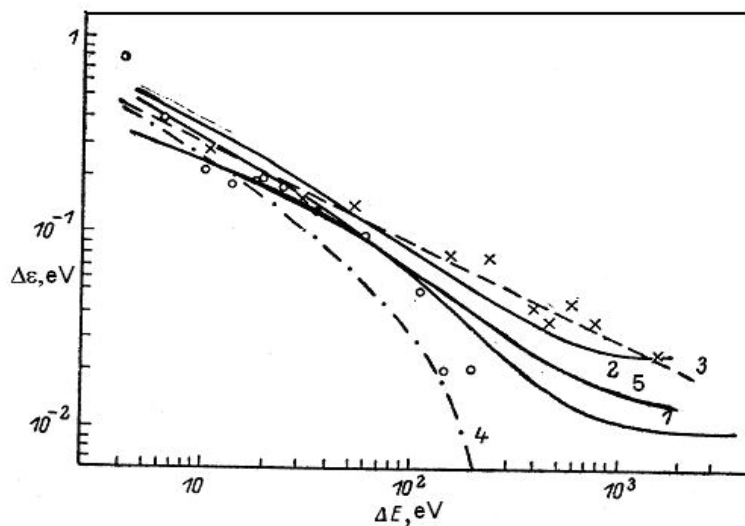


Fig. 4. The shift of the Auger line $L_3 - M_{23}M_{23}(^1D_2)$ in Ar: 1- [6], 2- [12], 3-[13,14], 4- [15], [5]-our results. Experiments: o- [16]; x- [17].

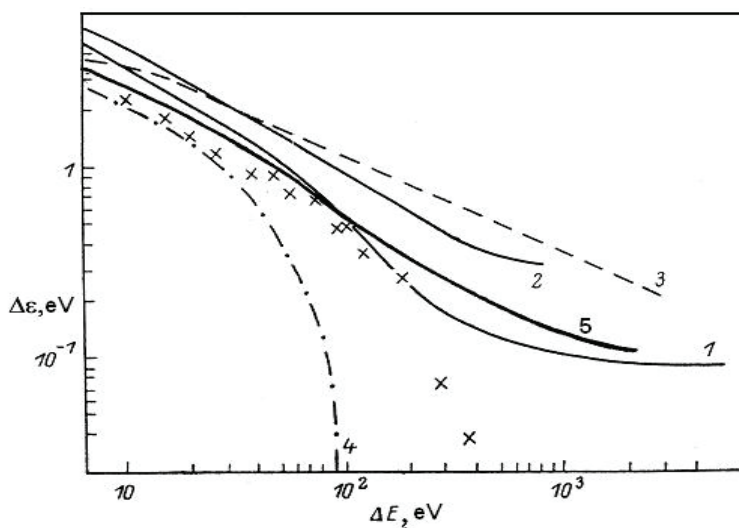


Fig. 5. The shift of the Auger line $M_{23} - M_{45}M_{23}(^1D_2)$ in Kr. 5-our results. Other results are the same as in Fig. 4. Experiments: x- [18].

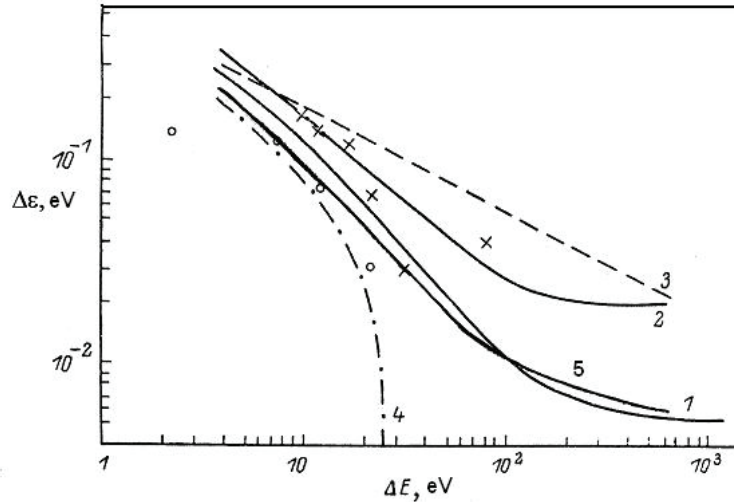


Fig. 6. The shift of the Auger line $N_5 - O_{23}O_{23}(^1S_0)$ in Xe. 5-our results. Other results are the same as in Fig. 4. Experiments: x-[16], o- [17].

4. CONCLUSION

The ionization of the inner shell of some atoms (*Ar, Kr, Xe*) is considered in the vicinity of their thresholds. The profiles of the Auger lines are calculated taking into account the PCI. In the improved calculation we have used the RPAE method for the calculations of the width of the Auger decay. The model of the PCI permits us to calculate the cross sections from the first principle. The obtained results are in agreement with experimental data. The collisions of this type are very important in the area of the nano-region the a better understanding of the basic physical processes and designed new materials.

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JONIZACIJA UNUTRAŠNJIH LJUSKI ATOMA ELEKTRONSKIM UDAROM

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U radu se razmatraju rezonantni procesi jonizacije unutrašnjih ljuski nekih atoma. Ova jonizacija nastaje nakon Ože raspada. Analizirali smo analitičke izraze za profile linija u elektronskom Ože spektru. Računali smo i pomeranje linija unutrašnjih nivoa Ože spektra atoma inertnih gasova.