# Calculation of Ar photoelectron satellites in the hard-x-ray region

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The intensities of photoelectron satellite lines, corresponding to the double core hole (DCH) states of Ar $1s$ ionization by hard x rays, are calculated using the many-body perturbation theory. Calculations support the interpretation of the most intense lines as the shake-up excitations $2p \to 4p$. It is demonstrated that the intensities of the spectrum lines corresponding to $4s$ (and $3d$) excited states in the DCH field can be explained only taking into account the knock-up process $2p \to 3d$ along with the shake-up process $1s \to 4s$ that accompanies $2p$ photoionization.

## I. INTRODUCTION

Recent experiments in hard-x-ray photoelectron spectroscopy (HAXPES) resulted in investigation of a particular type of photoelectron satellites [1] corresponding to final states with a double core hole (DCH), and one excited electron. Several years ago previous to that some of the DCH states in Ar $1s$ photoionization corresponding to excitations $2p \to 4p$ were discovered experimentally and their positions were calculated [2]. Well resolved structure in the DCH energy region [1] is the basis for theoretical calculation of electron correlations with high-energy transfer, which corresponds to HAXPES.

Along with strong lines, a very interesting result of [1] is the identification of excitations $1s \to 4s$ with extremely large energy transfer to the satellite and very small relative intensity, about $10^{-4}$ of that of the main line.

These measurements became possible due to the modern HAXPES technique in photoelectron spectroscopy. HAXPES is versatile for the investigation of bulk electronic structure of functional materials [3,4]. Theoretical calculations are required for a better understanding of the physics of this type of excitation. Due to a significant energy difference from traditional electron spectroscopy, physical phenomena related to HAXPES, e.g., nondipolar effects and interchannel correlations, should be specially considered for this energy region [5,6].

The satellite peaks in the photoelectron spectra appear due to many-electron correlations. Their investigation is important for understanding the many-body nature of the interaction of electromagnetic radiation with matter. Satellite spectra in the soft-x-ray region were investigated quite well [7–13]. Corresponding satellite intensities were calculated using the sudden approximation [14–17], the configuration interaction method [18], and the many-body perturbation theory [13,19,20]. The investigation of the decay of valence satellites into different continuum channels revealed a nonuniform lineshape broadening in different decay channels [21], which was predicted theoretically [22–24].

Two satellite series, $2p \to 4p,5p$ and $1s \to 4s$, identified in Ref. [1] correspond to large ($\sim 300$ eV) and very large ($\sim 3000$ eV) energy transfer due to many-electron correlations. The main aim of the present work is to calculate satellite intensities and to clarify some specific features of the satellite excitations in the case of large energy transfer. We discuss also the problem of extension of the existing many-electron photoionization theory to the HAXPES photon energy region and high-energy transfer to the satellite states. Also we calculate the energy positions of all the satellite series and for strong lines generally confirm their interpretations in Ref. [1]. As to the relatively weak lines, the interpretation of at least one of them proved to be different. It is demonstrated that it is exited via the knock-up process, instead of the shake-up channel.

## II. THEORY

Theoretical approaches to double ionization are usually based on perturbation theory, where the potential of a hole initially created by the photon is considered as a perturbation potential (see [25] and references therein). In the lowest order of many-body perturbation theory the relaxation of the core hole $k$, created in photoionization, is described by its transition to double-hole–one-particle states $i^{-1}j^{-1}s$. Photoionization with excitation of another electron is shown in Fig. 1(a). Note that for the monopole shake-up process one has $i = k$.

To account for these processes the self-energy $\Sigma_k(E)$ of the initial hole $k$ is calculated according to the following formula:

$$\mathrm{Re}\Sigma_k(E) = \sum_{ijs} \frac{\langle kj|U|is\rangle^2}{E - \varepsilon_i - \varepsilon_j + \varepsilon_s}. \tag{1}$$

Here $\langle kj|U|is\rangle$ is the Coulomb interelectron interaction matrix elements with exchange, and the sum (integral) runs over all final states $i^{-1}j^{-1}s$ including the discrete and continuum excited states $s$. One-electron energies of electrons and holes are denoted as $\varepsilon_i$, and $E$ stands for the energy parameter of the initial hole $k$. Radial parts of the Coulomb matrix elements and energies are calculated using the HARTREE-FOCK computer code [26]. The angular momentum coupling technique is applied to analytically calculate the angular parts of the Coulomb matrix elements [25,27,28].

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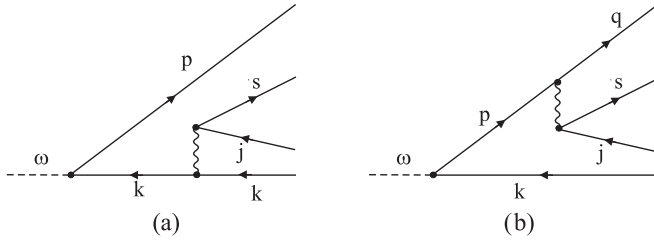*Corresponding author: vgyar@igic.ras.ru

FIG. 1. Many-body perturbation theory diagrams for two channels of a satellite excitation: (a) excitation by the core hole potential (the shake-up channel) and (b) excitation by the outgoing electron (the knock-up channel). A solid line with an arrow directed to the right (left) represents an electron (a hole). The dashed line denotes the interaction with a photon and a wavy line denotes the Coulomb interaction.

The positions of the lines in the spectrum are given by the solutions of the so-called Dyson equation [25]:

$$E = \varepsilon_k + \Sigma_k(E). \quad (2)$$

The line intensities are proportional to the spectroscopic factors that are defined by the following expression [25]:

$$f = \frac{1}{1 - \partial \Sigma_k / \partial E}. \quad (3)$$

Here the derivatives are taken at the solutions of Eq. (2). In the vicinity of the satellite under consideration, formulas (1) and (3) may be approximated by the following relation, corresponding to the second order of the perturbation theory [25]:

$$f_s = \frac{\langle kj|U|ks \rangle^2}{(\varepsilon_s - \varepsilon_j)^2}. \quad (4)$$

It is seen from formula (4) that in the direct (main) part of the Coulomb matrix element the core hole $k$ wave function overlaps with itself. As a result, for any monopole satellite excitation $j^{-1}s$ the dependence of the Coulomb integral upon $k$ is not very strong. For excitations from the valence shells the satellite intensities are usually about $10^{-2}$ of the main line intensity [7–13]. In this case the energy difference in the denominator of (4) is about 1 a.u. If the satellite is excited from Ar $2p$ shell, the energy denominator in Eq. (4) is about 10 a.u. Hence in the latter case one can expect for the satellites an intensity that is 100 times less, than in the former case, i.e., about $10^{-4}$ of the main line. This crude estimation agrees with the experimental results [1]. For the satellite excitation from the Ar $1s$ shell, whose binding energy is about 100 a.u., one can expect the spectroscopic factor values to be about $10^{-6}$ of the main line.

The same satellite states can be excited also by the outgoing photoelectron [see Fig. 1(b)]. The amplitude of this process is given by the following expression [13,25]:

$$A_{kqjs}(\omega) = \int_{\varepsilon_p} \frac{D_{kp}(\omega)U_{ps,qj}d\varepsilon_p}{\omega - \varepsilon_p + \varepsilon_k + i\delta} \delta(\omega - \varepsilon_q + \varepsilon_k - \varepsilon_s + \varepsilon_j). \quad (5)$$

In formula (5) the energy conservation is fulfilled for the final state $q$, while the photoionization amplitude $D_{kp}(\omega)$ is cal-

TABLE I. Theoretical photoionization cross sections of Ar $1s$ and Ar $2p$ shells for different photon energies.

| | Photon energy | | |
|---|---|---|---|
| | 3900 eV[a] | 3650 eV[b] | 700 eV[c] |
| Shell | Photoionization cross sections | | |
| Ar $1s$ | $48.0 \times 10^3$ b | $56.8 \times 10^3$ b | |
| Ar $2p$ | $1.84 \times 10^3$ b | | $366 \times 10^3$ b |

[a]Actual photon energy in Ref. [1].
[b]Formal photon energy that corresponds to the transfer of 250 eV to the $2p \to 4p$ excitation.
[c]Formal photon energy that corresponds to the transfer of 3200 eV to the $1s \to 4s$ excitation.

culated beyond the so-called energy conservation frame, i.e., for $\omega$ not necessarily equal to $\varepsilon_p - \varepsilon_k$. Photoionization cross sections with corresponding energy shifts were investigated in the RPAE (random phase approximation with exchange) approximation [25]. It was obtained that photoionization of any level by photon energy $\omega$ with energy transfer $\Delta E_s$ to another channel may be roughly approximated by the photoionization cross section of the level, but by photons of the energy $\omega - \Delta E_s$.

This outcome of [25] can be envisaged as follows. In the shake-up channel the kinetic energy of the photoelectron is $\Delta E_s$ less than in the main line channel, and the wave function with actual photoelectron energy must be used for the calculation of the dipole matrix element. This corresponds to the calculation of the photoionization cross section at photon energy $\omega - \Delta E_s$. Thus the formula for the satellite intensity relative to any reference photoelectron line $r$ can be presented as:

$$\tilde{f}_s = \frac{f_s \sigma_k(\omega - \Delta E_s)}{\sigma_r(\omega)}. \quad (6)$$

Here the spectroscopic factor $f_s$ is defined by formula (3). Note that in Ref. [1] and in the present work the reference line is Ar $1s$, and satellite excitations accompanying $1s$ and $2p$ photoionization are considered.

Table I presents the photoionization cross sections of Ar $1s$ and Ar $2p$ shells for different photon energies, calculated using the program from [29]. Photon energy 3900 eV corresponds to the one-electron photoionization. The photoionization cross section of the Ar $1s$ line at 3650 eV corresponds to the satellite excitation $2p \to 4p$. It is seen that this approach enhances the cross section by 18%. In the case of the Ar $2p$ line a transition from the photon energy 3900 eV to the energy 700 eV can be considered as a very rough approximation to the satellite excitation $1s \to 4s$ effect. Nevertheless, it is possible to conclude that in the case of the satellite excitation from the core shell, the photoionization cross section, which has to be used for the calculation of the satellite intensity, is significantly larger than that for the main line.

For the satellite excitations from valence shells one can use the photoionization cross sections beyond the energy conservation shell [25] or neglect the difference between $\sigma_k(\omega - \Delta E_s)$ and $\sigma_k(\omega)$. On the other hand, in the case of DCH states the energy difference $\Delta E_s$ is quite significant and cannot

TABLE II. Theoretical binding energies (eV) of Ar DCH states $(1s^{-1}2p^{-1})(^{2S+1}P_J)$ with one excited electron $nl$.

| DCH state | $nl = 4s^a$ | $nl = 4s^b$ | $nl = 4p^a$ | $nl = 4p^b$ | $nl = 4p^c$ | $nl = 5p^a$ | $nl = 5p^b$ |
|---|---|---|---|---|---|---|---|
| $(1s^{-1}2p^{-1})(^1P_1)nl$ | 3511.9 | 3511.5 | 3514.5 | 3514.3 | 3512.8 | 3518.6 | 3519.0 |
| $(1s^{-1}2p^{-1})(^3P_0)nl$ | 3504.6 | | 3504.6 | 3505.2 | 3503.3 | 3508.6 | 3509.8 |
| $(1s^{-1}2p^{-1})(^3P_1)nl$ | 3503.8 | 3501.4 | 3501.2 | 3504.0 | 3502.6 | 3507.6 | 3508.2 |
| $(1s^{-1}2p^{-1})(^3P_2)nl$ | 3499.6 | 3500.0 | 3502.0 | 3502.5 | 3500.9 | 3506.0 | 3506.6 |

[a]Theoretical values, corrected by 2.6 eV (see text).
[b]Experimental values (estimated from figure of [1]).
[c]Theoretical values [2].

be neglected. From formula (5) it is clear that when a satellite is excited by the outgoing electron, the main contribution to the amplitude (5) comes from the vicinity of the singularity of the integrand that corresponds to the energy conservation. In this case one can use in formula (5) photoionization amplitude $D(\omega)$ corresponding to the main line.

## III. RESULTS AND DISCUSSION

The calculations of the satellite excitation energies were performed within the $LSJ$ coupling scheme. The theoretical value of the relativistic $1s$ ionization energy 3208.9 eV, calculated as the difference of Dirac-Fock [30] total energies of Ar and Ar $1s^{-1}$ states, is a little bit larger than the experimental ionization energy, 3206.3 eV. To take into account this small systematic difference all theoretical binding energies of DCH states were shifted by the same value, 2.6 eV. The calculations in valence shells were performed using a nonrelativistic program [26] with the $LS$ coupling for all terms. To obtain the ionization energy of DCH states with relativistic corrections, the nonrelativistic values were shifted by the difference of the relativistic Ar $1s^{-1}2p^{-1}$ energy averaged over $2p_{1/2}$ and $2p_{3/2}$ holes and nonrelativistic configuration average Ar $1s^{-1}2p^{-1}$ energy. The value 11.78 eV of the multiplet splitting between $1s^{-1}2p^{-1}(^1P)$ and $1s^{-1}2p^{-1}(^3P)$ DCH states is significantly larger than the theoretical spin-orbit splitting of the $2p$-subshell value 2.59 eV. Spin-orbit splitting for the final states was calculated using graphical representation of the spin-orbit coupling weight factors [25,28] and the theoretical value of spin-orbit splitting of the $2p$ shell. Theoretical energies of the DCH states are compared with experiment in Table II.

The agreement between the theoretical binding energies and the experimental ones [1] confirms the validity of the $LSJ$ coupling scheme for the case under consideration.

Table III compares theoretical intensities of the satellites, accompanying Ar $1s$ photoionization with the experimental data [1,12]. There is no spin-orbit splitting in the case of a singlet channel $^1P_1$, and standard formulas for satellite intensities in $LS$ coupling [23] can be applied. For triplet series Table III compares theoretical results for the triplet case in $LS$ coupling [25] with the sum over three experimental components, which were estimated from Fig. 2 of Ref. [1]. The satellite intensities relative to the intensity of the Ar $1s$ line were calculated using formulas (1) and (3). Table III presents also the results corrected for the photoionization cross sections according to formula (6). The intensity of the satellite that corresponds to the excitation $3p \rightarrow 4p$ is in good agreement with experiment and theoretical data in sudden

approximation [12]. Table III shows that the satellite intensities for the excitations $2p \rightarrow 4p$ are also in good agreement with experiment [1]. The corrections by photoionization cross section are not significant in these two cases. The Coulomb matrix elements for the excitations $3p \rightarrow 4p$ and $2p \rightarrow 4p$ differ insignificantly and the ratio of intensities is almost exactly equal to the squared ratio of the excitation energies.

It was suggested in Ref. [1] that the state $1s^{-1}2p^{-1}(^1P_1)4s(^2P)$ is created as a shake-up excitation $1s \rightarrow 4s$, accompanying the $2p$ ionization. Our calculations under this assumption resulted in a very small value of the intensity, as is shown in Table III. There are several reasons for this. The squared energy denominator in Eq. (4) results in a factor $10^{-2}$ relative to the $1s^{-1}2p^{-1}4p$ satellites. Direct and exchange Coulomb integrals have different signs in this case. Note that the signs of the weight factors before the Coulomb and exchange integrals are the same in a singlet case and are different in a triplet case. In the case of the $4s$ satellite in the triplet channel, negative signs of the exchange integral and exchange part of the weight factor result in the same signs for direct and exchange terms. That is why the theoretical intensity of the $4s$ satellite in the triplet channel is two orders of magnitude larger than the intensity of the $4s$ satellite in the singlet channel. Even after correction of the Ar

TABLE III. Theoretical and experimental intensities of the shake-up satellites of Ar $1s$ photoionization (in units of $10^{-4}$ of Ar $1s$ photoelectron line).

| Final state | Formula (3) | Formula (6) | Expt. [1,12] |
|---|---|---|---|
| $1s^{-1}3p^{-1}(^1P+^3P)4p(^2S)^a$ | 680 | 680 | $\approx 600$ |
| $1s^{-1}2p^{-1}(^1P_1)4p(^2S)$ | 2.6 | 3.0 | $\approx 2.75$ |
| $5p(^2S)$ | 1.0 | 1.18 | $\approx 0.75$ |
| $6p(^2S)$ | 0.48 | 0.57 | $\approx 0.37$ |
| $1s^{-1}2p^{-1}(^3P_{0,1,2})4p(^2S)$ | 4.5 | 5.3 | $\approx 2.08$ |
| $5p(^2S)$ | 1.7 | 2.0 | $\approx 0.79$ |
| $1s^{-1}2p^{-1}(^1P_1)4s(^2P)$ | $0.30 \times 10^{-5b}$ | $0.60 \times 10^{-3c}$ | $\approx 0.33$ |
| $1s^{-1}2p^{-1}(^3P_{0,1,2})4s(^2P)$ | $0.96 \times 10^{-3b}$ | $0.19^c$ | $\approx 0.23$ |

[a]The sum of $1s^{-1}3p^{-1}(^1P)4p$ and $1s^{-1}3p^{-1}(^3P)4p$ states, whose theoretical intensities are 0.025 and 0.043 of the Ar $1s$ line intensity, respectively.
[b]Spectroscopic factors were multiplied by the ratio of photoionization cross sections $\sigma_{2p}/\sigma_{1s} = 0.0383$ (the photon energy is 3900 eV for both shells).
[c]Spectroscopic factors were multiplied by the ratio of photoionization cross sections $\sigma_{2p}/\sigma_{1s} = 7.63$ (the photon energy is 700 eV for the $2p$ shell and 3900 eV for the $1s$ shell).

TABLE IV. Intensities of the knock-up satellites of Ar $1s$ photoionization (in units of $10^{-4}$ of Ar $1s$ line) and binding energies relative to the state $1s^{-1}2p^{-1}(^1P)4s(^2P)$.

| Final state | $\Delta E_b$ (eV) | Intensity | Final state | $\Delta E_b$ (eV) | Intensity |
|---|---|---|---|---|---|
| $1s^{-1}2p^{-1}(^3P)4s(^2P)$ | 0.00 | 0.00056 | $1s^{-1}2p^{-1}(^1P)4s(^2P)$ | 0.0 | 0.0034 |
| $1s^{-1}2p^{-1}(^3P)3d(^2P)$ | −1.09 | 0.579 | $1s^{-1}2p^{-1}(^1P)3d(^2P)$ | −0.45 | 0.412 |
| $1s^{-1}2p^{-1}(^3P)3d(^2D)$ | −0.87 | 0.0060 | $1s^{-1}2p^{-1}(^1P)3d(^2D)$ | −0.87 | 0.0020 |
| $1s^{-1}2p^{-1}(^3P)3d(^2F)$ | −0.37 | 0.0016 | $1s^{-1}2p^{-1}(^1P)3d(^2F)$ | −0.34 | 0.113 |
| Total[a] | | 0.587 | Total[a] | | 0.530 |
| Total[b] | | ≈0.23 | Total[b] | | ≈0.33 |

[a]Theory, present work.
[b]Experiment [1].

$2p$ photoionization cross section for the energy of satellite excitation $1s \rightarrow 4s$ (see Table I) the theoretical intensity of the singlet $4s$ state is two orders of magnitude less than the experimental value (see Table III).

The states corresponding to the monopole shake-up excitations $1s \rightarrow 4s$ accompanying $2p$ ionization may also be obtained by dipole knock-up processes $2p \rightarrow 4s$ accompanying the $1s$ photoionization. The dipole part of the Coulomb interaction between the outgoing electron and the ionic core may also result in the excitation $2p \rightarrow 3d$. The intensities of knock-up processes were calculated using formula (5) for the actual coupling schemes. The total nonrelativistic energies were calculated self-consistently for all terms under consideration. Since we compare relative energies for singlet and triplet states separately, the nonrelativistic approach is sufficient in this case. Table IV presents the theoretical energies of $4s$ and $3d$ states in DCH potential and intensities of knock-up excitations. The calculations demonstrate that the energy differences between the $4s$ state and some terms of $3d$ states are less than the linewidth of the satellites, 0.6 eV [1] (see Table IV). The knock-up intensity for the state $1s^{-1}2p^{-1}(^1P)3d(^2P)$ is 0.412 and its energy shift from the state $1s^{-1}2p^1(^1P)4s(^2P)$ is 0.45 eV. The intensities of other states in a singlet channel are quite small. Hence it follows that the experimental intensity of the state labeled $4s$ in a singlet channel [1] is due to knock-up of the $2p$ electron to the $3d$ state.

On the other hand, in a triplet channel the energy splitting between the $4s$ state and the only state of significant intensity, $3d(^2P)$, is 1.09 eV, i.e., larger than the experimental linewidth. Hence it follows that the intensity of the $4s$ satellite in the triplet channel cannot be explained by the knock-up process. At the photon energy 3900 eV the photoionization cross section of the $2p$ shell is 26 times less than that of the $1s$ shell and the theoretical intensity of the $4s$ satellite in the triplet channel without correction for the energy transfer is too small (see Table III). The $2p$ photoionization cross section corrected for the energy transfer to the satellite excitation becomes 7.6 times larger than that of the $1s$ shell (see Table I) and the $4s$ triplet satellite intensity is in agreement with the experiment (see

Table III). Thus, in order to explain the intensities of some satellite states in the DCH field, the photoionization cross sections corrected for energy transfer to the satellites should be used and the knock-up process should be taken into account.

## IV. CONCLUSIONS

The high-resolution technique in the HAXPES region [1] permits to resolve the fine structure of previously known [2] shake-up excitations $2p \rightarrow 4p$ of Ar $1s$ ionization and to identify new and very small ($10^{-4}$ of the main line) excitations, whose symmetry corresponds to $1s \rightarrow 4s$ satellites of Ar $2p$ ionization. The latter ones present a type of electron correlation satellite in photoelectron spectroscopy with an extremely large (about 3000 eV) energy parameter. The results of our calculation using standard approaches of many-body perturbation theory [25] are in quantitative agreement with the experiment [1] and confirm the shake-up mechanism of the excitations from the $2p$ shell, accompanying the Ar $1s$ ionization.

The smallest lines, corresponding to $1s \rightarrow 4s$ excitations and identified for the first time in Ref. [1] are the subject of reconsideration of the many-body shake-up theory. It was shown in this paper that in order to explain intensities of the satellite excitations $1s \rightarrow 4s$ in the triplet channel, the photoionization cross sections, accounting for the energy transfer to the satellite, have to be used [25]. In the case under consideration it corresponds to a factor up to about 200.

It was also obtained that the energy positions of the $3d$ and $4s$ states in the DCH potential are quite close to each other and that the intensities of some knock-up processes, $2p \rightarrow 3d$, are of the same order as experimental satellite intensities in the $4s$ channel. Thus the smallest lines in the DCH spectra may be, most likely, due to the knock-up process. It means that the measurements performed in Ref. [1] permit us to obtain and identify not only the strong lines but gain important information from the low-intensity features of the measured spectrum.

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