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Interference shake-up effects in the resonant Auger decay of krypton

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Abstract

Parameters of the resonant 4p4p–3d$\varepsilon\ell$ Auger effect (RA) following the 3d–np ($n = 5, 6$) excitation in Kr were calculated with taking into account the interference between several resonant and direct non-resonant transition amplitudes. For the first time all individual lines of the extended RA spectrum which comprises both the $4p^4(^1D)5p$ and the $4p^4(^1D)6p$ groups of final ionic states were considered. It was revealed that each group contains individual lines where the interference contributions have different signs thus providing a weak interference effect on the average over the whole group. Interference effects are found to be more pronounced in the angular distribution of the RA products.

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The resonant Auger effect (RA) for intermediate shells of rare-gas atoms is an impressive example to study the dynamics of angular and spin momenta transfer in the photoionization process (see, e.g., review [1] and references therein). In RA the total and spin angular momenta of polarized photon transfer to the resonant intermediate state and in its decay are shared between the photoelectron and residual ion. An anisotropy of the process results in a noticeable difference of the angular distribution parameters of RA products for different final ionic states.

Till recent time the only experimental method to study RA was photoelectron spectroscopy. The Raman regime of excitation [2] in which the bandwidth of the exciting radiation is smaller than the natural width of the resonances was applied. The excitation energy was selected to sit exactly on the resonance and the principal attention was paid to the lowest excited resonant state which is more isolated in comparison with the higher ones. The intensities of the RA lines and the photoelectron distribution parameters, β_{el}, were measured for many final ionic states.

Theoretically, the step-wise model [3,4] was introduced to describe the RA. In it the RA effect was considered as excitation and following decay of the particular single resonance selected by the exciting-photon energy. Other possible pathways (i.e., non-resonant direct photoionization and photoionization via the neighboring resonances) were neglected.

In recent years a considerable experimental progress was achieved in studying the RA. The following new approaches were implemented: (i) measurement of the subsequent fluorescent decay of the final ionic states using the photon-induced fluorescence spectroscopy (PIFS) using the linear or circular polarized exciting synchrotron radiation [5,6]. The alignment, A_{20}, and orientation, O_{10}, parameters for the final ionic states were determined providing a complementary information about the relative contribution of the photoelectron partial waves; (ii) fine tuning of the exciting-photon energy, scanning thus the resonances in the Raman regime [7–10]; (iii) studying higher excitations than the first resonance [8–10].

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It was obtained that those pathways which were neglected in the step-wise model provide a contribution to the resulting transition amplitude which is clearly seen in the experiment. However, a strict ab initio theoretical calculation of this new phenomenon was still very insufficient.

In the present paper, we consider particularly the RA photoelectron spectrum measured by Kukk et al. [8] where the photoexcitation of the $3d^9np$ resonances ($n = 5, 6$) of Kr and their non-radiative decay to the different $4p^4(^1D)mp\ L_1S_1J_1$ ($m = 5, 6$) final ionic states were studied. The $n = m$ corresponds to the spectator RA case while $n \neq m$ are shake processes. The excitation energy was selected in the range between 92.2 and 92.8 eV. It is larger than the excitation energy of the first resonance R1: $3d^9_{5/2}5p_{3/2}$ ($\omega = 91.200$ eV) but was scanned smoothly between the two resonances, R2: $3d^9_{3/2}5p_{\mathrm{I}}$ ($\omega = 91.425$ eV) and R4: $3d^9_{5/2}6p_{3/2}$ ($\omega = 91.560$ eV). The resonance R3: $3d^9_{3/2}5p_{\mathrm{II}}$ ($\omega = 91.455$ eV) has low excitation probability and was excluded from the discussion. The identification of the resonances we use here is in accordance with our paper [10]. The dispersed intensities in [8] were summed over each of the two groups of closely-lying RA lines connected with the $4p^4(^1D)5p$ and $4p^4(^1D)6p$ final ionic states. The spectra obtained were analyzed using the fitting procedure under the following approximations: (i) each of the above groups of final ionic states was approximated as a single "group" state; (ii) each "group" state is expected to be populated either via the R2 or the R4 resonance.

It turned out that for each group the measured intensity was not equal to the sum of two Lorentzian curves. This means that the transition amplitudes via the R2 and R4 resonances evidently interfere with each other. The signs of the interference effects between or outside the R2 and R4 resonances were qualitatively explained analyzing the signs of the radial parts of excitation and decay transition amplitudes of the resonances to the final "group" state. However, a quantitative agreement between the fit spectrum and the measured one was achieved after additional fitting parameters had been introduced: either by the reduction of the interference between the R2 and R4 resonances or by adding a non-resonant photoionization channel. Moreover, as it was mentioned in [8], there are some lines inside those groups that display stronger interference than the group in average, but the consideration of those features were beyond the scope of the work.

In the present paper we calculate the dynamics of the RA transitions for each individual line entering the two above groups with the aim of describing the averaged interference effects observed in [8] and find the cases where the interference discussed leads to the clearly detected principal changes in the calculated values.

In our previous works [5,9,10] the intensities of the RA lines as well as the angular distribution parameters of photoelectron, alignment or orientation of the residual ion were ab initio calculated for the first time with taking into account all the interfering amplitudes entering Eq. (1) (here we refer to them as to calculated in INT model):

$$D(E_1J_1, \varepsilon\ell) = \langle E_1J_1, \varepsilon\ell|\mathbf{d}|0\rangle + \sum_R \frac{\langle E_1J_1, \varepsilon\ell|\mathbf{H}^{\mathrm{ee}}|R\rangle\langle R|\mathbf{d}|0\rangle}{(\varepsilon + E_1 - E) + \imath\Gamma(R)/2} \quad (1)$$

The details of the theoretical approach as well as the calculation technique was described in detail elsewhere [5,9,10]. The most essential points of the model are:

- The wavefunctions and energies of the initial, resonance and final states were calculated using the relativistic configuration-interaction (CI) method in intermediate-coupling scheme.
- All excited configurations stemming from the CI set by single and double electron excitations were accounted for. This changes both the diagonal (energies of the CI basis states) and non-diagonal (effective Coulomb interaction) matrix elements of the CI secular equation.
- The direct transition amplitude $\langle E_1J_1, \varepsilon\ell|\mathbf{d}|0\rangle$ was computed including the relaxation of the atomic orbitals within the sudden approximation where only the monopole 4p–mp excitation is taken into account.

In Refs. [5,9,10] we compared the results obtained within the INT approach with our data or the data from other theoretical papers obtained in the step-wise model. In this paper we intend to distinguish purely the manifestation of the interference terms in Eq. (1). Therefore, it is meaningful to compare the INT results with a calculation where the resonances overlap but do not interfere (below we refer to this model as to the statistical (STAT) one). Within the STAT model the RA line intensity is expressed as

$$\sigma = \sum_R \sigma^{(R)}, \quad (2)$$

where $\sigma^{(R)}$ is a cross section computed with the transition amplitude (1) containing the single term corresponding to the transition via the specific R-resonance (the direct non-resonant transition is also included in (2)).

The anisotropy parameters within the STAT model are calculated as quantities weighted over the $\sigma^{(R)}$. The equation for the β_{el} parameter is

$$\beta_{\mathrm{el}} = \sigma^{-1} \sum_R \beta_{\mathrm{el}}^{(R)} \sigma^{(R)}. \quad (3)$$

The formulae for A_{20} and O_{10} look similar. One should note that, in contrast to the step-wise model, the anisotropy parameters in the STAT model are energy dependent quantities.

Calculated intensities of the RA lines summed over the groups $4p^4(^1D)5p$ (left upper panel) or $4p^4(^1D)6p$ (right upper panel) are presented in Fig. 1 as functions of the exciting-photon energy. One can see that the interference of the R2 and R4 resonances manifests itself in both cases. The signs of the interference (constructive or destructive) are the same as obtained experimentally in [8], e.g., for the $4p^46p$ group interference is constructive between the R2 and R4 resonances