DOUBLE AUGER EFFECT IN THE MULTIPARTICLE PERTURBATION THEORY FRAMEWORK

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Within the framework of multiparticle perturbation theory (MPT), we investigate the correlation process of decay of an interior atomic vacancy accompanied by emission of two electrons simultaneously, i.e., the double Auger effect. In the lowest nonvanishing order of MPT, with respect to the interelectron interaction, expressions are obtained for calculation of the partial amplitudes and the probability of transitions in atoms with filled shells. Approximate formulas are discussed for the value of the probability in concrete transitions. Results are introduced and discussed for the numerical calculation of the double Auger transition $1s^{-1}\to 2s^{-2}2p^{-1}q_1q_2$ in Ne expressed in the Hartree–Fock basis of wave functions.

Usually the energy of a vacancy in a deep shell is much greater than the ionization potential of the external shells of a many-electron atom. Therefore as a result of its decay, emission is possible of not only one (usual Auger decay) but of two electrons – the double Auger decay. This was first detected in [1], where the charge spectrum of ions that form as a result of ionization of electron shells of Ne by Roentgen quanta ($\omega \sim 1.5$ keV) was investigated.

It was found that along with Ne^+ ions that formed under direct photoionization of the K and L shells, Ne^{+2} and Ne^{+3} ions also existed in the spectrum. Recording of Ne^+ ions is associated primarily with photoionization of the L-shell since formation of K-vacancies accompanies a high probability (~99% [2]) of Auger K–LL transitions. Radiative decay of 1s- or 2s-vacancies does not change the charge state of the ions. For the same reasons, the formation of double ions Ne^{+2} is caused primarily by K–LL transitions, since direct multiple ionization in the experiment carried out has low probability. The authors of the experiment associate the formation of ions of multiplicity greater than two (~25%) with two causes. A part of these ions (~2/3) forms as a result of "shakeoff" of outer-shell electrons by a sudden change in the self-consistent field of the atom under K-shell ionization, similar to the way this proceeds under β-decay of the nucleus [3]. The remaining part is caused by multielectron effects, namely, by the double Auger effect. Theoretical values realized in [1] gave qualitative agreement with experiment, although the quantitative result proved to be substantially too low.

We shall investigate the double Auger effect within the framework of multiparticle perturbation theory (MPT) in atoms with filled shells.

As a result of some process (photoionization, electron capture, etc.) let one electron be removed from an inner atomic shell i. It is possible that the energy released as a result of the filling of hole i with one of the outer-shell electrons goes to dislodge two other electrons (Fig. 1). The probability of such a process, i.e., of the double Auger transition $i\to f_1f_2f_3q_1q_2$, is nonzero only for calculation of the interelectron interaction. In the lowest nonvanishing order of perturbation theory in the Hartree–Fock basis of one-electron wave functions, the double Auger transition is described by the aggregate of Feynman diagrams shown in Fig. 2. Moreover, each of the diagrams represented, together with other time versions, implies three more exchanges.

A singularity of the double Auger effect is the possibility of arbitrary distribution of the transition energy $E = E_i - E_f$ (E_i and E_f are the initial and final energies of the ions) between two outgoing electrons q_1 and q_2. If we neglect the interaction between the

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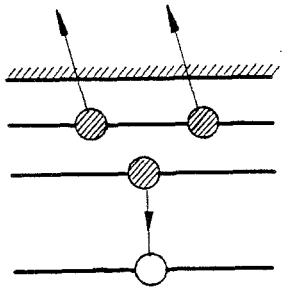

Fig. 1. Schematic representation of double Auger effect (the open circle is the original vacancy, the dark circles are the final vacancies).

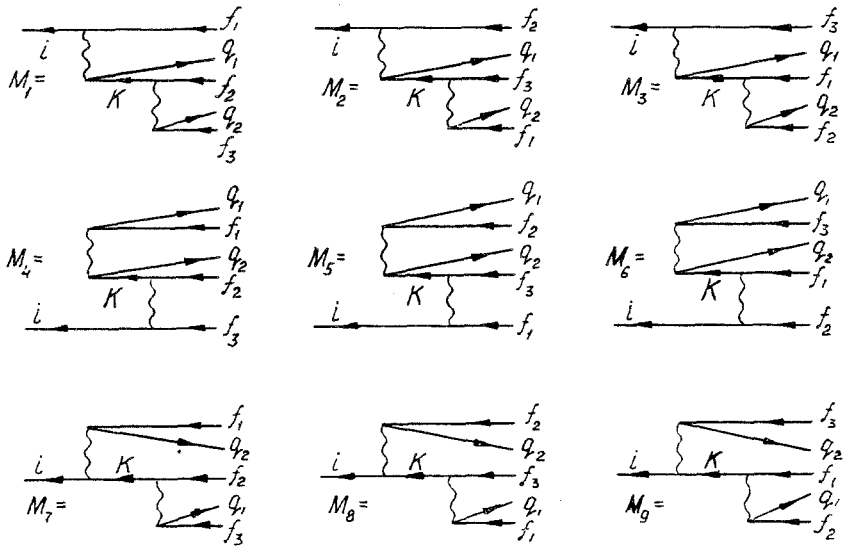

Fig. 2. Feynman diagrams of the double Auger effect. The straight lines with arrows to the left (right) denote propagation of holes (particles); the wavy lines denote the Coulomb interaction; the time increases from left to right.

Auger electrons, we get that the transition energy equals the sum of the energies of the outgoing electrons $E=\varepsilon_{q_1}+\varepsilon_{q_2}$.

The probability that the emitted electrons will have energy in the interval $(\varepsilon_{q_1}, \varepsilon_{q_1}+d\varepsilon_{q_1})$, $(\varepsilon_{q_2}, \varepsilon_{q_2}+d\varepsilon_{q_2})$ is determined by the expression

$$d\Gamma = 2\pi |M(\varepsilon_{q_1}, \varepsilon_{q_2})|^2 \delta(E-\varepsilon_{q_1}-\varepsilon_{q_2})\, d\varepsilon_{q_1} d\varepsilon_{q_2} \delta(E-E_i+E_f) \qquad (1)$$

($\hbar = m = e = 1$, energy in Ry), where $M(\varepsilon_{q_1}, \varepsilon_{q_2})$ is the probability density amplitude, equal to the sum of the partial amplitudes described by the diagrams in Fig. 2.

Final expressions for the partial amplitudes M_i, i= 1, 2, ..., 9, are suitable for numerical calculations of concrete transitions between states with vacancies in arbitrary shells i, f_1, f_2, f_3, obtained in the approximation of the LS-connection. The following order of composition of moments is chosen: $i[LS] \to f_1 f_2 [L_1 S_1] f_3 [L_2 S_2] q_1 [L_3 S_3] q_2 [L'S']$. These expressions contain angular and spin factors in the form of sums of products of 3j-, 6j-, and 9j-coefficients; because of inconvenience, it is not presented here [4]. Conditions under which the angular and spin factors are nonzero determine a selection rule in one-electron orbital and spin momenta, as well as in intermediate terms (L_1S_1), (L_2S_2), (L_3S_3). The selection rule in total orbital and spin momenta coincides with the general rules for nonradiative transitions: $L=L'$, $S=S'$, $M_L=M_L'$, $M_S=M_S'$. In particular, it turns out that for fixed electron configura-

tions and terms of the initial and final ions, the outgoing electrons can have a very wide (infinite) spectrum of values of orbital momenta. This complicates the calculation of the total probability of double Auger decay. However, in concrete transitions the determined physical arguments and model values permit us to avoid tedious calculations. These model approximations can be the following.

We assume first that the energy ratio of some partial amplitudes can vanish for an intermediate state $\kappa=\kappa_0>F$ of the continuous spectrum, for example, in M_4 for $\varepsilon_{\kappa_0} = \varepsilon_{f_2} + \varepsilon_{f_3} - \varepsilon_i$. The contribution of such a state determines the imaginary part of M_4

$$\operatorname{Im} M_4 = -\pi\left[<\kappa_0 i\,|\,r_{12}^{-1}\,|\,f_2 f_3 \times q_1 q_2\,|\,r_{12}^{-1}\,|\,f_1\kappa_0> + \text{exchange}\right].$$

If it dominates over contributions of other states, then we have the following value for the transition probability:

$$\Delta_1\Gamma = \Gamma_A^{(i)} \int_0^E \sigma_{\kappa f_1} d\varepsilon_\kappa, \tag{2}$$

where $\Gamma_A^{(i)}$ is the probability of transition $i\to f_2 f_3 \kappa_0$, accompanied by emission of a virtual Auger electron κ_0; $\sigma_{\kappa f_1}$ is the ionization cross-section of shell f_1 by electron κ_0.

Further, transitions are possible in which holes between the initial (i) hole and final (f_1, f_2, f_3) holes of the shell take immediate part. This occurs in the case when the energy ratio in some diagram vanishes for an intermediate hole state $\kappa = \bar{\kappa} \le F$. In order to calculate correctly the contribution of such a state to the transition probability, it is necessary to consider its total width $\Gamma_{\bar{\kappa}}$. For example, let this occur in diagram M_1. Then the contribution of state $\bar{\kappa}$ to the amplitude is determined by the expression

$$M_1(\kappa=\bar{\kappa}) = -i\,\frac{2}{\Gamma_{\bar{\kappa}}}\left[(\bar{\kappa} q_2\,|\,r_{12}^{-1}\,|\,f_2 f_3 \times i q_1\,|\,r_{12}^{-1}\,|\,f_1\bar{\kappa}> + \text{exchange}\right],$$

in which the matrix elements describe the amplitudes of successive (cascade) Auger transitions: 1) $i\to f_1\bar{\kappa} q_1$ and 2) $\bar{\kappa}\to f_2 f_3 q_2$. The contribution of the cascade mechanism to the probability density takes the form

$$\Delta_2\Gamma = \frac{2}{\pi}\int_0^E \frac{\Gamma_A^{(i)}\Gamma_A^{(\bar{\kappa})}}{\Gamma_{\bar{\kappa}}^2}\, d\varepsilon_{q_1}, \tag{3}$$

where $\Gamma_A^{(i)}$ and $\Gamma_A^{(\bar{\kappa})}$ are the probabilities of Auger decays 1 and 2. If the total width of vacancy $\bar{\kappa}$ is determined, in principle, its Auger width, i.e., $\Gamma_{\bar{\kappa}} \approx \Gamma_A^{(\bar{\kappa})}$, and furthermore, the integrand in (3) is small everywhere with the exception of a $\Gamma_{\bar{\kappa}}/2$-neighborhood of points $\varepsilon_1 = \varepsilon_{f_1} + \varepsilon_{\bar{\kappa}} - \varepsilon_i$ and $\varepsilon_2 = E - \varepsilon_1$, we obtain the value of the probability of a double Auger transition for the cascade mechanism of decay in the form

$$\Delta_2\Gamma = \frac{2}{\pi}\,\Gamma_A^{(i)}. \tag{4}$$

Thus, the probability of double Auger decay in this case can be equated to the probability of the usual Auger decay.

Finally, in some cases, in the amplitudes it is possible extract terms which can exceed others from the large values of the Coulomb integrals. Usually these are integrals containing two or more identical functions. As an example we shall take M_1 for $\kappa=f_2$, M_2 for $\kappa=f_1$, and M_9 for $\kappa=i$. Their contribution to the amplitude equals

$$\Delta_3 M = \{<iq_1\,|\,r_{12}^{-1}\,|\,f_1 f_2>\,|<f_2 q_2\,|\,r_{12}^{-1}\,|\,f_2 f_3> + <f_1 q_2\,|\,r_{12}^{-1}\,|\,f_1 f_3> -$$
$$- <iq_2\,|\,r_{12}^{-1}\,|\,if_3>]\}/(\varepsilon_{q_2} - \varepsilon_{f_3}) + \text{exchange} \approx (<iq_1\,|\,r_{12}^{-1}\,|\,f_1 f_2> -$$
$$- <iq_1\,|\,r_{12}^{-1}\,|\,f_2 f_1>)<\tilde{\tilde{q}}_2\,|\,\tilde{f}_3>,$$

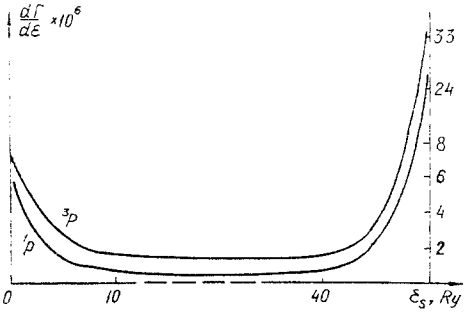

Fig. 3

where $<\tilde{\tilde{q}}_2|\tilde{f}_3>$ is the overlap integral between wave functions of Auger electron q_2 found in the field of an atom with two vacancies f_1 and f_2, and of hole f_3 found in the field of the initial vacancy i. The overlap is proportional to the change in the self-consistent field of the atom for Auger transition $i \to f_1 f_2 q_1$. Therefore the given approximation corresponds to the "shakeoff" model [1], in which a sudden change of the field for Auger decay of hole i with emission of a fast electron $q_1, \varepsilon_{q_1} \approx \varepsilon_{f_1} + \varepsilon_{f_2} - \varepsilon_i$, reduces with probability $\sim |<\tilde{\tilde{q}}_2|\tilde{f}_3>|^2$ to shakeoff of a second slow electron from shell f_3

$$\Delta_3 \Gamma = \Gamma_A^{(i)} \int_0^E |<\tilde{\tilde{q}}_2|\tilde{f}_3>|^2 d\varepsilon_{q_2}. \qquad (5)$$

The investigated approximations (2), (3), and (5) permit us on the basis of an analysis of the energy ratios and possible intermediate states to draw conclusions about the character of the energy spectrum of electrons emitted in concrete Auger transitions, and to obtain comparatively simply the probability values.

Concrete calculations with consideration of all diagrams of Fig. 2 are realized for transition $1s^{-1} \to 2s^{-2}2p^{-1}q_1q_2$ in a neon atom on the basis of a complex of programs [5, 6].

The wave functions of both Auger electrons are determined in the "frozen" framework field $2s^{-2}2p^{-1}$. Transition energy E = 50.512 Ry is calculated with consideration of the interaction of vacancies in the final state. This corresponds to calculation of specific classes of higher-order diagrams [7].

According to established selection rules, emitted pairs of electrons can have values of orbital momenta (lq_1, lq_2) equal to (0,1), (1,2), (2,3), etc. Calculated curves of the probability density that characterize the energy spectrum of the emitted electrons in transitions $1s^{-1} \to 2s^{-2}2p^{-1}q_s[^{1,3}P]q_p$ are presented in Fig. 3. They show that such a distribution of the transition energy is more probable between two Auger electrons for which one carries a large part of the energy and the other is slow. Moreover, the probability of emission of a slow p-electron is noticeably greater than of an electron with momentum $l=0$. The principal contribution in this region of energies (along the borders of the spectrum) is given by the "shakeoff" model, i.e., the q_s-electron is more likely to "shake off" from subshell $2s$ $(\sim |<\tilde{\tilde{q}}_s|\tilde{2s}>|^2)$, and q_p from the 2p subshell $(\sim |<\tilde{\tilde{q}}_p|\tilde{2p}>|^2)$. The cascade mechanism of transition is absent. The summed total probability of these transitions equals 0.342×10^{-2} eV, or 1.5% of the total width Γ_{1s} = 0.23 eV [2] of the 1s-hole. The value of the same probability in the "shakeoff" model (5) gives a much lower (by approximately a factor of 3) value, which agrees with the conclusions of [1].

An exact calculation of the transition probabilities accompanied by emission of other pairs of electrons has not been carried out. However, on the basis of the calculation of the previous transition and physical arguments based on approximate formulas (2)-(5), we can make the following estimates.

The principal contribution to the probability of decay is given by the region of small energies of one of the Auger electrons, where the "shakeoff" model works well. For decay of a 1s-hole in Ne, the electrons can shake off only from the 2s- or 2p-levels, whose wave functions enter into the overlap integral. From the resulting integrals only $<\tilde{\tilde{q}}_p|\tilde{2p}>$ can be

large enough, and the rest, i.e., $\langle\tilde{\tilde{q}}_d|\tilde{2s}\rangle$, $\langle\tilde{\tilde{q}}_d|\tilde{2p}\rangle$, $\langle\tilde{\tilde{q}}_f|\tilde{2s}\rangle$, $\langle\tilde{\tilde{q}}_f|\tilde{2p}\rangle$, etc. vanish for integration over the angular variables. Therefore, estimating the probability of transition $1s^{-1}\to 2s^{-2}2p^{-1}q_pq_d$ as $\approx 2/3\Gamma$ of transition $1s^{-1}\to 2s^{-2}2p^{-1}q_sq_p$, and the probabilities of transitions with emission of electrons having $l_q > 2$ as lower by an order of magnitude or more, we get an approximate value of the probability of double Auger decay of hole 1s to electron configuration $2s^{-2}2p^{-1}q_1q_2$ equal to 0.6×10^{-2} eV.

Assuming further that with roughly the same probability the double Auger decay of the 1s-hole reduces to configurations $2s^{-1}2p^{-2}q_1q_2$ and $2p^{-3}q_1q_2$, we get the value of the total width of the 1s-hole in Ne with respect to double Auger decay equal to 1.8×10^2 eV or ~7.8% of its total width.

This result characterizes part of the triple ions that form in the decay of the 1s-hole, and agrees sufficiently well with the values 8-10% obtained in experiment [1].

Thus, the conducted investigation shows that the processes of double Auger decay of vacancies contribute significantly to the formation of triple ions.

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