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RELATIVISTIC THEORY OF THE AUGER (AUTOIONIZATION) DECAY OF EXCITED STATES IN SPECTRA OF MULTICHARGED IONS

Relativistic method of calculating the characteristics of the Auger decay in the atomic spectra, based on the S-matrix Gell-Mann and Low formalism, is used for estimating the transition energies and autoionization probabilities in spectra of the Fe ion with one vacancy above the core $1s^22s^22p^63s^23p^6$.

1. The Auger decay is related to very key channel of decay of the excited atomic (molecular) states and attracts a great interest because of the importance for different applications in a plasma physics, physics of the ionized gases, quantum optics and photoelectronics [1–16]. When calculating the Auger decay characteristics it is usually used the two-step model [1–5]. Since the vacancy lifetime in an inner atomic shell is rather long (about 10^{-17} to 10^{-14}s), the atom ionization and the Auger emission are considered to be two independent processes. In the more correct dynamic theory of the Auger effect [1–5] the processes are not believed to be independent from one another. The fact is taken into account that the relaxation processes due to Coulomb interaction between electrons and resulting in the electron distribution in the vacancy field have no time to be over prior to the transition. In fact, a consistent Auger decay theory has to take into account correctly a number of correlation effects, including the energy dependence of the vacancy mass operator, the continuum pressure, spreading of the initial state over a set of configurations etc. [1–6]. Note that the effects are not described adequately to date, in particular , within the Auger decay theory [1–3]. One could remind that the inner shell excitation relaxes via resonant Auger electron or fluorescent photon emission. For example, the resonant Auger spectra of the halogens and noble gases were for the first time reported by Eberhardt *et al* and since then the resonant Auger spectra of noble gases have been studied extensively both experimentally and theoretically [1–8]. In particular, argon (chlorine) and corresponding like ions have attracted a lot of interest.

The most widespread theoretical studying is based on using the multi-configuration Dirac–Fock (MCDF) calculation [1–8]. The theoretical predictions based on MCDF calculations have been carried out within different approximations and remained hitherto non-satisfactory in many relations. Earlier [8–10] it has been proposed relativistic perturbation theory (PT) method of the Auger decay characteristics for complex atoms, which is based on the Gell-Mann and Low S-matrix formalism energy approach) and QED PT formalism [11–14]. The novel element consists in an using the optimal basis of the electron state functions derived from the minimization condition for the calibration-non-invariant contribution (the second order PT polarization diagrams contribution) to the imaginary part of the multi-electron system energy already at the first non-disappearing approximation of the PT [13]. Earlier it has been applied in studying the Auger decay characteristics for a set of neutral atoms, quasi-molecules and solids. Besides, the ionization cross-sections of inner shells in various atoms and the Auger electron energies in solids (*Na,Si etc*) were estimated. Here we will apply this approach to studying the autoionization decay probabilities in spectra of the multicharged ions on example of the Fe ion with one vacancy above the core $1s^22s^22p^63s^23p^6$.

2. Let us describe briefly the key aspects of the relativistic method to autoionization and Auger decay probabilities. Within the frame of PT approach [8,11,14] to the Auger effect description, the Auger transition probability and, accordingly, the Auger line intensity are

defined by the square of an electron interaction matrix element having the form:

$$V^{\omega}_{1234} = \left[(j_1)(j_2)(j_3)(j_4)\right]^{1/2} \times$$
$$\times \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathrm{Re}\, Q_{\lambda}(1234);$$
$$Q_{\lambda} = Q^{\mathrm{Qul}}_{\lambda} + Q^{\mathrm{Br}}_{\lambda}. \qquad (1)$$

The terms $Q^{\mathrm{Qul}}_{\lambda}$ and $Q^{\mathrm{Br}}_{\lambda}$ correspond to subdivision of the potential into Coulomb part $cos|\omega|r_{12}/r_{12}$ and Breat one, $cos|\omega|r_{12}\alpha_1\alpha_2/r_{12}$. The real part of the electron interaction matrix element is determined using expansion in terms of Bessel functions: :

$$\frac{\cos|\omega| r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \times$$
$$\times \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega| r_<) J_{-\lambda-1/2}(|\omega| r_>) P_{\lambda}(\cos \mathbf{r}_1 \mathbf{r}_2). \qquad (2)$$

where J is the 1st order Bessel function, $(\lambda)=2\lambda+1$. The Coulomb part $Q^{\mathrm{Qul}}_{\lambda}$ is expressed in terms of radial integrals R_{λ}, angular coefficients S_{λ} [4,11]:

$$\mathrm{Re}\,Q_\lambda^{\mathrm{Qul}} = \frac{1}{Z}\mathrm{Re}\left\{R_l\left(1243\right)S_\lambda\left(1243\right)+\right.$$
$$+R_\lambda\left(\tilde{1}24\tilde{3}\right)S_\lambda\left(\tilde{1}24\tilde{3}\right)+R_\lambda\left(1\tilde{2}4\tilde{3}\right)S_\lambda\left(1\tilde{2}4\tilde{3}\right)+$$
$$\left.+R_\lambda\left(\tilde{1}\tilde{2}4\tilde{3}\right)S_\lambda\left(\tilde{1}\tilde{2}4\tilde{3}\right)\right\}. \qquad (3)$$

As a result, the Auger decay probability is expressed in terms of $\mathrm{Re}Q_\lambda(1243)$ matrix elements :

$$\mathrm{Re}\,R_\lambda\left(1243\right)=$$
$$=\iint dr_1 r_1^2 r_2^2 f_1\left(r_1\right)f_3\left(r_1\right)f_2\left(r_2\right)f_4\left(r_2\right)Z_\lambda^{(1)}\left(r_<\right)Z_\lambda^{(1)}\left(r_>\right). \quad (4)$$

where f is the large component of radial part of single electron state Dirac function and function Z is :

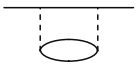
$$Z_\lambda^{(1)} = \left[\frac{2}{|\omega_{13}|\alpha Z}\right]^{\lambda+1/2}\frac{J_{\lambda+1/2}\left(\alpha|\omega_{13}|r\right)}{r^\lambda\Gamma\left(\lambda+3/2\right)}.$$

The angular coefficient is defined by standard way [8]. The other items in (3) include small components of the Dirac functions; the sign "~" means that in (3) the large radial component f_i is to be changed by the small g_i one and the moment l_i is to be changed by $\tilde{l}_i = l_i - 1$ for Dirac number $\varkappa_i > 0$ and l_i+1 for $\varkappa_i<0$. The Breat interaction is known to change considerably the Auger decay dynamics in some cases (c.f. [4]). The Breat part of Q is defined as the sum:

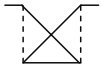
$$Q_\lambda^{\mathrm{Br}} = Q_{\lambda,\lambda-1}^{\mathrm{Br}} + Q_{\lambda,\lambda}^{\mathrm{Br}} + Q_{\lambda,\lambda+1}^{\mathrm{Br}}, \qquad (5)$$

where the contribution of our interest is determined as:

$$Q_\lambda^{\mathrm{Br}} = \frac{1}{Z}\mathrm{Re}\left\{R_\lambda\left(12\tilde{4}\tilde{3}\right)S_\lambda^l\left(12\tilde{4}\tilde{3}\right)+\right.$$
$$+R_\lambda\left(\tilde{1}\tilde{2}43\right)S_\lambda^l\left(1243\right)+R_l\left(\tilde{1}2\tilde{4}\tilde{3}\right)S_\lambda^l\left(\tilde{1}2\tilde{4}\tilde{3}\right)+$$
$$\left.+R_l\left(1\tilde{2}4\tilde{3}\right)S_\lambda^l\left(1\tilde{2}4\tilde{3}\right)\right\}. \qquad (6)$$

The Auger width is obtained from the adiabatic Gell-Mann and Low formula for the energy shift [13]. The contribution of the $\mathrm{A_d} =$  diagram to the Auger level width with a vacancy $n_\alpha l_\alpha j_\alpha m_\alpha$ is:

$$\sum_\lambda \frac{2}{(\lambda)(j_\alpha)}\sum_{\beta\gamma\le f}\sum_{k>f} Q_\lambda\left(\alpha k\gamma\beta\right)Q_\lambda\left(\beta\gamma k\alpha\right), \qquad (7)$$

while contribution of the $\mathrm{A_{ex}} =$  one is:

$$\frac{2}{(j_\alpha)}\sum_{\lambda_1\lambda_2}\sum_{\beta\gamma\le f}\sum_{k>f} Q_{\lambda_1}\left(\alpha k\gamma\beta\right)Q_{\lambda_2}\left(\beta\gamma k\alpha\right)\begin{Bmatrix} j_\alpha & j_\gamma & \lambda_2 \\ j_k & j_\beta & \lambda_1 \end{Bmatrix}. \quad (8)$$

The formulas (7),(8) define the full Auger level width. The partial items of the $\sum_{\beta\gamma}\sum_{k}$ sum answer to contributions of $\alpha^{-1}\to(\beta\gamma)^{-1}K$ channels resulting in formation of two new vacancies $\beta\gamma$ and one free electron k: $\omega_k=\omega_\alpha+\omega_\beta-\omega_\alpha$. The final expression for the width in the representation of jj-coupling scheme of single-electron moments has the form:

$$\Gamma(2j_1^o l_1^o, 2j_2^o l_2^o; J) = 2\sum_{j_k l_k}|\Gamma(2j_1^o l_1^o, 2j_2^o l_2^o; 1l_o, kjl)|^2 \quad (9)$$

Here the summation is made over all possible decay channels. The basis of electron state functions was defined by the solution of Dirac equation (integrated numerically using the Runge-Cutt method). The calculation of radial integrals $\mathbf{Re}R_\lambda(1243)$ is reduced to the solution of a system of differential equations [4]:

$$\left.\begin{aligned} y_1' &= f_1 f_3 Z_\lambda^{(1)}\left(\alpha|\omega|r\right)r^{2+\lambda}, \\ y_2' &= f_2 f_4 Z_\lambda^{(1)}\left(\alpha|\omega|r\right)r^{2+\lambda}, \\ y_3' &= \left[y_1 f_2 f_4 + y_2 f_1 f_3\right]Z_\lambda^{(2)}\left(\alpha|\omega|r\right)r^{1-\lambda}. \end{aligned}\right\} \qquad (10)$$

In addition, $y_3(\infty)=\mathbf{Re}R_\lambda(1243)$, $y_1(\infty)=X_\lambda(13)$. The system of differential equations includes also equations for functions $f/r^{|\varkappa|-1}$, $g/r^{|\varkappa|-1}$, $Z_\lambda^{(1)}$, $Z_\lambda^{(2)}$. The formulas for the auger decay probability include the radial integrals $R_\alpha(\alpha k\gamma\beta)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correct normalization of the function Ψ_k is a problem. The correctly normalized function should have the following asymptotic at $r\to0$ [4]:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to \left(\ddot{e}\dot{u}\right)^{-1/2}\begin{cases}\left[\grave{u}+\left(\acute{a}Z\right)^{-2}\right]^{-1/2}sin\left(kr+\ddot{a}\right), \\ \left[\grave{u}-\left(\acute{a}Z\right)^{-2}\right]^{-1/2}cos\left(kr+\ddot{a}\right).\end{cases} \qquad (11)$$

When integrating the master system, the function is calculated simultaneously:

$$N\left(r\right)=$$
$$=\left\{\pi\omega_k\left[f_k^2\left[\omega_k+\left(\alpha Z\right)^{-2}\right]+g_k^2\left[\omega_k+\left(\alpha Z^{-2}\right)\right]\right]\right\}^{1/2}.$$

It can be shown that at $r\to\infty$, $N(r)\to N_k$, where N_k is the normalization of functions f_k, g_k of continuous spectrum satisfying the condition (11).

The energy of an electron formed due to a transition jkl is defined by the difference between energies of an atom with a hole at the j level and double-ionized atom at kl levels in the final state:

$$E_A(jkl, {}^{2S+1}L_J) = E_A^+(j) - E_A^{2+}(kl, {}^{2S+1}L_J) \qquad (12)$$

To single out the above-mentioned correlation effects, the equation (12) can be presented as:

$$E_A(jkl, {}^{2S+1}L_J) = E(j) - E(k) - E(l) - \Delta(k,l; {}^{2S+1}L_J) \quad (13)$$

where the item Δ takes into account the dynamic correlation effects (relaxation due to hole screening with electrons etc.). Other details of the method and calculational procedure can be found in refs. [8–14].

3. Now let us describe some calculated data for the transitions energies and autoionization decay probabilities in the spectra of the multicharged ions on example of the Fe ion with one vacancy above the core $1s^22s^22p^63s^23p^6$. This ion of a great interest because of the high complexness of the spectrum and great actuality for astrophysical applications [4–7, 15,16]. As the final state of the studied system after autoionization decay is the three-quasiparticle, the general number of the decay channels is sufficiently large, so we are limited only by summarized probability of the autoionization decay for the state $1s^22s^22p^63s^23p^6$ with defi-

nite quantum numbers of vacancies n_1l_1 and n_2l_2. The detailed information about total number of channels is presented in ref. [17]. In table 1 we present values of the "i-f" transitions energies, calculated by us within ab initio QED PT, and also results of calculations within the MCDF (by Klapish et al), relativistic PT (RPT) with empirical zeroth approximation (by Ivanov et al) and available experimental data [12,15–17].

Table 1

The "i-f" transitions energies (in 10^2 cm^{-1}) , calculated within ab initio QED PT, MCDF and available experimental data.

N	i	f	Exp.[15]	MCDF	RPT	QED PT
1	$1s2s^22p^63s^23p$	$1s\ ^22s^22p^63s^2$	577000	577500	577200	577148
2	$1s2s^22p^63s^23p^2$	$1s\ ^22s^22p^63s^23p$	575700	576230	575910	575820
3	$1s2s^22p^63s^23p^3$	$1s\ ^22s^22p^63s^23p^2$	574400	575040	574940	574532
4	$1s2s^22p^63s^23p^4$	$1s\ ^22s^22p^63s^23p^3$	573400	573920	574360	573937
5	$1s2s^22p^63s^23p^5$	$1s\ ^22s^22p^63s^23p^4$	572400	572860	573520	572845
6	$1s2s^22p^63s^23p^6$	$1s\ ^22s^22p^63s^23p^5$	571430	571886	572550	572124

Analysis of the data in table 1 allow to make the following conclusions. Firstly, the accurate account of the complicated inter-electron (vacancy) correlations plays a critical role not only for acceptable quantitative agreement between theory and experiment, however, it is of the principal importance for right interpretation of the corresponding transitions in the spectra. Secondly, the presented in ref.[15] interpretation of the experimental highly ionized iron spectra, probably, is not fully correct because of the high complexness these spectra and, besides, using the DF calculation results for the corresponding interpretation. In fact in our opinion, the experimental data, in particular, for the "5" and "6" transitions (see table 1) are probably not correct and corresponding to other transitions. The difference between the RPT and QED PT data is connected with using the a little different basises of the relativistic wave functions. In our ab initio approach calculation it has been used the QED method [13]. In refs. [12,16] it has been used the empirical zeroth approximation, which naturally accounts for the main (not all) part of the inter-particle correlations contribution. In the table 2 we listed the values for probabilities of decay of the FeX states with vacancy $1s_S$, obtained within our approach (QED PT) with using the optimized basises (OB) of the one-quasiparticle wave functions and calculation data within the RPT with empirical zeroth approximation (without optimization of basises (WOB) of the wave functions) [12].

Table 2

Probabilities of decay of the FeX states with vacancy $1s_S$: QED PT –OB (A- our data); RPT-WOB (B) [12].

	n_2l_2			
method	A B	A B	A B	A
n_1l_1	2s	2p	3s	3p
2s	399+14 42+14	131+14 14+15	130+14 14+14	198+14
2p		264+15 28+15	158+14 17+14	722+14
3s			834+12 90+12	243+13
3p				612+13

Note: the mantissa and decimal order of value are given: $42+14=0.42\cdot10^{14}$;

The analysis of the presented data in the table 2 shows that our results are less than the corresponding data from ref. [12,16] at ~5%. This fact can be explained by using the specially optimized basises of the one-quasiparticle wave functions (it is in fact corresponding to degree of account for the multi particle exchange-correlation effects) in our scheme. In refs. [12,16] it had been used the formalism of relativistic PT with the empirical zeroth approximation, and optimization of the one-quasi-particle wave functions basises is not specially fulfilled, though using the empirical information about corresponding one-quasiparticle atomic ion allows indirectly take into account the correlation corrections. The great experience of using the relativistic QED perturbation theory [4,6,11–14] shows that the basis optimization, as a rule, improves averagely the atomic parameters values at 5–20%. Earlier an application of our scheme to studying the Auger decay characteristics for a set of neutral atoms, quasi-molecules and solids, the ionization cross-sections of inner shells in various atoms etc has demonstrated a reasonably well agreement with available sufficiently exact experimental data. So, we believe that the received results should be considered as quite acceptable and very useful for many applications. At last, it is obvious that the further experimental studying of the corresponding spectra is of a great importance.

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RELATIVISTIC THEORY OF THE AUGER (AUTOIONIZATION) DECAY OF EXCITED STATES IN SPECTRUM OF MULTICHARGED ION

Abstract.
Relativistic method of calculating the characteristics of the Auger decay in the atomic spectra, based on the S-matrix Gell-Mann and Low formalism and QED perturbation theory, is used for estimating the transition energies and autoionization probabilities in spectra of the Fe ion with one vacancy above the core $1s^22s^22p^63s^23p^6$.
Key words: autoionization decay, multicharged ion, relativistic theory

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РЕЛЯТИВИСТСКАЯ ТЕОРИЯ ОЖЕ (АВТОИОНИЗАЦИОННОГО) РАСПАДА ВОЗБУЖДЕННЫХ СОСТОЯНИЙ В СПЕКТРЕ МНОГОЗАРЯДНОГО ИОНА

Резюме.
Релятивистский метод расчета характеристик Оже распада в атомных спектрах, который основывается на S-матричном формализме Гелл-Мана и Лоу и КЭД теории возмущений, использован для оценки энергий переходов вероятностей автоионизационного распада в спектре иона Fe с одной вакансией над остовом $1s^22s^22p^63s^23p^6$.
Ключевые слова: автоионизационный распад, многозарядный ион, релятивистская теория

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РЕЛЯТИВІСТСЬКА ТЕОРІЯ ОЖЕ (АВТОІОНІЗАЦІЙНОГО) РОЗПАДУ ЗБУДЖЕНИХ СТАНІВ У СПЕКТРІ БАГАТОЗАРЯДНОГО ІОНУ

Резюме.
Релятивістський метод розрахунку характеристик Оже розпаду в атомних спектрах, який базується на S-матричному формалізмі Гелл-Мана та Лоу і КЕД теорії збурень, використано для оцінки енергій переходів та ймовірностей авто іонізаційного розпаду в спектрі іону Fe з однією вакансією над остовом $1s^22s^22p^63s^23p^6$.
Ключові слова: автоіонізаційний розпад, багатозарядний іон, релятивістська теорія