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CASCADE OF AUGER TRANSITIONS IN SPECTRUM OF XENON: THEORETICAL DATA

The energy parameters of the Auger transitions for the xenon atomic system are calculated within the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order density functional approximation. The results are compared with reported experimental data as well as with those obtained by semiempirical method. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory zeroth order that significantly provides a physically reasonable agreement between theory and experiment.

1. Introduction

Development of the novel experimental methods in a modern Auger- spectroscopy allows to open new interesting features especially for the heavy complex atomic systems. It is easily to understand that a synchrotron radiation sources provide an effective way to ionize deep core hole States in heavy multielectron systems (e.g. [1]). As result, new advanced data on the energy and spectral parameters of the complex atomic systems can be obtained.

Let us remind following to ref . [2] that studies in modern atomic physics (spectroscopy, spectral lines theory, theory of atomic collisions etc), astrophysics, plasma physics, laser physics and quantum and photo-electronics requires an availability of sets of correct data on the energetic, spectroscopic and structural properties of atoms, including the data on the Auger transitions [1-8]. The kinetic energy of the ejected Auger electron is measured by Auger-electron spectroscopy (AES). Sensing the Auger spectra in atomic systems and solids gives the important data for the whole number of scientific and technological applications. So called two-step model is used most widely when calculating the Auger decay characteristics [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 [2,3] 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 [1-19]. The most widespread theoretical studying the Auger spectra parameters is based on using the multi-configuration Dirac-Fock (MCDF) calculation [2,3]. The theoretical predictions based on MCDF calculations have been carried out within different approximations and remained hitherto non-satisfactory in many relations. Earlier [8-13] 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 [4-7]. The novel element consists in 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. 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 were estimated. Here we apply the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order density functional approximation is applied to determination of the energy parameters of the Auger transitions of the xenon atomic system.

2. The theoretical method

In Refs. [2, 8-17] the fundamentals of the relativistic many-body PT formalism have been in detail presented, so further we are limited only by the key elements, following the cited Refs. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In Refs. [2-13, 19-38] there is realized field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix M diagonalization. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the M. The complex secular matrix M is represented in the form [2,9,10]:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \quad (1)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}, M^{(3)}$ those of the one-, two- and three-QP diagrams respectively. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent 1QP contributions. The optimized 1-QP representation is the best one to determine the zeroth approximation. In the relativistic energy approach [4-9], which has

received a great applications during solving numerous problems of atomic, molecular and nuclear physics (e.g., see Refs. [10-13]), the imaginary part of electron energy shift of an atom is directly connected with the radiation decay possibility (transition probability). An approach, using the Gell-Mann and Low formula with the QED scattering matrix, is used in treating the relativistic atom. The total energy shift of the state is usually presented in the form:

$$\Delta E = Re\Delta E + i\,\Gamma/2\,, \quad (2)$$

where Γ is interpreted as the level width, and the decay possibility $P = \Gamma$. The imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as [4]:

$$Im\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V_{\alpha n\alpha n}^{|\omega_{\alpha n}|}\,, \quad (3)$$

where $(\alpha>n>f)$ for electron and $(\alpha<n<f)$ for vacancy. Under calculating the matrix elements (3) one should use the angle symmetry of the task and write the expansion for potential $\sin|\omega|r_{12}/r_{12}$ on spherical functions as follows [4]:

$$\frac{\sin|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0}^{\infty} (\lambda) J_{\lambda+\frac{1}{2}}(|\omega|r_1).$$
$$\cdot J_{\lambda+\frac{1}{2}}(|\omega|r_1) J_{\lambda+\frac{1}{2}}(|\omega|r_2) P_\lambda(\cos r_1 r_2) \quad (4)$$

where J is the Bessel function of first kind and $(\lambda)= 2\lambda + 1$. This expansion is corresponding to usual multipole one for probability of radiative decay.

Within the frame of QED PT approach the Auger transition probability and the Auger line intensity are defined by the square of an electron interaction matrix element having the form [4]:

$$V_{1234}^\omega = [(j_1)(j_2)(j_3)(j_4)]^{\frac{1}{2}} \sum_{\lambda\mu} (-1)^\mu \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times Re\, Q_\lambda(1234);$$

$$Q_\lambda = Q_\lambda^{\text{Qul}} + Q_\lambda^{\text{Br}} \cdot \qquad (5)$$

The terms Q_λ^{Qul} and Q_λ^{Br} 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:

$$\frac{cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda) J_{\lambda+1/2}(|\omega|r_<) J_{-\lambda-1/2}(|\omega|r_>) P_\lambda(\cos \mathbf{r_1 r_2}) \qquad (6)$$

where J is the 1$^{\text{st}}$ order Bessel function, $(\lambda)=2\lambda+1$.

The Coulomb part Q_λ^{Qul} is expressed in terms of radial integrals R_λ, angular coefficients S_λ [4]:

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

$$\left. + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\,\tilde{2}\,\tilde{4}\,\tilde{3})S_\lambda(\tilde{1}\,\tilde{2}\,\tilde{4}\,\tilde{3})\right\} \qquad (7)$$

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

$$\text{Re}\,R_\lambda(1243) = \iint dr_1 r_1^2 r_2^2 f_1(\eta)f_3(\eta)f_2(r_2)f_4(r_2)Z_\lambda^{(1)}(r_<)Z_\lambda^{(1)}(r_>) \qquad (8)$$

where f is the large component of radial part of single electron state Dirac function; function Z and angular coefficient are defined in Refs. [4-7]. The other items in (7) include small components of the Dirac functions; the sign «~» means that in (7) 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 æ$_1 > 0$ and l_i+1 for æ$_i < 0$. The Breat part of Q is defined in [4,11]. The Auger width is obtained from the adiabatic Gell-Mann and Low formula for the energy shift [4].

The direct contribution to the Auger level width with a vacancy $n_\alpha l_\alpha j_\alpha m_\alpha$ is as follows:

$$\sum_\lambda \frac{2}{(\lambda)(j_\alpha)} \sum_{\beta\gamma \le f}\sum_{k > f} Q_\lambda(\alpha k\gamma\beta)Q_\lambda(\beta\gamma k\alpha), \qquad (9)$$

while the exchange diagram contribution is:

$$\frac{2}{(j_\alpha)} \sum_{\lambda_1\lambda_2}\sum_{\beta\gamma \le f}\sum_{k > f} Q_{\lambda_1}(\alpha k\gamma\beta)Q_{\lambda_2}(\beta\gamma k\alpha)\begin{Bmatrix} j_\alpha & j_\gamma & \lambda_2 \\ j_k & j_\beta & \lambda_1 \end{Bmatrix} \cdot \qquad (10)$$

The partial items of the $\sum\limits_{\beta\gamma}\sum\limits_k \widehat{}$ sum answer to contributions of $\alpha^{-1} \rightarrow (\beta\gamma)^{-1}K$ channels resulting in formation of two new vacancies $\beta\gamma$ and one free electron k: $\omega_k = \omega_\alpha + \omega_\beta - \omega_\alpha$.

The calculating of all matrix elements, wave functions, Bessel functions etc is reduced to solving the system of differential equations. The formulas for the autoionization (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 wave functions is very important, namely, they should have the following asymptotic at $r \rightarrow 0$:

$$\left.\begin{array}{c} f \\ g \end{array}\right\} \rightarrow (\lambda\omega)^{-1/2}\left\{\begin{array}{l} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} sin(kr + \delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} cos(kr + \delta). \end{array}\right. \qquad (12)$$

The important aspect of the whole procedure is an accurate accounting for the exchange-correlation effects. We have used the generalized relativistic Kohn-Sham density functional [8-17] in the zeroth approximation of relativistic PT; naturally, the perturbation operator contents the operator (7) minus the cited Kohn-Sham density functional. Further the wave functions are corrected by accounting of the first order PT contribution. Besides, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which is reduced to minimization of the gauge dependent multielectron contribution $Im\Delta E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels.

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

$$E_A(jkl, {}^{2S+1}L_J) = E_A^+(j) - E_A^{2+}(kl, {}^{2S+1}L_J)$$
(13)

To single out the above-mentioned correlation effects, the equation (13) can be presented as [8,9]:

$$E_A(jkl, {}^{2S+1}L_J) = E(j) - E(k) - E(l) - \Delta(k,l; {}^{2S+1}L_J),$$
(14)

where the item Δ takes into account the dynamic correlation effects (relaxation due to hole screening with electrons etc.) To take these effects into account, the set of procedures elaborated in the atomic theory [8-13] is used. All calculations are performed on the basis of the modified numeral code Superatom (version 93).

3. Results and conclusion

Below the energy parameters of the Auger transitions for the xenon are presented and compared with the experimental data as well as with those obtained by semiempirical and perturbation theory methods. In table 1 we present data on the initial and final states of the most intense $4d^{-2}\rightarrow4d^{-1}5p^{-2}$ and $4d^{-1}5p^{-2}\rightarrow5p^{-}4$ Auger transitions in the neutral xenon.

Our theoretical data (the relativistic many-body PT) and the theoretical semiempirical data by Jonauskas et al [1], and relativistic perturbation theory data [9] for the energies of the Auger transitions are also given.

The analysis of the presented results in table 1 results in the conclusions that the précised description of the Auger processes requires the detailed accurate accounting for the exchange-correlation effects, including the particle-hole interaction, screening effects and iterations of the mass operator.

Table 1. Calculated and experimental energies of the Auger transitions E_k for Xe (see text)

Initial state	Final state	E_{th} [1]	E_{th}, [9]	E_{th}, our	E_{ex} [1]
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^1D) $^2F_{5/2}$	31.5	31.3	31.2	
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^3P) $^2F_{7/2}$	31.2	31.0	30.9	30.8
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^1D) $^2G_{9/2}$	30.9	30.6	30.5	
$4d^{-2}$ $^1D_2$	$4d^{-1}5p^{-2}$ (^3P) $^2D_{5/2}$	30.5	30.3	30.2	30.3
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^3P) $^2D_{3/2}$	30.1	30.0	29.9	29.9
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^1D) $^2D_{5/2}$	29.3	29.2	29.1	
$4d^{-2}$ $^1D_2$	$4d^{-1}5p^{-2}$ (^1D) $^2F_{7/2}$	29.1	29.1	29.0	29.1
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^1D) $^2F_{7/2}$	29.1	29.1	29.1	
$4d^{-2}$ $^3F_4$	$4d^{-1}5p^{-2}$ (^3P) $^4F_{9/2}$	29.1	29.1	29.1	
$4d^{-2}$ $^3F_4$	$4d^{-1}5p^{-2}$ (^3P) $^4F_{5/2}$	28.4	28.3	28.2	
$4d^{-2}$ $^3F_4$	$4d^{-1}5p^{-2}$ (^3P) $^2F_{5/2}$	28.1	28.0	28.2	28.3
$4d^{-2}$ $^1G_4$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{5/2}$	27.8	27.8	27.8	27.9
$4d^{-2}$ $^3F_2$	$4d^{-1}5p^{-2}$ (^1D) $^2G_{9/2}$	27.4	27.3	27.2	27.1
$4d^{-2}$ $^3P_1$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{5/2}$	27.0	26.9	26.8	
$4d^{-2}$ $^3F_4$	$4d^{-1}5p^{-2}$ (^3P) $^2F_{5/2}$	26.5	26.5	26.4	26.5
$4d^{-2}$ $^1D_2$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{3/2}$	26.1	26.2	26.1	
$4d^{-2}$ `$^1G_4$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{3/2}$	26.1	26.2	26.1	
$4d^{-2}$ $^3P_2$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{5/2}$	25.9	26.0	25.9	
$4d^{-2}$ $^3F_4$	$4d^{-1}5p^{-2}$ (^1D) $^2G_{9/2}$	25.6	25.9	25.8	-
$4d^{-2}$ $^3F_2$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{5/2}$	24.3	24.6	24.6	24.7
$4d^{-2}$ $^3F_4$	$4d^{-1}5p^{-2}$ (^1S) $^2D_{5/2}$	22.5	22.9	22.8	

The relativistic many-body PT approach provides physically reasonable results in comparison with the fine experimental results due to a considerable extent to more correct accounting for complex inter electron exchange-correlation effects. It is important to note that using more correct gauge-invariant procedure of generating the relativistic orbital bases in the zeroth approximation of the consistent relativistic perturbation theory is directly connected with correctness of accounting for the exchange-correlation effects. The further theoretical progress can be reached by the next refinement of theoretical procedure.

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Key words: relativistic theory, Auger spectroscopy, xenon

Чернышев А.С., Ефимова Е.А., Буяджи В.В.. Никола Л.В.

КАСКАД ОЖЕ-ПЕРЕХОДОВ В СПЕКТРЕ КСЕНОНА: ТЕОРЕТИЧЕСКИЕ ДАННЫЕ

Резюме. Энергетические параметры оже-переходов для атомной системы ксенона рассчитаны в рамках комбинированного релятивистского энергетического подхода и релятивистской многочастичной теории возмущений с приближением функционала плотности нулевого порядка. Результаты сравниваются с экспериментальными результатами, а также с полуэмпирическими теоретическими данными. Важный момент связан с учетом вкладов сложных многочастичных обменных корреляционных 'ффектов и использованием оптимизированного одноквазичастичного представления в нулевом приближении многочастичной теории возмущений, что определяет физически разумное согласие между теорией и экспериментом.

Ключевые слова: релятивистская теория, Оже-спектроскопия, ксенон

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КАСКАД ОЖЕ-ПЕРЕХОДІВ В СПЕКТРІ КСЕНОНА: ТЕОРЕТИЧНІ ДАНІ

Резюме. Енергетичні параметри оже-переходів для атомної системи ксенону обчислені на основі комбінованого релятивістського енергетичного підходу і релятивістської багаточастинкової теорії збурень з наближенням функціонала щільності нульового порядку. Результати порівнюються з експериментальними результатами, а також з напівемпіричними дтеоретичними даними. Важливий момент пов'язаний з урахуванням вкладів складних багаточасткових обмінних кореляційних ефектів та з використанням оптимізованого одноквазічастічного уявлення в нульовому наближенні релятивістської багаточастинкової теорії збурень, що визначає фізично певну згоду між теорією і експериментом.

Ключові слова: релятивістська теорія, Оже-спектроскопія, ксеон.