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RELATIVISTIC APPROACH TO THE RECOIL INDUCED EXCITATION AND IONIZATION OF IONS DURING CAPTURE OF NEUTRON

The relativistic energy approach is adapted to description of the recoil-induced excitation and ionization in atoms due to a neutron capture. The data for transition probabilities to different electronic states, induced by a neutron capture, are presented for some ions.

The paper is devoted to carrying out new adequate consistent relativistic approach to the recoil-induced excitation and ionization in atoms and ions due to the neutron capture and alpha-particle. In last years a development of methods of the laser spectroscopy allowed observing and further using the little changes in structure of atomic and molecular spectra resulted from the corresponding alteration of the internal state of a nucleus or because of the cooperative neutron-electron-gamma-nuclear processes, including the neutron capture [1–20]. The neutron capture phenomenon is responsible for complicated and rich physics of the different excitation and ionization processes in the electron shells of the atoms and ions [1–8]. The first references to the neutral recoil are originated from the known classical papers by Migdal and Levinger (look the detailed description of the history and corresponding models in refs. [1,2]), who evaluated approximately the ionization of an atom undergoing a sudden recoil in due to neutron impact and in a radioactive disintegration respectively. Gol'dansky-Letokhov-Ivanov have estimated an influence of the electron shell on velocity of recharging the metastable nucleus during the muon and neutron capture within simple qualitative models [2,3] and found the cited effect to be very small. The neutral recoil situation differs radically from processes involving a charged particle for which the sudden recoil approximation is often invalid (look, for example, refs. [1–3, 10–14]). An attractive situation arises under the transition to heavy multicharged ions because of changing the energy and geometric parameters of the electron shell. The character of interaction with a nucleus may change strongly, opening new channels of electron-nuclear processes [7–9]. Such effects as the electron-positron pair production (during the nucleus recharging) etc. are added to traditional channels of the nucleus excited state decay Here one could mention the processes of capture of neutron or alpha particle by atom or ion [1,2,4]. It is easily imagine a situation when this process becomes by energetically possible only after removal of the strongly bound electron in the initial state. It is known that it's possible the transfer of part of a nuclear energy to the atom or molecule electron shells under radiating (absorption) the γ quanta by a nucleus.

The different simple models (look, for example, refs. [1–4, 5–9,13–19]) were developed to evaluate the different cooperative processes channels, in particular, excitation or ionization of an atom, the electronic redistribution of an atom induced a sudden recoil of its nucleus occurring when a neutral particle is either emitted (γ-radioactivity) or captured (neutron capture for instance). The consistent QED approach to cited processes has been developed in refs. [9–12,19–21].

Here we adapt a relativistic energy approach [10,11,19–22] to the recoil-induced excitation and ionization in atoms (ions) due to the neutron capture. As method of calculation of the correlated electron wave functions, we use the QED perturbation theory (PT) on inter electron interaction [24–27].

Let us describe the key moments for the quantum approach to the recoil-induced excitation and ionization in atoms due to some particle capture [11–13]. The initial state of system being a discrete state, it is clear that two phenomena can occur after the momentum transfer to the final nucleus: an excitation to a final discrete state of the daughter system or an ionization, the final state lying in the continuum. The transition amplitude matrix element is given by the overlap between initial state (nuclear charge Z) and final state (nuclear charge Z') in a Galilean boost of velocity $\boldsymbol{v}$. The overlap in the momentum space is as follows:

$$\int d\vec{p}\ \Phi_i(\vec{p},Z)\Phi_f^*(\vec{p}+\vec{k},Z') \tag{1}$$

where subscript i, f represent the set of quantum numbers of the initial and final states and $\hbar\boldsymbol{k}=m\boldsymbol{v}$ is the recoil momentum of electron accompanying the resulting nucleus and having kinetic energy equal to $(ka_0)^2Ry$. The energy E_R of the recoiling nucleus of mass M_R is:

$$E_R=\frac{M_R}{m_e}(k\,a_0)^2R_{yd} \tag{2}$$

The function $\Phi_i(\vec{p},Z)$ is related to the function $\Psi_i(r,Z)$ as:

$$\Phi_i(\vec{p},Z)=(2\pi)^{-\frac{3}{2}}\int d\vec{r}e^{-i\vec{p}\cdot\vec{r}}\Psi_i(\vec{r},Z) \tag{3}$$

So, using these relations the overlap is defined by:

$$b_{if}=\int d\vec{r}\quad \Psi_i(\vec{r},Z)e^{-i\vec{k}\cdot\vec{r}}\Psi_f^*(\vec{r},Z') \tag{4}$$

The probability of populating state f starting from state i is given by $P_{if}=|b_{if}|^2$. As we are dealing in multielectron systems, one can write the wave function of system as:

$$\psi(\gamma LSM_L M_S)=\sum_i a_i\Phi(\gamma_i LSM_L M_S) \quad (5)$$

The extension of eq.(4) to two-electron system is:

$$b_{if}=\int d\vec{r}_1\int d\vec{r}_2\Psi_i(\vec{r}_1;\vec{r}_2;Z)e^{-ik(z_1+z_2)}\Psi_f^*(\vec{r}_1,\vec{r}_2;Z') \quad (6)$$

where the Oz-axis of the coordinate system is chosen along the $\boldsymbol{k}$ direction. The two-electron recoil operator $R=exp[-ik(z_1+z_2)]$ matrix element between the correlated electronic wave functions of the form (5) is written in standard form [1,22]:

$$(\overline{\Psi}(\gamma' L'S'M_S^{/})\,|\,R\,|\,\Psi(\gamma LSM_L M_S))=$$
$$=(\Psi(\gamma LSM_L M_S)\,|\,R^*\,|\,\overline{\Psi}(\gamma' L'S'M_L^{/}M_S^{/}))=$$
$$=\sum_{i,j}a_i^*\overline{a}_j\left\langle\Phi(\gamma_i LSM_L M_S)\,|\,R^*\,|\,\overline{\Phi}(\gamma_j L'S'M_L^{/}M_S^{/})\right\rangle \quad (7)$$

It could be reduced to the direct and exchange contributions:

$$\frac{1}{\sqrt{(1+\delta_{\rho_a l_a\rho_b l_b})(1+\delta_{\rho_c l_c\rho_d l_d})}}\times$$
$$\times\,[R\,(ab,\,cd)+(-1)^{la+lb-L-S}\,R(ba,\,cd)] \quad (8)$$

where $R(ij\,,\,rt)\equiv\langle\,(\rho_i\,l_i\,)_1\,(\rho_j l_j)_2 LSM_L\,M_S\,|R^*\,|$
$\overline{(\rho_r l_r)_1(\rho_l l_l)_2 L'S'M_L^{/}M_S^{/}}\rangle$

The plane wave function development can be used for each one-electron recoil operator:

$$R=e^{-ik(z_1+z_2)}=\sum_{l,l'=0}^{\infty}(-i)^{l+l'}(2l+1)(2l'+1)\times$$
$$\times j_l(kr_1)j_{l'}(kr_2)C_0^{(l)}(1)C_0^{(l')}(2) \quad (9)$$

where $C_m^{(l)}=\sqrt{(4\pi)/(2l+1)}Y_{lm}$. The one-electron reduced matrix element brings some simplification taking the target in its ground state $1s^{21}S$:

$$\langle(\rho_i l_i)_1(\rho_j l_j)_2{}^1S_{00}\,|\,R^*\,|\,\overline{(\rho_r l_r)_1(\rho_l l_l)_2{}^1L_{00}^{/}}\rangle=(-1)^{lr-ll}$$
$$\sqrt{2L'+1}\sum_{l,l'}^{\infty}i^{l+l'}(2l+1)(2l'+1)\sum_{m=-l_{\min}}^{+l_{\min}}(l_i\,\|\,C^{(l)}\,\|\,l_r)(l_j\,\|\,C^{(l')}\,\|\,l_l)$$
$$\times\begin{pmatrix}l_i & l_j & 0\\ m & -m & 0\end{pmatrix}\begin{pmatrix}l_r & l_l & L'\\ m & -m & 0\end{pmatrix}\begin{pmatrix}l_i & l & l_r\\ -m & 0 & m\end{pmatrix}$$
$$\begin{pmatrix}l_j & l' & l_l\\ m & 0 & -m\end{pmatrix}$$
$$\times\int_0^{\infty}drP_{\rho_r l_r}(r)j_l(kr)\overline{P_{\rho_r l_r}}(r)\quad\int_0^{\infty}drP_{\rho_l l_j}(r)j_{l'}(kr)\overline{P_{\rho_l l_l}}(r) \quad (10)$$

All notations in eq. (10) are standard. The matrix element on correlated electron functions is calculated according to the formula:

$$\sum_{f,i}|<\Psi_f\,|\,R\,|\,\Psi_i>|^2=\sum_{f_1,f_2}|<\Phi_{f1f2}\,|\,R\,|\,\Phi_{i1i2}>+$$
$$+\sum_{n_1n_2}\frac{<\Phi_{f1f2}\,|\,V\,|\,\Phi_{n1n2}><\Phi_{n1n2}\,|\,R\,|\,\Phi_{i1i2}>}{E_{n_1n_2}^0-E_{f_1f_2}^0}+\ldots \quad (11)$$

where E^0 and Φ are the eigen values and eigen functions of the Coulomb hamiltonian, V is operator of the electrostatic interaction between electrons; its matrix elements are equal to difference between direct and exchange integrals. Such an approach allows accounting for the inter-electron correlation in the initial and final states with high degree of accuracy. [25–27].

It should be strictly noted that, generally speaking, the presented above formulas are acceptable for treating the non-relativistic atomic systems (say, hydrogen, helium etc). Consistent and qualitatively adequate description of the cooperative processes in multicharged ions (essentially relativistic systems) requires using the the QED formalism, in particular, the relativistic energy approach, based on the S-matrix Gell-Mann and Low formalism and QED PT (the basises are in details presented in refs. [10,11,19], look standard QED [20–23]). To calculate transition amplitude it is necessary to use the basis's of the correlated relativistic Dirac bi-spinors. To construct such basis we use formalism of the QED PT on the inter-electron interaction [9,21,24].

In the QED PT the matrix elements of the interaction operator between two-electron states give the standard contribution of the first order (energy matrice M):

$$M_1^{(2)}=\left\langle n_1l_1j_1\quad n_2l_2j_2\,[J]\right|V_{\rm int}\left|n_4l_4j_4\quad n_3l_3j_3\,[J]\right\rangle=$$
$$=P_1P_2(-1)^{1+j_2+j_4+J}\times$$
$$\times\left[(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)\right]^{1/2}\times$$
$$\times\sum_{i,k}\sum_a\begin{Bmatrix}j_ij_kJ\\ j_2j_1a\end{Bmatrix}\left(\delta_{i,3}\delta_{k,4}+(-1)^J\,\delta_{i,4}\delta_{k,3}\right)Q_a \quad (12)$$

where, as usually, $P_1=\begin{cases}1 & \text{for}\quad n_1l_1j_1\neq n_2l_2j_2\\ 1/2 & \text{for}\quad n_1l_1j_1=n_2l_2j_2\end{cases}$,

$$P_2=\begin{cases}1 & \text{for}\quad n_3l_3j_3\neq n_4l_4j_4\\ 1/2 & \text{for}\quad n_3l_3j_3=n_4l_4j_4\end{cases}$$

The variable Q_a ($Q_\lambda=Q_\lambda^{\rm Qul}+Q_\lambda^{\rm Br}$) contains the Coulomb and Breit parts and is standardly expressed through the radial integrals R_λ and angle coefficients S_λ., The detailed expressions can be found, for example, in ref. [24]. In particular, one could write for the Coulomb part (in the Coulomb units)

$$Q_\lambda^{\rm Qul}=\frac{1}{Z}\left\{R_l(1243)S_\lambda(1243)+R_\lambda\left(\tilde{1}24\tilde{3}\right)S_\lambda\left(\tilde{1}24\tilde{3}\right)\right.$$
$$\left.+R_\lambda\left(1\tilde{2}\tilde{4}3\right)S_\lambda\left(1\tilde{2}\tilde{4}3\right)+R_\lambda\left(\tilde{1}\tilde{2}\tilde{4}\tilde{3}\right)S_\lambda\left(\tilde{1}\tilde{2}\tilde{4}\tilde{3}\right)\right\}. \quad (13)$$

Here there used the notations: the large component of the Dirac wave function is denoted as 1 (2,3,4), the little component — as $\left(\tilde{1}\tilde{2}\tilde{4}\tilde{3}\right)$, i.e. with "wave" symbol. For example, one of the

integrals in Eq. (13) is as follows:

$$R_\lambda(1243)=$$
$$=\iint dr_1r_1^2r_2^2f_1(r_1)f_3(r_1)\times$$
$$\times f_2(r_2)f_4(r_2)Z_\lambda^{(1)}(r_<)Z_\lambda^{(1)}(r_>). \quad (14)$$

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

The Breit part is as follows [24]:

$$Q_\lambda^{\mathrm{Br}} = Q_{\lambda,\lambda-1}^{\mathrm{Br}} + Q_{\lambda,\lambda}^{\mathrm{Br}} + Q_{\lambda,\lambda+1}^{\mathrm{Br}}, \quad (15)$$

where

$$Q_\lambda^{\mathrm{Br}} = \frac{1}{Z}\mathrm{Re}\left\{R_\lambda\left(12\tilde{4}\tilde{3}\right)S_\lambda^l\left(12\tilde{4}\tilde{3}\right)+ R_\lambda\left(\tilde{1}\tilde{2}43\right)S_\lambda^l(1243)+R_l\left(\tilde{1}2\tilde{4}3\right)S_\lambda^l\left(\tilde{1}2\tilde{4}3\right)+ +R_l\left(1\tilde{2}4\tilde{3}\right)S_\lambda^l\left(1\tilde{2}4\tilde{3}\right)\right\}. \quad (16)$$

Further it should be mentioned that the angle part of the matrix element $S(1243)$ is factorized on the indexes 1, 3 and 2, 4 and can be presented by the following way:

$$\left.\begin{aligned} &S_\lambda^{(1)}(1243)=(\lambda)(-1)^{\lambda+l+1}S_\lambda^l(13)S_\lambda^l(24),\\ &S_\lambda^{(1)}(13)=(-1)^{l_3+j_3}(ll_1l_3)\times\\ &\times\begin{pmatrix} j_3 & j_1 & \lambda\\ -1/2 & 1/2 & 0\end{pmatrix}\left\{\frac{1}{\sqrt{2\lambda(\lambda+1)}}\times\right.\\ &\left[(-1)^{j_1+j_3+\lambda}(j_3)+(j_1)\right]\begin{pmatrix}\lambda & 1 & l\\ -1 & 1 & 0\end{pmatrix}+\\ &\left.\times+(-1)^{l_3+j_1+\lambda}\begin{pmatrix}\lambda & 1 & l\\ 0 & 0 & 0\end{pmatrix}\right\}. \end{aligned}\right\} \quad (17)$$

The available in Eq. (17) $3j$ symbols are expressed by the known standard analytical formulas.

We have performed studying the transition probabilities to different electronic states, which are induced during the capture of a neutron by the ^3He, $^{39}Ar^{16+}$ ions. The atom ^4He resulting from the neutron capture by ^3He recoils with a 99keV energy. The higher recoil energy 1,6MeV is corresponding to K=3,99. According to ref. [12], at K=1 the total population of the three first series ^1S,^1P and ^1D reaches as much as ~98%. The dominating channel is excitation to discrete state (57%) and then the channel for ionization of one electron (38%). It differs from situation of higher recoil energies, as then the double-ionization processes become dominant. We will not present the probabilities data as the relativistic values are practically identical to results by Glushkov et al and Wauters et al, where non-relativistic approaches (PT and B-spline approach) are used to define the correlated wave functions [12,14]. Thus, the relativistic effects have to be not important for He atomic system. The relativistic effects however became important for heavy multicharged He-like ions. In a case of He-like ion $^{139}Ar^{16}$ the binding energy of electrons is much higher in comparison with neutral He. We firstly carried out the calculation of the transition probabilities for this ion and defined (look table 1) that at K=5 the total population of the three first series ^1S,^1P and ^1D reaches as much as ~69% and it differs drastically from situation of the neutral He.

Table 1

Transition probabilities (in %) to different electronic states by capture of a neutron by $^{139}Ar^{16+}$

	ΣP (K=5)			
Final States	^1S	$^1P^0$	^1D	^1S+^1P+^1D
Discrete states	56,6595	11,8841	0,3318	68,8754
Autoionizing states	0,5811	0,2508	1,0094	1,8413
Ionization of one electron	2,7214	18,9950	6,3182	28,0346
Double ionization	0,3306	0,3361	0,5815	1,2482
SUM	60,2926	31,4660	8,2409	99,9995

It has been found that at relatively high recoil energies ~28% probability transfer from the discrete spectrum population mechanism to single-ionization. It is relatively new situation in the recoil induced ionization of the atomic systems by a neutron capture. Obviously, the experimental studying the processes considered and determination of the corresponding probabilities in a case of the high Z-charged ions is of a great importance.

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RELATIVISTIC APPROACH TO THE RECOIL INDUCED EXCITATION AND IONIZATION OF IONS DURING CAPTURE OF NEUTRON

Abstract.
The relativistic energy approach is adapted to description of the recoil-induced excitation and ionization in atoms due to a neutron capture. The data for transition probabilities to different electronic states, induced by a neutron capture, are presented.
Key words: atom ionization probability, capture of neutron, energy approach

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РЕЛЯТИВИСТСКИЙ ПОДХОД К ОПИСАНИЮ ЭФФЕКТОВ ВОЗБУЖДЕНИЯ И ИОНИЗАЦИИ В ИОНАХ ВСЛЕДСТВИЕ ЗАХВАТА НЕЙТРОНА

Резюме.
Релятивистский энергетический подход адаптирован к задаче описания возбуждения и ионизации в атомах и ионах, индуцированных отдачей вследствие захвата нейтрона. Представлены данные вероятностей переходов в различные электронные состояния, индуцированные захватом нейтрона, для ряда ионов.
Ключевые слова: вероятность ионизации, захват нейтрона, энергетический подход

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РЕЛЯТИВІСТСЬКИЙ ПІДХІД ДО ОПИСУ ЕФЕКТІВ ЗБУДЖЕННЯ ТА ІОНІЗАЦІЇ В ІОНІХ ЗАВДЯКИ ЗАХОПЛЕННЮ НЕЙТРОНУ

Резюме.
Релятивістський енергетичний підхід адаптовано до опису збудження та іонізації в атомах та іонах, індукованих віддачею завдяки захопленню нейтрону. Представлені дані ймовірностей переходів у різні електронні стани, які індуковані захопленням нейтрону, для ряду іонів.
Ключові слова: імовірність іонізації, захоплення нейтрону, енергетичний підхід