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Consistent quantum theory of recoil induced excitation and ionization in atoms during capture of neutron

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Abstract. We present a consistent new theoretical scheme for the calculation of recoil-induced excitation and ionization in atoms and ions during the emission or capture of a neutral particle (neutron) or alpha particle. The perturbation theory on inter electron interaction as a method of the calculation of correlated electron wave functions is used. The numerical results for transition probabilities to different electronic states, induced by capture of a neutron by ^{3}He, $^{19}Ne^{8+}$ are presented.

1. Introduction

The aim of this paper is to present a new consistent scheme for the calculation of recoil-induced excitation and ionization in atoms and ions during the emission or capture of a neutral particle (neutron) or alpha-particle. In last years a development of the laser spectroscopy methods allowed the observing and further using little changes in structure of atomic and molecular spectra resulted from the corresponding alteration of internal state of a nucleus [1–13]. The alteration of atomic or molecular states must be manifested in the quantum transitions, for example, in the spectrum of γ-radiation of a nucleus or during the neutral or charged particle capture. It has been estimated the influence of electron shell on the velocity of re-charging metastable nuclei [2, 3] and this effect has been found to be very little. Another more attractive situation occurs for heavy multicharged ions because of the changing the energy and geometric parameters of electron shells. The character of interaction with a nucleus may change strongly. The new channels of electron-nuclear processes can be opened [7–9]. One could mention the processes of capture of neutron or alpha particle by an atom or ion [6–8]. It is easily imagine the situation when this process becomes by energetically possible only after the removal of 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 first references to the neutral recoil are due to Migdal [14] and Levinger [15], who evaluated approximately the ionization of an atom undergoing a sudden recoil due to neutron impact and in a radioactive disintegration respectively (c.f. also [12, 13]). The neutral recoil situation differs radically from processes involving a charged particle for which the sudden recoil approximation is often invalid (c.f. [12, 13]). The different simple models (c.f. [16–23] were

developed to evaluate the excitation or ionization of an atom, the electronic redistribution of an atom induced by a sudden recoil of its nucleus occurring when a neutral particle is either emitted (γ-radioactivity) or captured (neutron capture for instance). Using the simple wave functions without the account of main correlation effects does not allow to get the adequate quantitative results. In more sophisticated calculational schemes variational wave functions with great number of parameters or multiconfigurational wave functions are used. In fact, the quality of electron wave functions determines the advantages or disadvantages of any theoretical approach.In refs. [12,13] a consistent B-spline set approach has been realized and evaluated from a detailed comparison with the analytical results. In this paper we present a new theoretical scheme for the calculation of recoil-induced excitation and ionization in atoms (ions) during the emission or capture of a neutral particle (neutron) or alpha particle. As method of the calculation of correlated electron wave functions, we use the perturbation theory on inter electron interaction [5, 24–27]. An advantage of this approach is connected with direct account of the main electron correlations in the initial and final states. This approach has been successfully used in the calculations of the oscillator strengths, radiative widths, cross-sections of photo-excitation and photoionization of two- and multi-electron systems with excitation of residual ion to different states (c.f.[4,5,7–11,24–27]). Here the numerical results for transition probabilities to different electronic states, induced by capture of a neutron by ^{3}He, ^{19}Ne^{8+} are presented.

2. The calculation of transition probabilities induced by capture of a neutron

Our main aim is to present a new consistent theoretical scheme for the calculation of recoil-induced excitation and ionization in atoms and ions due to a capture of neutron or alpha-particle. 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. According to standard quantum-mechanical theory (c.f. [7, 12, 13]), the transition amplitude matrix element is given by the overlap between the initial state (strictly saying, with a nuclear charge Z) and the final state (with a nuclear charge Z') in a Galilean boost of velocity v. The overlap in the momentum space is as [13]:

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

where subscript i and f represent the set of quantum numbers of the initial and final states and $\hbar k = mv$ is the recoil momentum of the electron accompanying the resulting nucleus and having a kinetic energy equal to $(ka_0)^2$Ry. Further we use the definition: $K = ka_0$ The energy E_R of the recoiling nucleus of mass M_R is:

$$E_R = \frac{M_R}{m_e}(ka_0)^2\mathrm{Ry}d. \tag{2}$$

The function $\Phi_i(\overrightarrow{p},Z)$ is related to the function $\Psi_i(\overrightarrow{r},Z)$ written in the configuration space through the well known Fourier transform relation:

$$\Phi_i(\overrightarrow{p},Z) = (2\pi)^{-3/2}\int d\overrightarrow{r}\,\exp(-i\overrightarrow{p}\cdot\overrightarrow{r})\Psi_i(\overrightarrow{r},Z). \tag{3}$$

So, using these relations the overlap is defined by:

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

The probability of populating state 'f' starting from state 'i' is given by $P_{if} = |b_{if}|^2$. As further we are dealing in with two-electron atoms and ions, one can write the wave function of system as follows:

$$\psi(\gamma LSM_L M_S) = \sum_i a_i \Phi(\gamma_i LSM_L M_S). \tag{5}$$

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

$$b_{if} = \int d\overrightarrow{r_1} \int d\overrightarrow{r_2} \Psi_i(\overrightarrow{r_1}, \overrightarrow{r_2}; Z) \exp[-ik(z_1 + z_2)] \Psi_f^*(\overrightarrow{r}, \overrightarrow{r_2}; Z'), \tag{6}$$

where the Oz-axis of the coordinate system is chosen along the $\overrightarrow{k}$ direction. The matrix element of the two-electron recoil operator:

$$R = \exp[-ik(z_1 + z_2)]$$

between correlated electronic wave functions (5) is written as follows (c.f. [13]):

$$\begin{aligned}[\overline{\Psi}(\gamma' L' S' M'_S)|R|\Psi(\gamma LSM_L M_S)] = [\Psi(\gamma LSM_L M_S)|R^*|\overline{\Psi}(\gamma' L' S' M'_L M'_S)] = \\ = \sum_{i,j} a_i^* \overline{a}_j \langle \Psi(\gamma_i LSM_L M_S)|R^*|\overline{\Psi}(\gamma_j L' S' M'_L M'_S)\rangle.\end{aligned} \tag{7}$$

It could be reduced to the direct and exchange contributions:

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

where

$$R(ij,rl) = \langle (\rho_i l_i)_1 (\rho_j l_j)_2 LSM_L M_S|R^*|\overline{(\rho_r l_r)_1 (\rho_l l_l)_2} L' S' M'_L M'_S\rangle.$$

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

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

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 $1s^2\ {}^1S$:

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

All notations in Eq. (10) are standard. In order to calculate the transition amplitude it is necessary to use the basis of correlated wave functions. The quality of electronic functions

Table 1. Transition probabilities (in %) to different electronic states by capture of a neutron by ^{3}He

Final states	$\sum P(\mathrm{K}=1)$ present paper ^{1}S	^{1}P^0	^{1}D	^{1}S+^{1}P+^{1}D
Discrete states	50.559	5.5101	0.1113	56.1804
Autoionizing states	0.3419	0.1518	1.0601	1.5538
Ionization of one electron	3.5564	27.3392	6.8169	37.7125
Double ionization	0.4880	0.9525	1.0154	2.4559
TOTAL	54.9453	33.9536	9.0037	97.9026

defines an accuracy of calculating the ionization and excitation probabilities in atom (ion) during a capture of particle. In order to construct the basis of correlated wave functions we use the formalism of perturbation theory on the inter-electron interaction [5,24–27]. The matrix elements on correlated electron functions are calculated according to the formula:

$$\sum_{f,i} |\langle \Psi_f | R | \Psi_i \rangle|^2 =$$

$$= \sum_{f_1,f_2} \left| \Phi_{f_1,f_2} | R | \Phi_{i_1,i_2} \rangle + \sum_{n_1,n_2} \frac{\langle \Phi_{f_1,f_2} | V | \Phi_{n_1,n_2} \rangle \langle \Phi_{n_1,n_2} | R | \Phi_{i_1,i_2} \rangle}{E^0_{n_1,n_2} - E^0_{f_1,f_2}} + \right. \tag{11}$$

$$\left. + \sum_{m_1,m_2} \frac{\langle \Phi_{i_1,i_2} | V | \Phi_{m_1,m_2} \rangle \langle \Phi_{m_1,m_2} | R | \Phi_{i_1,i_2} \rangle}{E^0_{m_1,m_2} - E^0_{i_1,i_2}} \right|^2 ,$$

where E^0 and Φ are the eigenvalues and eigenfunctions of the Coulomb Hamiltonian, V is the operator of electrostatic interaction between electrons; their matrix elements are equal to difference between the direct and exchange integrals. Summation on indexes n and m includes integration on the continuum states too. It is very important to note that our approach allows accounting for inter-electron correlation in the initial and final states with high degree of accuracy (c.f. [5,24]). Strictly saying, we are accounting for the inter electron correlations in the first order on the parameter $1/Z$. It is obvious that the account for the next perturbation theory order can increase an accuracy. Calculation of all matrix elements has been carried out with using our atomic code (c.f. [4,5,7–11,25–27].

3. Results and discussion

The numerical results for transition probabilities to different electronic states have been obtained for processes of capture of a neutron by ^{3}He, ^{19}Ne^{8+} and for α+^{4}He$\rightarrow^8$Be^{2+} reaction. All results are presented in Tables 1–4. At first we consider the case, when K = 1.

The atom ^{4}He resulting from the neutron capture by ^{3}He recoils with 99 keV energy. The higher recoil energy 1.6 MeV is corresponding to K = 3.99. The calculation has shown that at K= 1 the total population of three first series ^{1}S, ^{1}P, and ^{1}D reaches as much as $\sim$ 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 [8, 13]. This is in an excellent agreement with data of Wauters *et al*. [13], where a consistent B-spline set approach to the calculation of correlated wave functions has been used.

Table 2. Transition probabilities (in %) to different electronic states by capture of a neutron by ^{3}He

	$\sum P$(K = 3.99) present paper			
Final states	^{1}S	^{1}P^0	^{1}D	^{1}S+^{1}P+^{1}D
Discrete states	0.0964	0.0025	0	0.099
Autoionizing states	0.0102	0.0024	0.0025	0.015
Ionization of one electron	1.0453	1.6212	1.6805	4.347
Double ionization	4.4035	11.710	13.735	29.849
TOTAL	5.555	13.336	15.518	34.310

Table 3. Transition probabilities (in %) to different electronic states by capture of a neutron by ^{19}Ne^{8+}

	$\sum P$(K = 1) present paper			
Final states	^{1}S	^{1}P^0	^{1}D	^{1}S+^{1}P+^{1}D
Discrete states	97.8767	1.3845	0.003	99.2642
Autoionizing states	0.0019	0.0031	0.0038	0.0088
Ionization of one electron	0.037	0.7063	0.012	0.722
Double ionization	0.0004	0.0037	0.0009	0.005
TOTAL	97.8827	2.0976	0.0197	100.00

Table 4. Transition probabilities (in %) to different electronic states by capture of a neutron by ^{19}Ne^{8+}

	$\sum P$(K = 5) present paper			
Final states	^{1}S	^{1}P^0	^{1}D	^{1}S+^{1}P+^{1}D
Discrete states	67.327	14.9598	0.47	76.757
Autoionizing states	0.3902	0.2415	0.7492	1.381
Ionization of one electron	1.4854	14.4080	4.2036	20.097
Double ionization	0.2270	0.2184	0.4688	0.90
TOTAL	63.430	29.831	5.892	99.15

For the He-like ion ^{19}Ne^{8+} the binding energy of electrons is much higher in comparison with neutral He. The calculation has shown that at K = 1 (the recoil energy 472 keV) the total population of three first series ^{1}S, ^{1}P, and ^{1}D reaches as much as $\sim 99\%$ and other processes are almost non-existent (see Table 3). It differs drastically from situation of higher recoil energies, as $\sim 20\%$ probability transfer from the discrete spectrum population mechanism to single-ionization (c.f. [13]).

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