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SENSING THE RECOIL INDUCED EXCITATION AND IONIZATION IN ATOMS AND IONS DUE TO THE CAPTURE OF NEUTRON AND ALPHA-PARTICLE

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Abstract

SENSING THE RECOIL INDUCED EXCITATION AND IONIZATION IN ATOMS AND IONS
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New theoretical scheme for sensing the recoil-induced excitation and ionization in atoms and ions due to the neutron capture and alpha particle is proposed. As method of calculation of the correlated electron wave functions, the perturbation theory on inter electron interaction is used. The numerical results for transition probabilities to different electronic states, induced by capture of a neutron by ^3He , $^{19}\text{Ne}^{8+}$ and for $\alpha+^4\text{He}\rightarrow^8\text{Be}^{2+}$ reaction are presented.

Key words: sensing, recoil in atom, ionization probability, capture of neutron, alpha-particle

Анотація

ДЕТЕКТУВАННЯ ЕФЕКТІВ ЗБУДЖЕННЯ ТА ІОНІЗАЦІЇ В АТОМАХ ТА ІОНАХ,
ІНДУКОВАНИХ ВІДДАЧЕЮ ЗАВДЯКИ ЗАХОПЛЕННЮ НЕЙТРОНУ
ТА АЛЬФА ЧАСТИНКИ

С. В. Малиновська

Запропоновано нову теоретичну схему детектування ефектів збудження та іонізації в атомах та іонах, індукованих віддачею завдяки захопленню нейтрону і альфа частинки. Як метод розрахунку корельованих електронних хвильових функцій використано метод, який базується на теорії збурень по між електронній взаємодії. Представлені чисельні оцінки імовірностей переходів у різні електронні стани, які індуковані захопленням нейтрону ^3He , $^{19}\text{Ne}^{8+}$, та в реакції $\alpha+^4\text{He}\rightarrow^8\text{Be}^{2+}$.

Ключові слова: детектування, віддача в атомі, імовірність іонізації, захоплення нейтрону, альфа частинка.

*Аннотация***ДЕТЕКТИРОВАНИЕ ЭФФЕКТОВ ВОЗБУЖДЕНИЯ И ИОНИЗАЦИИ В АТОМАХ И ИОНАХ, ИНДУЦИРОВАННЫХ ОТДАЧЕЙ ВСЛЕДСТВИЕ ЗАХВАТА НЕЙТРОНА И АЛЬФА ЧАСТИЦЫ***С. В. Малиновская*

Предложена новая теоретическая схема детектирования эффектов возбуждения и ионизации в атомах и ионах, индуцированных отдачей вследствие захвата нейтрона и альфа-частицы. В качестве метода расчета коррелированных электронных волновых функций использован метод, базирующийся на теории возмущений по межэлектронному взаимодействию. Представлены численные оценки вероятностей переходов в различные электронные состояния, индуцированные захватом нейтрона ${}^3\text{He}$, ${}^{19}\text{Ne}^{8+}$, и в реакции $\alpha + {}^4\text{He} \rightarrow {}^8\text{Be}^{2+}$.

Ключевые слова: детектирование, отдача в атоме, вероятность ионизации, захват нейтрона, альфа-частица.

1. Introduction

Paper is devoted to carrying out new scheme for sensing 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 because of the corresponding alteration of the internal state of a nucleus [1-12]. It should be mentioned a selective photoionization of atoms with the isomer nucleus and possibility of the quick physical separation of the isomer nuclei. Any alteration of the atomic or molecular state must be manifested in the quantum transitions, for example, in a spectrum of the γ -radiation of a nucleus or due to the neutral or charged particle capture. The influence of the electron shell on velocity of recharging the metastable nucleus has been estimated [3] and this effect has been found to be very small. 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 [1,4,5]. To traditional channels of the nucleus excited state decay, such effects are added as the electron-positron pair production (during the nucleus recharging) etc. Here one could mention the processes of capture of neutron or alpha particle by atom or ion [6-8]. 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 atom or mole-

cule electron shells under radiating (absorption) the γ quanta by a nucleus. The first references to the neutral recoil are due to Migdal (1941) and Levinger (1953), who evaluated approximately the ionization of an atom undergoing a sudden recoil in due to neutron impact and in a radioactive disintegration respectively (c. f. [1]). The neutral recoil situation differs radically from processes involving a charged particle for which the sudden recoil approximation is often invalid (c. f. [5-7]). Different simple models (c. f. [1-3, 6-8]) were developed to evaluate the 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). Here a new theoretical scheme for sensing the recoil-induced excitation and ionization in atoms (ions) due to the neutron capture and alpha-particle is proposed. As method of calculation of the correlated electron wave functions, the perturbation theory on inter electron interaction is used. The numerical results for transition probabilities to different states, induced by capture of neutron by ${}^3\text{He}$, ${}^{19}\text{Ne}^{8+}$ and for $\alpha + {}^4\text{He} \rightarrow {}^8\text{Be}^{2+}$ reaction are given

2. Calculating transition probabilities induced by capture of a neutron and alpha-particle

Our main purpose is present new high precise theoretical scheme for sensing the recoil-induced excitation and ionization in atoms and ions due to the neutron capture and 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. [1,7]), 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 \mathbf{v} . The overlap in the momentum space is as follows:

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

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

$$E_R = \frac{M_R}{m_e} (ka_0)^2 R_{yd} \quad (2)$$

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

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

So, using these relations the overlap is defined by:

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

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

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

All notations in eq. (10) are standard. To calculate transition amplitude it is necessary to use the basis's of correlated wave functions. The quality of electronic functions defines an accuracy of calculating the ionization and excitation probabilities in atom (ion) during a capture of particle. To construct such basis we use formalism of the per-

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

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

$$b_{if} = \int d\vec{r}_1 \int d\vec{r}_2 \Psi_i(\vec{r}_1; \vec{r}_2; Z) e^{-i\mathbf{k} \cdot (\mathbf{z}_1 + \mathbf{z}_2)} \Psi_f^*(\vec{r}_1, \vec{r}_2; Z') \quad (6)$$

where the Oz-axis of the coordinate system is chosen along the \mathbf{k} direction. The two-electron recoil operator $R = \exp[-i\mathbf{k} \cdot (\mathbf{z}_1 + \mathbf{z}_2)]$ matrix element between the correlated electronic wave functions of the form (5) is written in standard form {c. f. 1,6}):

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

It could be reduced to the direct and exchange contributions:

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

where $R(ij, rt) \equiv (c_i l_i)_1 (c_j l_j)_2 LSM_L M_S | R^* | (\rho_r l_r)_1 (\rho_l l_l)_2 L' S' M'_L M'_S$

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

$$\begin{aligned} R &= e^{-i\mathbf{k} \cdot (\mathbf{z}_1 + \mathbf{z}_2)} = \sum_{l, l'=0}^{\infty} (-i)^{l+l'} (2l+1) \times \\ & \times (2l'+1) j_l(kr_1) j_{l'}(kr_2) C_0^{(l)}(1) C_0^{(l')}(2) \end{aligned} \quad (9)$$

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 $1s^2 1S$:

turbation theory on the inter-electron interaction [12-15]. The matrix element on correlated electron functions is calculated according to the formula:

$$\sum_{f,i} |\langle \Psi_f | R | \Psi_i \rangle|^2 = \sum_{f_1, f_2} |\langle \Phi_{f_1 f_2} | R | \Phi_{i_1 i_2} \rangle|^2 +$$

$$+ \sum_{n_1 n_2} \frac{\langle \Phi_{f1f2} | V | \Phi_{n1n2} \rangle \langle \Phi_{n1n2} | R | \Phi_{i1i2} \rangle}{E_{n_1 n_2}^0 - E_{f_1 f_2}^0} + \quad (11)$$

$$+ \sum_{m_1 m_2} \frac{\langle \Phi_{i1i2} | V | \Phi_{m1m2} \rangle \langle \Phi_{m1m2} | R | \Phi_{i1i2} \rangle}{E_{m_1 m_2}^0 - E_{i_1 i_2}^0} |^2$$

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. Summation on indexes n and m includes also integration on the continuum. It is very important to note that such an approach allows accounting for inter electron correlation in the initial and final states with high degree of accuracy (c. f. [15]). Strictly saying, we are accounting for inter electron correlation's in the first order on parameter $1/Z$. It is obvious that accounting for next perturbation theory order can increase the accuracy. Calculation of all matrix elements has been carried out according to papers [11-15].

3. Results and discussion

The numerical results for transition probabilities to different electronic states have been received for processes of capture of a neutron by ^3He , $^{19}\text{Ne}^{8+}$ and for $\alpha + ^4\text{He} \rightarrow ^8\text{Be}^{2+}$ reaction. All results are presented in tables 1-3. At the beginning we considered a case, when $K=1$. The atom ^4He resulting from the neutron capture by ^3He recoils with a 99keV energy. The higher recoil energy 1,6MeV is corresponding to $K=3,99$. Calculation has shown that at $K=1$ the total population of the three first series $^1S, ^1P$ and 1D 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%).

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

Final States	$\Sigma P (K=3,99)$ present paper			
	1S	$^1P^0$	1D	$^1S + ^1P + ^1D$
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	13,7350	29,849
SUM	5,555	13,336	15,418	34,31

This is in an excellent agreement with data of Wauters et al [7], where the B-spline approach to

calculating the correlated wave functions has been used. At higher recoil energy ($K=3,99$) the double ionization processes become dominant $\sim 30\%$ (see table 1). The next object of studying is He-like ion $^{19}\text{Ne}^{8+}$. It is obvious that the binding energy of electrons is much higher for this ion in comparison with neutral He. Calculation has shown that at $K=1$ (the recoil energy 472 keV) the total population of the three first series $^1S, ^1P$ and 1D reaches as much as $\sim 99\%$ and other processes are almost non-existent. In table 2 we present the transition probabilities for $K=5$ (the recoil energy 11,8MeV). The recoil energy increase by going from $K=1$ to $K=5$ leads to a drastic change of the energy redistribution. Namely, there is a $\sim 20\%$ probability transfer from the discrete spectrum population mechanism to single-ionization processes (see table 2).

Table 2.
Transition probabilities (in %) to different electronic states by capture of a neutron by $^{19}\text{Ne}^{8+}$

Final States	$\Sigma P (K=3,99)$ present paper			
	1S	$^1P^0$	1D	$^1S + ^1P + ^1D$
Discrete states	1,4128	0,7224	0,0576	2,193
Autoionizing states	0,2430	1,2350	0,7198	2,198
Ionization of one electron	1,3965	6,5280	8,1402	16,065
Double ionization	2,5027	4,8506	6,5004	13,854
SUM	5,555	13,336	15,418	34,31

In table 3 we present calculated transition probabilities (in %) to different electronic states for $\alpha + ^4\text{He} \rightarrow ^8\text{Be}^{2+}$ reaction. The value of K is equal 3,99 that is corresponding to the recoil energy of 3,16MeV. This situation fits with a 6,32 MeV initial energy of the alpha particle with a ^4He nucleus attached to the laboratory frame. It is obvious that the sudden recoil approximation holds for a neutral particle capture or emission and could remain valid for a process involving a nuclear charge change at very high energies.

Comparison of data from table 3 with data of table 2 shows that the total population probabilities are identical for the neutron capture of He and $\alpha + \text{He}$ reaction. But, the effect of the nuclear charge change ($Z'=2Z$) is manifested in difference of distributions between the states populated for the two collisional systems. It is in a qualitative agreement with available literature data (c. f. [7]). So, we have proposed a new theoretical scheme for sensing the recoil-induced excitation and ionization in atoms and ions due to the neutron capture and alpha particle.

Table 3.
Transition probabilities (in %) to different
electronic states for $\alpha+^4\text{He}\rightarrow^8\text{Be}^{2+}$ reaction

Final States	ΣP (K=3,99) present paper			
	1S	$^1P^0$	1D	$^1S+^1P+^1D$
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