ФІЗИЧНІ, ХІМІЧНІ ТА ІНШІ ЯВИЩА, НА ОСНОВІ ЯКИХ МОЖУТЬ БУТИ СТВОРЕНІ СЕНСОРИ

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SENSING FORBIDDEN TRANSITIONS IN SPECTRA OF SOME HEAVY ATOMS AND MULTICHARGED IONS: NEW THEORETICAL SCHEME

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Abstract. It has been carried out sensing and calculating the energies and oscillator strengths of some forbidden atomic transitions in spectra of heavy atoms and multicharged ions on the basis of new relativistic scheme within gauge-invariant quantum electrodynamics (QED) perturbation theory (PT).

Keywords: sensing forbidden atomic transitions, heavy atoms and multicharged ions, new relativistic approach

ВИЗНАЧЕННЯ ЗАБОРОНЕНИХ ПЕРЕХОДІВ У СПЕКТРАХ ДЕЯКИХ ВАЖКИХ АТОМІВ ТА БАГАТОЗАРЯДНИХ ІОНІВ: НОВА ТЕОРЕТИЧНА СХЕМА

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Анотація. Виконано розрахунок енергій, імовірностей та сил осциляторів заборонених атомних переходів у спектрах декотрих важких атомів та багатозарядних іонів на основі нової релятивістської схеми в межах калібровочно-інваріантної КЕД теорії збурень.

Ключові слова: детектування заборонених атомних переходів, важкі атоми та багатозарядні іони, нова релятивістська схема

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ОПРЕДЕЛЕНИЕ ВЕРОЯТНОСТЕЙ ЗАПРЕЩЕННЫХ ПЕРЕХОДІВ В СПЕКТРАХ НЕКОТОРЫХ ТЯЖЕЛЫХ АТОМОВ И МНОГОЗАРЯДНЫХ ИОНОВ: НОВАЯ ТЕОРЕТИЧЕСКАЯ СХЕМА

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Аннотация. Выполнен расчет вероятностей и сил осцилляторов запрещенных атомных переходов в спектрах некоторых сложных тяжелых атомов и многозарядных ионов на основе новой релятивистской схемы в рамках калибровочно-инвариантной КЭД теории возмущений.

Ключевые слова: детектирование запрещенных атомных переходов, тяжелые атомы и многозарядные ионы, новая релятивистская схема

1. Introduction

The experimental and theoretical studying of the radiation transition characteristics of a whole number of atomic systems, which are interesting and perspective from the point of view of the quantum electronics and photoelectronics, is in last years of a great importance (c.f.[1-27]). It is also very important for search the optimal candidates and conditions for realization of the X-ray lasing. Besides, the forbidden atomic transitions are attracting from the point of view of sensing new physics behind the well known standard model.

The well known multi-configuration Dirac-Fock (MCDF) approach is widely used in calculations of the atoms and ions. It provides the most reliable version of calculation for atomic systems. Nevertheless, as a rule, detailed description of the method for studying role of the relativistic, gauge-invariant contributions, nuclear effects is lacking. Serious problems are connected with correct definition of the high-order correlation corrections, QED effects etc. The further improvement of this method is connected with using the gauge invariant procedures of generating relativistic orbitals basis's and more correct treating the nuclear and QED effects [1-7]. In references [1-7] it has been developed a new ab initio approach to calculating spectra of atomic systems with account of relativistic, correlation, nuclear, QED effects, based on the gauge-invariant QED PT [4] and new effective procedures for accounting the nuclear and radiative corrections [5-7]. Here we use propose a new relativistic scheme for determination and sensing the forbidden atomic transitions basing on the gauge-invariant QED perturbation theory formalism [5]. As object of studying the heavy atoms and Ne-, Zn-like multicharged ions are considered. one of the its versions [18] for calculating the Earlier it has been carried theoretical studying energy spectra, theoretical determination of the energies and oscillator strengths of some electric dipole transitions in spectrum of the rare-earth atom of Eu [27].

2. New relativistic approach to sensing and determination of the forbidden atomic transition probabilities

Let us describe in brief the important moment of our theoretical approach. As usually, the wave functions zeroth basis is found from the Dirac equation solution with potential, which includes the core ab initio potential, electric, polarization potentials of nucleus (the gaussian form for charge distribution in the nucleus is used). All correlation corrections of the PT second and high orders (electrons screening, particle-hole interaction etc.) are accounted for. The wavefunction for a particular atomic state

$$\Psi(\Gamma PJM) = \sum_{r}^{NCF} c_r \Phi(\gamma_r PJM) \qquad (1)$$

is obtained as the above described self-consistent solutions of the Dirac–Fock type equations. Configuration mixing coefficients c_r are obtained through diagonalization of the Dirac Coulomb Hamiltonian

$$H_{DC}=\Sigma_i c\alpha_i p_i + (\beta_i-1)c^2 - V_c(r|nlj)+ \\ +V_{ex}-V_{nucl}(r|R) + \Sigma_{i>j} \exp(i\omega r_{ij})(1-\alpha_1\alpha_2)/r_{ij}. \qquad (2)$$

In this equation the potential:

$$V(r)=V_c(r|nlj)+V_{ex}+V_{nucl}(r|R). \qquad (3)$$

This potential includes the electrical and polarization potentials of the nucleus. The part V_{ex} accounts for exchange inter-electron interaction. The main exchange effect are taken into account in

the equation. The rest of the exchange-correlation effects are accounted for in first two PT orders by the total inter-electron interaction [4]. The effective electron core density (potential V_c) is defined by iteration algorithm within gauge invariant QED procedure [4].

Consider the one-quasiparticle system. A quasiparticle is a valent electron above the core of closed electron shells or a vacancy in the core. In the lowest second order of the EDPT a non-zeroth contribution to the imaginary part of electron energy Im ΔE (the radiation decay width) is provided by relativistic exchange Fock diagram. In the fourth order of the QED PT there are diagrams, whose contribution into the ImΔE accounts for the core polarization effects. It is on the electromagnetic potentials gauge (the gauge non-invariant contribution). Let us examine the multielectron atom with one quasi-particle in the first excited state, connected with the ground state by the radiation transition. In the zeroth QED PT approximation we, as usually (c.f.[2-4]),use the one electron bare potential

$$V_{\mathrm{N}}(r) + V_{\mathrm{C}}(r), \tag{4}$$

with $V_{\mathrm{N}}(r)$ describing the electric potential of the nucleus, $V_{\mathrm{C}}(r)$, imitating the interaction of the quasi-particle with the core. The core potential $V_{\mathrm{C}}(r)$ is related to the core electron density $\rho_{\mathrm{C}}(r)$ in a standard way. The latter fully defines the one electron representation. Moreover, all the results of the approximate calculations are the functionals of the density $\rho_{\mathrm{C}}(r)$. In ref.[4] the lowest order multielectron effects, in particular, the gauge dependent radiative contribution for the certain class of the photon propagator calibration is treated. This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criterion in the searching for the optimal one-electron basis of the PT. The minimization of the density functional Im ΔE_{ninv} leads to the integral differential equation for the ρ_{c}, that can be solved using one of the standard numerical codes. In ref. [4] authors treated the function ρ_{c} in the simple analytic form with the only variable parameter b and substituted it to (6). More accurate calculation requires the solution of the integral differential equation for the ρ_{c} [21,26,27].

The probability is directly connected with imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as follows:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \tag{5}$$

where $\sum_{\alpha>n>f}$ – for electron and $\sum_{\alpha<n\le f}$ – for vacancy. The potential V is as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega| r_{12}}{r_{12}} \times \\ \times(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1). \tag{6}$$

The separated terms of the sum in (5) represent the contributions of different channells and a probability of the dipole transition is:

$$\Gamma_{б_n} = \frac{1}{4p}\cdot V^{|\omega_{б_n}|}_{б_n \alpha_n}. \tag{7}$$

The corresponding oscillator strength : $gf = \lambda^2_g \cdot \Gamma_{\alpha_n} / 6.67\cdot 10^{15}$, where g is the degeneracy degree, λ is a wavelength in angstrems (Å). Under calculating the matrix elements (5) one could use the angle symmetry of the task and write the expansion for potential $\sin|\omega|r_{12}/r_{12}$ on spherical functions as follows:

$$\frac{\sin|\omega| r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \times \\ \times\sum_{\lambda=0}^{\infty}(\lambda) J_{\lambda+1/2}(|\omega| r_1) J_{\lambda+1/2}(|\omega| r_2) P_\lambda(\cos \mathbf{r}_1\mathbf{r}_2), \tag{8}$$

where J –is the Bessell function of first kind and $(\lambda) = 2\lambda + 1$. This expansion is corresponding to usual multipole one for probability of radiative decay. Substitution of the expansion (7) to matrix element of interaction gives as follows:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)[\times \\ \times^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathrm{Im}\, Q_\lambda(1234); \\ Q_\lambda = Q^{\mathrm{Qul}}_\lambda + Q^{\mathrm{Br}}_\lambda. \tag{9}$$

where j_i are the entire single electron momentums, m_i — their projections; Q^{Qul}_λ is the Coulomb part of interaction, Q^{Br}_λ - the Breit part. The Coulomb part Q^{Qul}_λ is expressed in terms of radial integrals R_λ, angular coefficients S_λ [2,5]:

$$\mathrm{Re}\, Q^{\mathrm{Qul}}_\lambda = \frac{1}{Z}\mathrm{Re}\{R_l(1243)S_\lambda(1243) + \\ + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3}) + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + \\ + R_\lambda(\tilde{1}\tilde{2}43)S_\lambda(\tilde{1}\tilde{2}43)\}. \tag{10}$$

As a result, the Auger decay probability is ex-

pressed in terms of Re$Q_\lambda(1243)$ matrix elements [9]:

$$\mathrm{Re}\,R_\lambda(1243) = \iint dr_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1) \times \\ \times f_2(r_2) f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>). \quad (11)$$

where f is the large component of radial part of single electron state Dirac function and function Z is [5]:

$$Z_\lambda^{(1)} = \left[\frac{2}{|\omega_{13}|\alpha Z}\right]^{\lambda+1/2} \frac{J_{\lambda+1/2}(\alpha|\omega_{13}|r)}{r^\lambda \Gamma\left(\lambda+\frac{3}{2}\right)}. \quad (12)$$

The angular coefficient is defined by standard way [7]. 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 ж$_1$> 0 and l_i+1 for ж$_i$<0. The Breat interaction is known to change considerably the Auger decay dynamics in some cases (c.f. [5]). The Breat part of Q is defined as the sum:

$$Q_\lambda^{\mathrm{Br}} = Q_{\lambda,\lambda-1}^{\mathrm{Br}} + Q_{\lambda,\lambda}^{\mathrm{Br}} + Q_{\lambda,\lambda+1}^{\mathrm{Br}}, \quad (13)$$

where the contribution of our interest is determined as:

$$Q_\lambda^{\mathrm{Br}} = \frac{1}{Z}\mathrm{Re}\left\{R_\lambda(12\tilde{4}\tilde{3}) S_\lambda^l(12\tilde{4}\tilde{3}) + \right. \\ + R_\lambda(\tilde{1}\tilde{2}43) S_\lambda^l(1243) + R_l(\tilde{1}2\tilde{4}\tilde{3}) S_\lambda^l(\tilde{1}2\tilde{4}\tilde{3}) + \\ \left. + R_l(1\tilde{2}4\tilde{3}) S_\lambda^l(1\tilde{2}4\tilde{3})\right\}. \quad (14)$$

Radial parts F and G of two components of the Dirac function for electron, which moves in the potential $V(r,R)+U(r,R)$, are defined by solution of the Dirac equations (PT zeroth order). All calculations are carried out using the effective Dirac-Superatom-ISAN code developed by Ivanov-Ivanova-Glushkov [1-6].

3. Results and conclusions

We have carried out sensing and calculating probabilities of the magnetic dipole (M1) and electric quadrupole (E2) forbidden transitions for Ne-, Zn-like multicharged ions (Z=32-92) and single ionized atom of Hg. In all calculations we used the Ivanov-Ivanova model potential [1] with defining its parameter within above described an initio QED procedure [2]. In fact this potential imitated the self-consistent Dirac-Fock potential. All details can be found in refs. [1-6, 21]. In table 1,2 we present the energies and E2 probabilities of the $5d^96s^2(D_{5/2},D_{3/2})$- $5d^{10}6s$ ($S_{1/2}$) transition in Hg^+. For comparison we listed in this table the theoretical Hartree-Fock (HF), Dirac-Fock (DF) and DF (with fitting to experimental transition energies) values by Ostrovsky-Sheynerman and experimental data by Moore (NBS, Washington) [23-25]. In table 3 we present the oscillator strengths of the $4s^2(^1S_0)$- 4s4p ($^1P^0_1$) transition in the Zn-like multicharged ions. The same calculation was carried out for Ne-like ions (Z=22-92). For comparison we listed in this table the theoretical Hartree-Fock (HF), Dirac-Fock (DF), DF (with fitting to experimental transition energies) and model potential (MP) data.

Table 1
The energies of the $5d^96s^2(D_{5/2},D_{3/2})$- $5d^{10}6s$ ($S_{1/2}$) transition in Hg^+ (in Ry)

Method	E_{6s}	$D_{3/2}$- $S_{1/2}$	$D_{5/2}$- $S_{1/2}$
HF	-1.07	0.863	0.863
DF	−1.277	0.608	0.460
This work	−1.377	0.462	0.325
Experiment	−1.378	0.461	0.324

Table 2
The E2 probabilities of the $5d^96s^2(D_{5/2},D_{3/2})$- $5d^{10}6s$ ($S_{1/2}$) transition in Hg^+ (in s^{-1})

Method	$D_{3/2}$- $S_{1/2}$	$D_{5/2}$- $S_{1/2}$
HF	1360	1360
DF	257.0	77.4
DF (exp. E)	63.9	13.3
This work	54.53	11.84
Experiment	53.5±2.0	11.6±0.4

In table 4 we present the M1 and E2 transitions probabilities in some Zn-like ions [23-25,28]. The detailed tables of the transitions energies and probabilities, oscillator strengths for Zn-like (Z=32-92 and Ne-like (Z=22-92) are presented in ref. [29].

Analysis of the obtained data allows to make the following conclusions. Firstly, one can see that our approach provides physically reasonable agreement with experiment and significantly more advantagable in comparison with standard Dirac-Fock method and the Hartree-Fock approximation approach. Secondly, we have checked that the results for oscillator strengths, obtained within our approach in different photon propagator gauges (Coulomb, Babushkon, Landau gauges) are practically equal, that is provided bu using an effective QED energy procedure [4]. Thirdly, calculation has confirmed the great role of the interelectron correlation effects of the second and higher QED PT orders, namely,

effects of the interelectron polarization interaction and mutual screening.

Table 3

The oscillator strengths of $4s^2(^1S_0)$- 4s4p ($^1P^0_1$) transition in the Zn-like ions

Ion	Method	f_L	f_V
Ga^+	DF	1.89	1.98
	HF	2.30	2.01
	DF2	1.97	1.95
	MP	1.68	1.73
	Our	1.862	1.861
	Exp.	1.85 ± 0.15	1.85 ± 0.15
As^{3+}	DF	1.87	1.86
	Our	1.575	1.574
	Exp.	1.56 ± 0.23	1.56 ± 0.23
Kr^{6+}	DF	1.75	1.71
Gd^{34+}	DF	1.12	1.10
Yb^{40+}	DF	1.12	1.10
Au^{40+}	DF	1.18	1.15
Pb^{52+}	DF	1.21	1.18
U^{62+}	DF	1.37	1.31
	HF	1.41	1.47
	Our	1.333	1.332
	Exp.	1.31 ± 0.05	1.31 ± 0.05

Table 4

The M1 and E2 transitions probabilities in some Zn-like ions: (a) $4s4p\left(^3P^0_2\right)\rightarrow 4s4p\left(^3P^0_1\right)$; (b) $4s4p\left(^1P^0_1\right)\rightarrow 4s4p\left(^3P^0_2\right)$ (our data)

Trans.	M1 (a)	E2 (a)	M1 (b)	E2 (b)
Kr^{6+}	0.072(1)	0.034(-2)	0.033(2)	0.041(1)
Cd^{18+}	0.048(4)	0.132(1)	0.055(4)	0.034(3)
Xe^{24+}	0.042(5)	0.025(3)	0.034(5)	0.232(3)
Gd^{34+}	0.081(6)	0.118(4)	0.047(6)	0.047(5)
Yb^{40+}	0.039(7)	0.399(5)	0.145(6)	0.026(6)
Zn	0.028(8)	0.104(6)	0.119(7)	0.029(7)
Pb^{52+}	0.047(8)	0.067(7)	0.215(7)	0.058(7)
U^{62+}	0.036(9)	0.059(8)	0.128(8)	0.101(8)

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