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

PHYSICAL, CHEMICAL AND OTHER PHENOMENA, AS THE BASES OF SENSORS

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NEW NUMERICAL APPROACH IN SENSING RADIATIVE TRANSITIONS PROBABILITIES IN SPECTRA OF SOME COMPLEX IONS

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Abstract. It has been carried out sensing and calculating the energies and oscillator strengths of some radiative transitions in spectra of complex ion on the basis of new numerical relativistic scheme within gauge-invariant perturbation theory.

Keywords: sensing radiative transitions, complex ions, relativistic approach

НОВИЙ ЧИСЕЛЬНИЙ ПІДХІД ДО ВИЗНАЧЕННЯ РАДІАЦІЙНИХ ПЕРЕХОДІВ У СПЕКТРАХ ДЕКОТРИХ СКЛАДНИХ ІОНІВ

Т. О. Флорко

Резюме. Виконано розрахунок енергій, імовірностей та сил осциляторів ряду радіаційних переходів у спектрі складних іонів на основі нової чисельної релятивістської схеми в межах калібровочно-інваріантної теорії збурень.

Ключові слова: детектування радіаційних переходів, складні іони, релятивістська схема

НОВЫЙ ЧИСЛЕННЫЙ ПОДХОД К ОПРЕДЕЛЕНИЮ ВЕРОЯТНОСТЕЙ РАДИАЦИОННЫХ ПЕРЕХОДОВ В СПЕКТРАХ НЕКОТОРЫХ СЛОЖНЫХ ИОНОВ

Т. А. Флорко

Резюме. Выполнен расчет вероятностей и сил осцилляторов ряда радиационных переходов в спектре сложных ионов на основе новой численной релятивистской схемы в рамках калибровочно-инвариантной теории возмущений.

Ключевые слова: детектирование радиационных переходов, сложные ионы, 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.[1-11]). 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. 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, correlation, radiative effects [1-8]. In references [7-9] 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 relativistic PT and new effective procedures for accounting the nuclear and radiative corrections. Here we propose a new numerical relativistic scheme for radiative transitions basing on the gauge-invariant QED perturbation theory formalism [7-9] and the ideas of the Refs. [9-11]. We study the spectrum of energy levels and the probability of E2 and M1 forbidden radiative transitions between the low-lying configurations 3s23p5, 3s3p63p43d, 3p44s singly ionized argon atom. It should be noted that the spectral information on rare gas atoms and ions, in particular, neon, and argon, is crucial, for example, for diagnostic laboratory plasma [1-5]. The unknown atoms and ions are present in a tokamak plasma, stellator. Finally, the atoms and ions of argon found in astrophysical objects (nebulae, stars, etc.) [1,2]. From a theoretical point of view, the desired atoms and ions are a class of highly complex systems due to the high sensitivity of the calculated energies and transition probabilities for the quality and completeness of both relativistic and correlation effects.

2. New relativistic approach to sensing and determination of the radiative 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 [9]. The wave function for a particular atomic state [10]:

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

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

$$H_{DC}=\Sigma_i \{c\alpha_i p_i + (\beta_i-1)c^2 - Z/r + V(r|nlj)\} + \\ + \Sigma_{i>j} \exp(i\omega r_{ij})(1-\alpha_1\alpha_2)/r_{ij}. \quad (2)$$

In this equation the potential:

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

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 [9]. The effective electron core density (potential V_c) is defined by iteration algorithm within gauge invariant QED procedure [2,7].

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 [2,7]. In the zeroth QED PT approximation we, as usually (c.f.[9]), use the one electron bare potential

$$V_N(r) + V_C(r), \quad (4)$$

with $V_N(r)$ describing the electric potential of the nucleus, $V_C(r)$, imitating the interaction of the quasi-particle with the core. The core potential $V_C(r)$ is related to the core electron density $\rho_C(r)$ 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 $\rho_C(r)$. In ref.[7] 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. [7] 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 [2,9].

In order to define the probability of radiative transition we have used energy approach [6,7]. In this approach 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:

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

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

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

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

$$\Gamma_{\alpha_n} = \frac{1}{4\pi}\cdot V^{|\omega_{\alpha_n}|}_{\alpha_n\alpha_n}. \quad (7)$$

According to [6,7], a matrix element in (7) is written as follows:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2}\sum_{\lambda\mu}(-1)^{\mu}\begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \\ \times \mathrm{Im}\,Q_\lambda(1234); \quad Q_\lambda = Q^{\mathrm{Qul}}_\lambda + Q^{\mathrm{Br}}_\lambda. \quad (8)$$

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

$$Q_\lambda^{\mathrm{Qul}} = \frac{1}{Z}\{R_l(1243)S_\lambda(1243) + R_\lambda(\tilde{1}243)S_\lambda(\tilde{1}243) +$$
$$+ R_\lambda(1\tilde{2}43)S_\lambda(1\tilde{2}43) + R_\lambda(\tilde{1}\tilde{2}43)S_\lambda(\tilde{1}\tilde{2}43)\} \quad (9)$$

where f is the large component of radial part of single electron state Dirac function; the sign «~» means that in (10) 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 Breit part of Q is defined as the sum:

$$Q_\lambda^{\mathrm{Br}} = Q_{\lambda,\lambda-1}^{\mathrm{Br}} + Q_{\lambda,\lambda}^{\mathrm{Br}} + Q_{\lambda,\lambda+1}^{\mathrm{Br}}, \quad (10)$$

where the contribution of our interest is determined as:

$$Q_\lambda^{\mathrm{Br}} = \frac{1}{Z}\mathrm{Re}\{R_\lambda(12\tilde{4}\tilde{3})S_\lambda^l(12\tilde{4}\tilde{3}) + R_\lambda(\tilde{1}\tilde{2}43)S_\lambda^l(1243) +$$
$$+ R_l(\tilde{1}2\tilde{4}3)S_\lambda^l(\tilde{1}2\tilde{4}3) + R_l(1\tilde{2}4\tilde{3})S_\lambda^l(1\tilde{2}4\tilde{3})\}. \quad (11)$$

All calculations are performed using modified Superatom code developed by Ivanov et al [6-10].

3. Results and conclusions

We have considered the energy and transition probabilities for the 39 low-lying levels of the ArII: 3s23p5, 3s3p6, 3p43d, 3p44s. These states are in the PT formalism treated as 1 - and 3-QP state electron (4s, 3d) ($3p^{-1}$ vacancy) over the core of the filled electron shells 3s23p6. The structure of the low-lying levels ArII includes two odd levels with total angular momentum J = 1/2, J = 3/2 configuration 3s23p5 and 37 excited levels with J = 1/2, J = 3/2 configurations 3s3p6, 3p43d, 3p44s. Among these levels of the excited states with only the levels with J< 5/2 chance of E1 radiative transition to the ground state of the ion. On levels with J = 7/2 chance of M2 transition to the ground state. On levels with J = 7/2, 9/2 (eg, configuration 3p43d) possible inhibition of E2 and M1 transitions to lower lying levels of the same parity. Secular matrix as usual including states with the same total angular momentum and of the same parity. Interaction QP-frame described by the potential (3), actually simulates DF potential self-consistent field. The effects of polarization interaction QPs through polarizable core and screening (antiscreening in case of an electron-vacancy interactions) were taken into account as part of the procedure described above [2,7-9,12,13]. Table 1 shows the theoretical values of the excitation energies (in cm-1) for some levels with J = 5/2, calculated in various approximations: MCDF theory, MCDF theory plus accounting for the Breit corrections (MCDF+Breit), our theory and the experimental data [14]. In general, our theory provides a perfectly acceptable description of the structure of the spectrum, in most cases, more accurate than alternative MCDF methods. However, for some of the terms (for example, $3s^23p^4(^1D)3d^2S^e_{1/2}$, $3s^23p^4(^1S)3d^2D^e_{5/2}$, $3s^23p^4(^1S)3d^2D^e_{3/2}$) computation error is large enough and far beyond the standard spectroscopic, which is evidence of very strong inter-configuration interaction in the spectrum of the ion Ar+. Apparently, an adequate description of these terms requires a significant expansion of the secular matrix to account also high-lying configurations. We believe that in the spectrum of the studied ion there is an effect of the so-called "plunging" configurations of 3p4p4d and others. These configurations for the corresponding ion perturb the discrete spectrum, significantly increasing the interaction configurations.

Table 1. The excitation energies (in cm-1) levels with J = 5/2 in various approximations: MCDF (with accounting different numbers of additionally accounted configurations), MCDF+ Breit, our theory data and the experimental data (look text).

Level	MCDF	MCDF 4*l*(SD)	MCDF+ Breit	Our data	Experiment
$3s3p^6\ ^2S^e_{1/2}$	112307	110781	108772	108754	108721
$3s^23p^4(^3P)3d^4D^e_{1/2}$	137892	135584	133154	132965	132737
$3s^23p^4(^3P)4s\ ^4P^e_{1/2}$	139843	138088	135756	135673	135601
$3s^23p^4(^3P)3d\ ^4P^e_{1/2}$	157482	151676	148453	147441	147228

Table 2. Probability of M1 (s^{-1}) of the forbidden transitions in the spectrum AgII calculated in the method MCDF+ Breit (a) and our approach (b)

The initial state	The final state	a	b
$3s^23p^{52}P^o_{1/2}$	$3s^23p^{52}P^o_{3/2}$	5.46(-2)	5.34(-2)
$3s^23p^4(^1D)3d^2G^e_{9/2}$	$3s^23p^4(^3P)3d^2F^e_{7/2}$	1.50(-2)	1.39(-2)
$^2G^e_{7/2}$	$^2F^e_{7/2}$	4.28(-2)	4.12(-2)
$3s^23p^4(^3P)3d^4F^e_{9/2}$	$^4D^e_{7/2}$	4.11(-2)	3.98(-2)
$3s^23p^4(^1D)3d^2F^e_{7/2}$	$3s^23p^4(^1D)3d^2G^e_{7/2}$	1.24(-2)	1.01(-2)
$3s^23p^4(^3P)3d^4F^e_{7/2}$	$3s^23p^4(^3P)3d^4D^e_{7/2}$	3.36(-2)	3.23(-2)
$3s^23p^4(^1D)3d^2G^e_{7/2}$	$^4F^e_{5/2}$	5.30(-2)	5.18(-2)
$^2G^e_{9/2}$	$^4F^e_{7/2}$	6.87(-2)	6.69(-2)
$^2G^e_{7/2}$	$^4F^e_{7/2}$	8.73(-2)	8.52(-2)
$^2F^e_{7/2}$	$^2F^e_{5/2}$	3.67(-2)	3.55(-2)
$3s^23p^4(^3P)3d^2F^e_{7/2}$	$^4D^e_{5/2}$	2.48(-2)	2.32(-2)
$^2F^e_{7/2}$	$^4D^e_{7/2}$	1.05(-1)	0.92(-1)

Table 2 lists the data on M1 probability of the forbidden transitions between the levels of low-lying configurations in the spectrum AgII, calculated using the methods of the MCDF+ Breit and our theory. The only available experimental value of the probability of 5.32×10^{-2}=5.32(-2) M1 transition. $3s^23p^{52}P^o_{1/2}$ - $3s^23p^{52}P^o_{3/2}$ is consistent with our value (error ~ 0.4%), while the error in the calculation by the MCDF method is about 3%.

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. Secondly, calculation has confirmed the great role of the interelectron correlation effects of the second and higher PT orders, namely, effects of the interelectron polarization interaction and mutual screening.

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