ОПТИЧНІ, ОПТОЕЛЕКТРОННІ І РАДІАЦІЙНІ СЕНСОРИ

OPTICAL, OPTOELECTRONIC AND RADIATION SENSORS

PACS 32.15RM; УДК 539.184

SENSING RADIATIVE TRANSITIONS PROBABILITIES IN SPECTRA OF SOME Ne-LIKE ULTICHARGED IONS

A. V. Glushkov, T. A.Florko, A. V. Ignatenko, D. E.Sukharev

Odessa State Environmetal University, Odessa
I. I.Mechnikov Odessa National University, Odessa

SENSING RADIATIVE TRANSITIONS PROBABILITIES IN SPECTRA OF SOME Ne-LIKE ULTICHARGED IONS

A. V. Glushkov, T. A.Florko, A. V. Ignatenko, D. E. Sukharev

Abstract. On the basis of new relativistic scheme within gauge-invariant quantum electrodynamics (QED) perturbation theory (PT) it has been carried out sensing and calculating the energies and probabilities of some radiative transitions in spectra of the complex Ne-like multicharged ions, plasma of which is of a great interest as an active medium for new short-wave lasers.

Keywords: sensing radiative atomic transitions, Ne-like multicharged ions

ВИЗНАЧЕННЯ ІМОВІРНОСТЕЙ РАДІАЦІЙНИХ ПЕРЕХОДІВ У СПЕКТРАХ ДЕЯКИХ Ne-ПОДІБНИХ БАГАТОЗАРЯДНИХ ІОНІВ

О. В. Глушков, Т. О. Флорко, Г. В. Ігнатенко, Д. Є.Сухарев

Анотація. На основі нової релятивістської схеми в межах калібровочно-інваріантної КЕД теорії збурень виконано розрахунок ймовірностей радіаційних переходів у спектрах декотрих складних неоно-подібних багатозарядних іонів, плазма яких представляє інтерес як активне середовище короткохвильових лазерів.

Ключові слова: детектування радіаційних атомних переходів, неоно-подібні багатозарядні іони

ОПРЕДЕЛЕНИЕ ВЕРОЯТНОСТЕЙ РАДИАЦИОННЫХ ПЕРЕХОДІВ В СПЕКТРАХ НЕКОТОРЫХ Ne-ПОДОБНЫХ МНОГОЗАРЯДНЫХ ИОНОВ

А. В. Глушков, Т. А. Флорко, А. В. Игнатенко, Д. Е. Сухарев

Аннотация. На основе новой релятивистской схемы в рамках калибровочно-инвариантной КЭД теории возмущений выполнен расчет вероятностей радиационных атомных переходов в спектрах некоторых сложных неоно-подобных многозарядных ионов, плазма которых представляет интерес как активная среда для коротковолновых лазеров.

Ключевые слова: детектирование радиационных атомных переходов, неоно-подобные многозарядные ионы

1. Introduction.

Traditionally an investigation of spectra, spectral, radiative and autoionization characteristics for heavy and superheavy elements atoms and multicharged ions is of a great interest for further development atomic and nuclear theories and different applications in the plasma chemistry, astrophysics, laser physics, etc. (see Refs. [1–13]). Theoretical methods of calculation of the spectroscopic characteristics for heavy atoms and ions may be divided into a few main groups. First, the well known, classical multi-configuration Hartree-Fock method (as a rule, the relativistic effects are taken into account in the Pauli approximation or Breit hamiltonian etc.) allowed to get a great number of the useful spectral information about light and not heavy atomic systems, but in fact it provides only qualitative description of spectra of the heavy and superheavy ions . Second, the multi-configuration Dirac-Fock (MCDF) method is the most reliable version of calculation for multielectron systems with a large nuclear charge. In these calculations the one- and two-particle relativistic effects are taken into account practically precisely. The calculation program of Desclaux (the Desclaux program, Dirac package) is compiled with proper account of the finiteness of the nucleus size. However, a studying of complicated multielectron multicharged ions with a great contribution of the exchange-correlation effects by standard methods is connected with great principal and calculational problems. Though, in last years there is a great progress in this topic.

The isoelectronic sequence of neon has been especially thoroughly investigated, but nevertheless remains of interest because of the spectra of Ne-like ions are the source of the most important information for the solution of a wide variety of problems in the hot, dense, thermonuclear plasmas spectroscopy, physics of the shortwave lasers etc. The detailed analysis of spectra of the Ne-like ions has been performed, for example, in Refs. [2,11-17]. In Refs. [11-13] it has been used the relativistic PT with the empirical zeroth approximation, and optimization of the one-quasiparticle wave functions bases is not specially fulfilled, though using the empirical information about corresponding one-quasiparticle atomic ion energies allowed indirectly take into account the correlation corrections. In this paper we have used an advanced relativistic energy approach [3,14] within gauge-invariant QED perturbation theory and carried out sensing and calculating the energies and probabilities of some radiative transitions in spectra of the complex Ne-like multicharged ions, plasma of which is of a great interest as an active medium for new short-wave lasers. Some interesting possibilities can be found in refs. [2-4,10,18-20].

2. An advanced relativistic energy approach to determination of the radiative transition probabilities

Let us describe in brief the important moment of the used theoretical approach. An advanced relativistic energy approach is in details presented in our previous refs. [2-4,14-17]. Following to these refs, let us note that, as usually, the relativistic PT wave functions zeroth basis is found from the Dirac equation solution with potential, which includes the core ab initio potential, electric potentials of nucleus. All correlation corrections of the PT second and high orders (electrons screening, particle-hole interaction etc.) are accounted. Configuration mixing coefficients c_r are obtained through diagonalization of the Dirac Coulomb Hamiltonian:

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

In this equation the potential:

$$V(r)=V_c(r|nlj)+V_{ex}+V_{nucl}(r|R). \quad (2)$$

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 [3,4]. The effective electron core density (potential V_c) is defined by iteration algorithm within gauge invariant QED procedure [2,3,14]. 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 [14]. It is on the electromagnetic potentials gauge (the gauge non-invariant contribution Im δE_{ninv}). 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. [14] authors treated the function ρ_c in the simple analytic form with the only variable parameter b and substituted it to (2). More accurate calculation requires the solution of the integral differential equation for the ρ_c [2-4].

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 [6,12]:

$$\operatorname{Im} \Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\leq f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}, \qquad (3)$$

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

$$V_{ijkl}^{|\omega|} = \int dr_1 dr_2 \varnothing_i^*(r_1) \varnothing_j^*(r_2) \frac{\sin|\omega| r_{12}}{r_{12}} (1-\alpha_1\alpha_2) \varnothing_k^*(r_2) \varnothing_l^*(r_1) \qquad (4)$$

The separated terms of the sum in (3) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha_n} = \frac{1}{4\pi} \cdot V_{\alpha_n \alpha_n}^{|\omega_{\alpha_n}|} \qquad (5)$$

The corresponding oscillator strength : $gf = \lambda_g^2 \cdot \tilde{A}_{\alpha_n} / 6.67 \cdot 10^{15}$, where g is the degeneracy degree, g is a wavelength in angstrems (Å). Under calculating the matrix elements (3) 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:

$$\frac{\sin|\omega| r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0}^{\infty} (\lambda) J_{\lambda+\frac{1}{2}}(|\omega| r_1) J_{\lambda+\frac{1}{2}}(|\omega| r_2) P_\lambda(\cos \mathbf{r}_1 \mathbf{r}_2) \qquad (6)$$

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 (5) to matrix element of interaction gives as follows:

$$V_{1234}^{\omega} = [(j_1)(j_2)(j_3)(j_4)]^{\frac{1}{2}} \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times \mathbf{Im}\, Q_\lambda(1234),$$

$$Q_\lambda = Q_\lambda^{\text{Qul}} + Q_\lambda^{\text{B}}, \qquad (7)$$

where j_i are the entire single electron momentums, m_i – their projections; Q_λ^{Qul} is the Coulomb part of interaction, Q_λ^{B} - the Breit part. The Coulomb part Q_λ^{Qul} is expressed in terms of radial integrals R_λ, angular coefficients S_λ [12]:

$$\begin{aligned} \operatorname{Im} Q_\lambda^{\text{Qul}} = \frac{1}{Z} \operatorname{Re} \{ & R_l(1243) S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3}) S_\lambda(\tilde{1}24\tilde{3}) \\ & + R_\lambda(1\tilde{2}\tilde{4}3) S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3}) S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3}) \}. \end{aligned} \qquad (8)$$

As a result, the decay probability is expressed in terms of ReQ_λ(1243) matrix elements:

$$\operatorname{Im} R_\lambda(1243) = \int dr_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1) f_2(r_2) f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>) . \qquad (9)$$

where f is the large component of radial part of the Dirac function and function Z is [12]:

$$Z_{\lambda}^{(1)} = \left[\frac{2}{|\omega_{\text{ж}}|\alpha Z}\right]^{\lambda+1/2} \frac{J_{\lambda+1/2}(\alpha|\omega_{\text{ж}}|r)}{r^{\lambda}\Gamma(\lambda+3/2)}. \qquad (10)$$

The angular coefficient is defined by standard way [12]. The other items in (8) include small components of the Dirac functions; the sign «~» means that in (8) 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 $æ_i<0$. AN account of the Breit interaction may considerably change the decay dynamics in some cases [3]. The Breit part of Q is defined following to Refs. [12]. All calculations are carried out using the effective "Superatom-ISAN" code initially developed by Ivanov and coworkers (see Refs. [2-4, 6,11-16]).

3. Results and conclusions

In tables 1 and 2 we present the values of probabilities of the transitions between levels of the configurations $2s^22p^53s$,3d,4s,4d and $2s2p^63p$,4p in the Ne-like ions of the Ni XIX and Br XXVI (in s^{-1}; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP) [11-13]; c1 – REA-PT data (without account of the correlation corrections); c2 – REA-PT data (with account of the correlation); exp.- experimental data (and Refs. [2-4,11-13] therein).

Table 1 Probabilities of radiation transitions between levels of the configurations $2s^22p^53s$,3d,4s,4d and $2s2p^63p$,4p in the Ne-like ion of Ni XIX (in s^{-1}; total angle moment J=1): a – the MCDF method; b- relativistic PT with the empirical zeroth approximation (RPTMP); c1,2 – REA PT data (without and with account of the correlation corrections); exp.- experimental data (see text).

Analysis of the presented data shows that the REA-PT method provides a physically reasonable agreement between theoretical and experimental data. Let us note that the transition probabilities values in the different photon propagator gauges are practically equal (see comments in Refs. [1,2,14,21]). An account of the correlation effects is of a great importance to provide the spectroscopic accuracy. The received set of the data is principally important for investigations of the possible laser effect in a plasma of the studied Ne-like ions.

Table 2. Probabilities of radiation transitions between levels of the configurations $2s^22p^53s$,3d,4s,4d and $2s2p^63p$,4p in the Ne-like ion of Br XXVI (in s^{-1}; total angle moment J=1): a – the DF method; b- RPTMP; c1,2 – REA PT data (without and with account of the correlation corrections); exp.- experimental data.

Level J=1	Exp.	a-MCDF	b-RPTMP	c1-REA PT	c2-REA PT
$2p_{3/2}3s_{1/2}$	7.6+11	9.5+11	1.3+12	9.7+11	8.1+11
$2p_{1/2}3s_{1/2}$	6.0+11	1.8+12	1.0+12	7.6+11	6.2+11
$2p_{3/2}3d_{3/2}$	1.4+11	2.2+11	1.5+11	1.7+11	1.4+11
$2p_{3/2}3d_{5/2}$	1.2+13	2.1+13	1.2+13	1.5+13	1.2+13
$2p_{1/2}3d_{3/2}$	3.2+13	4.8+13	3.6+13	4.0+13	3.3+13
$2s_{1/2}\ 3p_{1/2}$	-	-	8.5+11	9.5+11	8.1+11
$2s_{1/2}\ 3p_{3/2}$	-	-	5.1+12	5.6+12	4.7+12
$2p_{3/2}4s_{1/2}$	3.3+11	-	3.6+11	4.1+11	3.4+11
$2p_{1/2}4s_{1/2}$	2.0+11	-	3.0+11	3.1+11	2.4+11
$2p_{3/2}4d_{3/2}$	4.5+10	-	5.2+10	5.4+10	4.8+10
$2p_{3/2}4d_{5/2}$	8.3+12	-	8.3+12	9.2+12	8.2+12
$2p_{1/2}4d_{3/2}$	8.1+12	-	7.9+12	8.9+12	8.0+12
$2s_{1/2}4p_{1/2}$			-	6.3+11	5.7+11
$2s_{1/2}4p_{3/2}$			-	2.7+12	2.4+12

Level *J*=1	Exp.	a-MCDF	b-RPTMP	c1-QED PT	C2-QED PT
$2p_{3/2}3s_{1/2}$	4.5+12	6.2+12	4.4+12	5.5+12	4.4+12
$2p_{1/2}3s_{1/2}$	3.1+12	4.8+12	2.8+12	3.6+12	2.7+12
$2p_{3/2}3d_{3/2}$	2.8+11	3.9+11	2.9+11	3.5+11	2.8+11
$2p_{3/2}3d_{5/2}$	6.1+13	8.0+13	6.3+13	7.5+13	6.1+13
$2p_{1/2}3d_{3/2}$	8.6+13	9.5+13	8.7+13	9.9+13	8.6+13
$2s_{1/2}\ 3p_{1/2}$	3.9+12	-	4.2+12	4.7+12	4.0+12
$2s_{1/2}\ 3p_{3/2}$	1.4+13	-	1.5+13	1.8+13	1.4+13
$2p_{3/2}4s_{1/2}$	1.1+12	-	1.2+12	1.5+12	1.1+12
$2p_{1/2}4s_{1/2}$	2.1+12	-	2.5+12	2.8+12	2.3+12
$2p_{3/2}4d_{3/2}$	2.8+10	-	7.3+10	6.9+10	6.3+10
$2p_{3/2}4d_{5/2}$	-	-	2.8+13	2.7+13	2.3+13
$2p_{1/2}4d_{3/2}$	2.0+13	-	2.2+13	2.3+13	2.0+13
$2s_{1/2}4p_{1/2}$	2.5+12	-	-	2.9+12	2.6+12
$2s_{1/2}4p_{3/2}$	7.1+12	-	-	8.9+12	8.0+12

References

1. Grant I. P., Relativistic Quantum Theory of Atoms and Molecules, Theory and Computation, Springer Series on Atomic, Optical, and Plasma Physics.- Berlin: Springer, Berlin.— 2007.— Vol.40.— P.587–626.
2. Glushkov A. V., Advanced relativistic energy approach to radiative decay processes in multielectron atoms and multicharged ions// Advances in the Theory of Quantum Systems in Chemistry and Physics.— Berlin: Springer.-2012 — Vol.28. — P.51–74.
3. Glushkov A. V., Relativistic quantum theory. Quantum mechanics of atomic systems.- Odessa: Astroprint, 2008. — 700P.
4. Glushkov A. V., Lovett L., Florko T. A., et al, Gauge-invariant QED perturbation theory approach to studying the nuclear electric quadrupole moments, hyperfine structure constants for heavy atoms and ions// Frontiers in Quantum Systems in Chemistry and Physics.-Berlin: Springer. — 2008. — Vol.18. — P.505–522.
5. K. G. Dyall, K. Faegri, Jr. Introduction to Relativistic Quantum Theory.- Oxford University Press, 2007.-680P.
6. Ivanova E. P., Ivanov L. N., Aglitsky E.V., Modern trends in spectroscopy of multicharged ions// Physics Rep.-1991.-Vol.166,N6. — P.315–390.
7. Dorofeev D. L., Zon B. A., Kretinin I. Y., Chernov V. E., Method of the Quantum Defect Green's Function for Calculation of Dynamic Atomic Polarizabilities// Opt. Spectr.-2005.-Vol. 99.-P. 540-548.
8. Sahoo B. K., Gopakumar G., Chaudhuri R. K. , Das B. P., Merlitz H., Mahapatra U.S., Makherjee D., Magnetic dipole hyperfine interactions in ^{137}Ba^{+} and the accuracies of neutral weak interaction matrix elements// Phys.Rev.A-2003.-Vol.68.-P.040501.
9. Derevianko A., Porsev S. G., Dressing lines and vertices in calculations of matrix elements with the coupled-cluster method and determination of Cs atomic properties// Phys.Rev. A. — 2005. — Vol.71. — P.032509.
10. Safronova U. I., Safronova M. S., Third-order relativistic many-body calculations of energies, transition rates, hyperfine constants, and blackbody radiation shift in ^{171}Yb^{+}//Phys. Rev. A. — 2009.-Vol.79.-P.022512.
11. Glushkov A. V., Ivanova E. P. Theoretical Study of Multicharged Ions Spectra of F- and Ne- Isoelectronic Sequence// J.Quant.Spectr. Rad.Transfer. — 1986.-Vol.36, N2.-P.127-145.
12. Ivanova E. P., Ivanov L. N., Glushkov A. V.,

Kramida A. E. High order corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-like and Ne-like ions //Phys.Scripta –1985.-Vol.32,N4.-P.512-524.

13. Ivanova E. P., Gulov A. V. Theoretical investigation of the neon isoelectronic sequence// Atom.Data.Nucl.Data.Tabl. — 1991. — Vol.49. — P.1–64.
14. Glushkov A. V., Ivanov L. N. Radiation decay of atomic states: atomic residue and gauge non-invariant contributions // Phys. Lett.A.— 1992. — Vol.170,N1. — P.33-37
15. Glushkov A. V., Relativistic calculation and extrapolation of oscillator strengths in Fr-like ions by model potential method// Opt. Spectr. — 1991. — Vol.70. — P.952–955.
16. Glushkov A. V., Relativistic calculation of oscillator strengths in multicharged ions with single electron above closed shells core// Opt. Spectr.— 1992. — Vol.72. — P.542–547.
17. Florko T. A., Loboda A. V., Svinarenko A. A., Sensing forbidden transitions in spectra of some heavy atoms and multicharged ions: new theoretical scheme// Sensor Electr. and Microsyst. Techn. — 2009. — N3. — P.10-15.
18. Bieron J., Froese-Fischer C., Fritzsche S., Pachucki K., Lifetime and hyperfine structure of the $^3D_2$ state of radium //J. Phys.B:At.Mol. Opt.Phys.— 2004. — Vol.37. — P.L305–311
19. Khetselius O. Y., Hyperfine structure of radium// Photoelectronics.— 2005.— Vol.14.— P.83–85.
20. Gurnitskaya E. P., Heavy ion storage ring experimental and theoretical determination of the lifetimes for the iron ion levels// Photoelectronics.—2005.—Vol.14.—P.50–54.
21. Kunisz M. D., Coulomb approximation oscillator strengths for some transitions in rare earths// Acta Phys.Polon.—1982.—Vol.a62.— P.285–296.

Стаття надійшла до редакції...