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SENSING THE OPTIMAL PLASMA PARAMETERS FOR X-RAY LASING: DEBYE SHIELDING APPROACH CALCULATION OF ELECTRON-COLLISION EXCITATION CROSS-SECTIONS FOR PLASMA IONS

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Summary

SENSING THE OPTIMAL PLASMA PARAMETERS FOR X-RAY LASING: CALCULAION OF ELECTRON-COLLISION STRENGTHS FOR AR-LIKE PLASMA

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A new high-accuracy theoretical spectroscopy scheme is used for sensing the laser plasma parameters. Within the uniform energy approach, it is carried out debye shileding approach calculation of cross-sections of electron-collisional excitation for ions of Ba in Ar-plasma.

Key words: sensing plasma parameters, debye shileding approach, electron-collisional excitation cross-section

Резюме

ДЕТЕКТУВАННЯ ОПТИМАЛЬНИХ ПАРАМЕТРІВ ПЛАЗМИ ДЛЯ РЕАЛІЗАЦІЇ ЛАЗЕРНОГО ЕФЕКТУ У РЕНТГЕНІВСЬКОМУ ДІАПАЗОНІ: РОЗРАХУНОК СИЛ ЕЛЕКТРОННИХ ЗІТКНЕНЬ ДЛЯ AR-ПОДІБНОЇ ПЛАЗМИ

О. В. Глушков, Е. П. Гурницька, Д. О. Корчевський, А. В. Лобода

Нова теоретична схема використана у задачі детектування параметрів лазерної плазми. Вперше отримані дані про перерізи електронного збудження за рахунок зіткнень для іонів Ba в аргоновій плазмі з використанням наближення дебаєвсьного екранювання.

Ключові слова: детектування параметрів плазми, наближення дебаєвсьного екранювання , переріз збудження за рахунок електронних зіткнень

Резюме

ДЕТЕКТИРОВАНИЕ ОПТИМАЛЬНЫХ ПАРАМЕТРОВ ПЛАЗМЫ ДЛЯ РЕАЛИЗАЦИИ ЛАЗЕРНОГО ЭФФЕКТА В РЕНТГЕНОВСКОМ ДИАПАЗОНЕ: РАСЧЕТ СИЛ ЭЛЕКТРОННЫХ СТОЛКНОВЕНИЙ ДЛЯ AR-ПОДОБНОЙ ПЛАЗМЫ

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Новая теоретическая схема использована в задаче детектирования и диагностики параметров лазерной плазмы. Впервые получены данные о сечениях электронно-столкновительного возбуждения для ионов Ba в аргоновой плазме с использованием приближения дебаевского экранирования.

Ключевые слова: детектирование параметров плазмы, приближение дебаевского экранирования, сечение электрон-столкновительного возбуждения.

The properties of laser-produced hot and dense plasmas, known as laser plasma, have drawn considerable attention ove the last two decades through the recent laser-fusion studies [1-14]. Similar interest is also stimulated by importance of this information for correct determination of the characteristics for plasma in thermonuclear (tokamak) reactors, searching new mediums for X-ray range lasers. The X-ray laser problem has stimulated a great number of papers devoting to development of theoretical methods for the modelling the elementary processes in a collisionally pumped plasma. In ref. [10-14] two new consistent relativistic and QED versions for calculations of the spectroscopic characteristics of the multicharged ions in plasma have been developed. Ih this paper we use them for sensing and diagnostics of the laser plasma parameters, i.e. within the uniform energy approach we have defined the cross-sections of electron-collisional excitation for ion of Ba in Ar-plasma. The key momet of present calculation is the using the Debye shielding approximation. It is a main difference from the analogous calculation for Ne-like [11-13] and Ar-like [17] ions. Recent advances in ultra-short laser technologies have shown laser plasmas tyo be a favourable source of quantum emission. In such extremely dense laser plasmas an electronic temperature of T_e=0,1-10 keV and a particle density of $r_e=10^{21}$-10^{25}cm^{-3} can be achieved. This suggests that the electronic structrue of atoms in plasmas is larely perturbed by a strong interactions with nearby charged particles. Recent studies report emission lines from several hydrogen-like atoms exhibiting a red spectral shift in the range of 0,07-3,7 eV and significant line broadening [3].

Let us present the key moments of the new consistent perturbation theory (PT) version for calculation of the electron collision strengths and rate coefficients of electron-collisional excitation for ions in a plasma [12-14]. It bases on the gauge invariant QED energy approach to construsction of the relativictic functions basis's [15,16] and using the Green's function method for accounting of the complex exchange-correlation, radiation and others corrections. Within the Gell-Mann and Low approach with the QED scattering matrix (c.f.[9,10,14]) the secular matrix elements are already complex in the second order of the perturbation theory (PT). The imaginary parts are connected with the radiation decay (radiation) possibility. The total energy shift of the state is usually presented in the form: DE = ReDE + i ImDE, Im DE = -G/2, where G is interpreted as the level width, and the decay possibility P = G. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to calculation and diagonalization of the complex matrix M. Usually one uses for this purpose a one-electron Hamiltonian with a central potential that can be treated as a bare potential in the formally exact QED PT. The bare potential includes the electric potential of the atomic nucleus and some model potential that is to be compensated for in all orders of PT. There are many well-known attempts to find the more fundamental optimization principles for the bare one-electron Hamiltonian. The minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels is proposed in [14] as "ab initio" optimization principle (see below). In our calculations of different characteristics we dealt with atoms and ions having one, two or three quasi-particles (electron or vacancies) outside the core of

closed electron shells. For example, the excited states {Ne]$3s^2 3p^5$nl of the Ar-like ion is a two-quasi-particle (2QP) state. It is usually accepted, as the bare potential, a potential including the electric nuclear potential V_N and some parameterized potential V_C, that imitates the interaction of closed-shell electrons with quasi-particles. The parameters of the model bare potential are chosen so as to generate accurate eigen-energies of all one-quasi-particle (1QP) states, i.e. $3s3p^6$, $3s^2 3p^5$ states of the Cl-like ion and $3s^2 3p^6$nl states of K-like ions, with the same nucleus. Usually the experimental one-quasi-particle energies are used for determination of parameters of the model potential (c.f.[8-10,15,16]).

In the Debye-Huckel theory of plasmas the interaction potential between two-charged particles in plasmas is modelled by a Yukawa-type potential [3]:

$$V(r_a, r_b) = \frac{Z_a Z_b}{|r_a - r_b|} \exp(-\mu |r_a - r_b|) \qquad (1)$$

where r_a,r_b represent respectively the spatial coordinates of particles A and B and Z_a,Z_b define the charges. The comparison of the Yukawa-type potential with a Coulombic potential shows that the effect of plasma is modelled by the shielding parameter m that describes the shape of the long-range potential. This shielding parameter is given as a function of temperature T and the charge density n by $\mu = (e^2 n / \varepsilon_o k_B T)^{1/2}$, where n is given as the sum of the electron-density N_e and the ion density N_k of the k-th ion species having the nuclear charge q_k as $n = N_e + \sum_k q_k^2 N_k$. Under typical laser plasma conditions of T~ 1keV and n~10^{22}cm^{-3}, the m patameter is of the oreder0,1 in atomic uinit. This is our case. Since m patameter is scaled by the square-root of the ratio *n/T*, both of a hot-dense plasma and a low-density warm plasma cam be characterized by m. By introducing the Yukawa-type electron0nuclear attraction and electron-electron repulsion potentials, the electronic Hamiltonian for an N-electron atom in a plasma is thus given in atomic units as (c.f.[3]):

$$H = \sum_{i=1}^{N} (\alpha c p_i - \beta c^2) - \sum_{i=1}^{N} \frac{Z}{|r_i|} \exp(-\mu |r_i|) + \sum_{i>j}^{N} \frac{1}{|r_i - r_j|} \exp(-\mu |r_i - r_j|) \qquad (2)$$

In the PT second order the energy shift is expressed in terms of two-electron matrix elements:

$$V(1,2;4,3) = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)} \times (-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \times \sum_{\lambda,\mu} (-1)^{\mu} \begin{bmatrix} j_1 \ldots\ldots j_3 \ldots \lambda \\ m_1 . - m_{3 \ldots} \mu \end{bmatrix} \begin{bmatrix} j_2 \ldots\ldots j_4 \ldots \lambda \\ m_2 . - m_4 .. \mu \end{bmatrix} \times (Q_\lambda^{Qul} + Q_\lambda^{Br}) \qquad (3)$$

Here Q_λ^{Qul} , Q_λ^{Br} are corresponding to the Coulomb and Breit inter-electron interaction, which expresses through the radial integrals of the Coulomb (Yukawa) inter-electron interaction [11,13]. To calculate all necessary matrix elements one must use the basis's of the 1QP relativistic functions. In many calculations of characteristics of the atomic elementary processes it has been shown that adequate description of these characteristics requires using the optimized basis's of wave functions. In ref. [15] it has been proposed "ab initio" optimization principle for construction of cited basis's. There is used the minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels. The details of procedure can be found in [15]. Here we briefly describe the key moments. In the fourth order of QED PT there appear diagrams, whose contribution into the ImdE accounts for the core polarization effects (polarization of the closed shell core by the quasi-particle). This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). Let us examine the multi-electron atom with 1QP in the first excited state, connected with the ground state by the radiation transition. In the zeroth order of QED PT we use the one-electron bare potential $V_N(r) + V_C(r)$. The core potential $V_C(r)$ is related to the core electron density $r_C(r)$ in a standard way [15,16]. Moreover, all the results of the approximate calculations are the functionals of the density $r_C(r)$. The minimization of the density functional $Im\ DE_{ninv}$ leads to the integral differential equation for the r_c, that is numerically solved. In result one can get the optimal one-electron basis of PT. Below we first use such a basis in calculation of the electron-collision cross-sections and strengths. Further we briefly discuss the energy approach in scattering theory 11,12] and give main formulas. We briefly outline the main idea using, as an example, the

collisional de-excitation of the Ar-like ion: $((3j_{iv})^{-1}4j_{ie}[J_iM_i],\ e_{in}) \to (F_o, e_{sc})$. Here F_o is the state of the ion with closed shells (ground state of the Ar-like ion); J_i is the total angular moment of the initial target state; indices *iv, ie* are related to the initial states of vacancy and electron; indices e_{in} and e_{sc} are the incident and scattered energies, respectively to the incident and scattered electrons. It is convenient to use the second quantization representation. In particular, the initial state of the system "atom plus free electron" can be written as

$$|I>=a_{in}^{+}\sum_{m_{iv},m_{ie}} a_{ie}^{+}a_{iv}\Phi_o C_{m_{ie},m_{iv}}^{J_i,M_i} \qquad (4)$$

Here $C_{m_{ie},m_{iv}}^{J_i,M_i}$ is the Clebsh-Gordan coefficient. Final state is: $|F>=a_{sc}^{+}\Phi_o$, where Φ_o is the state of an ion with closed electron shells (ground state of Ar-like ion), $|I>$ represents three-quasiparticle (3QP) state , and $|F>$ represents the one-quasiparticle (1QP) state. For the state (1) the scattered part of energy shift *Im* D*E* appears first in the PT second order in the form of integral over the scattered electron energy e_{sc}:

$$\int d\varepsilon_{sc} G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc})/(\varepsilon_{sc}-\varepsilon_{iv}-\varepsilon_{ie}-\varepsilon_{in}-i0) \qquad (5)$$

with $$Im\mathrm{D}E=\mathrm{p}\,G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc}) \qquad (6)$$

Here *G* is a definite squired combination of the two-electron matrix elements (2). The value s=-*2 Im*D*E* represents the collisional cross-section if the incident electron eigen-function is normalized by the unit flow condition and the scattered electron eigen-function is normalized by the energy d function. The collisional strength $\Omega(I \to F)$ is connected with the collisional cross section s by expression (c.f. [10,11]):

$$\sigma(I \to F)=\frac{\Omega(I \to F)\cdot\pi}{\{(2J_i+1)\varepsilon_{in}[(\alpha Z)^2\varepsilon_{in}+2]\}} \qquad (7)$$

Here and below the Coulomb units are used; 1 C.u. $\approx 27{,}054Z^2$ eV, for energy; 1 C.u.$\approx 0{,}529\cdot 10^{-8}/Z$ cm, for length; 1 C.u. $\approx 2{,}419\cdot 10^{-17}/Z^2$ sec for time. The collisional de-excitation cross section is:

$$\sigma(IK \to 0)=2\pi\sum_{j_{in},J_{sc}}(2j_{sc}+1)\times$$
$$\times\{\sum_{j_{ie},j_{iv}}<0\,|\,j_{in},j_{sc}\,|\,j_{ie},j_{iv},J_i>B_{ie,iv}^{IK}\}^2 \qquad (8)$$

Here $B_{ie,iv}^{IK}$ is a real matrix of eigen-vectors coefficients, which is obtained after diagonalization of the secular energy matrix. The amplitude like combination in (8) has the following form:

$$<0\,|\,j_{in},j_{sc}\,|\,j_{ie},j_{iv},J_i>=\sqrt{(2j_{ie}+1)(2j_{iv}+1)}\times$$
$$\times(-1)^{j_{ie}+1/2}\times\sum_{\lambda}(-1)^{\lambda+J_i}\times$$
$$\times\{\delta_{\lambda,J_i}/(2J_i+1)Q_\lambda(sc,ie;iv,in)+$$
$$+\begin{bmatrix} j_{in}\ldots j_{sc}\ldots J_i \\ j_{ie}\ldots j_{iv}\ldots\ldots\lambda \end{bmatrix} Q_\lambda(ie;in;iv,sc)\} \qquad (9)$$

In (9) values Q_λ^{Qul} and Q_λ^{Br} are defined in ref. [11]. For the collisional excitations from ground state (inverse process) one must consider $a_{in}^{+}\Phi_0$ as the initial state and

$$|F>=a_{sc}^{+}\sum_{m_{fe},m_{fv}} a_{fe}^{+}a_{fv}\Phi_o\tilde{C}_{m_{fe},m_{fv}}^{J_f,M_f} \qquad (10)$$

as a final state. The cross-section is as follows:

$$\sigma(0 \to IF)=2\pi(2J_f+1)\sum_{j_{in},j_{sc}}(2j_{sc}+1)\cdot$$
$$\cdot\{\sum_{j_{fe},j_{fv}}B_{fe,fv}^{FK}<j_{fe},j_{fv}J_f\,|\,j_{in},j_{sc}\,|\,0>\}^2 \qquad (11)$$

The different normalization conditions are used for the incident and for the scattered electron wave functions. Upon the normalization multipliers one gets symmetrical expressions for the excitation and de-excitation, saving the weight multiplier $(2J_f+1)$ in (11). The expression for the cross-section of the collisional excited-excited *IK-IF* transition can be found in [13]. The details of the whole numerical procedure of calculation of the collisional cross-section and strength can be found in [11-17]. It is worthwhile to indicate that the energy approach with using the optimal one-electron basis of PT first is used by us for description of elementary electron processes in collisionally pumped plasma. We applied our approach to estimate of the electron collisional excitation cross-sections, strengths of the electron-collisional excitation for some Ar-like ions. To test our theory we earlier [12] compared our calculations results on collisional cross-sections for Ne-like iron with known calculations. Comparison with experimental energies encourages us to believe in the accuracy for highly excited states for which there is no experimental information. Our results on electron collision strengths from the ground state for Ar -like barium are presented in table 1 for two approximations: i). the Coulombic-type (C) potentials approximation; ii). the Yukawa-type (Yu) potentials one (1).

Table 1

Calculated electron-collisional excitation cross-sections (s) for Ar-like barium for two values of incident electron energy 5,8keV (Units are 10^{-21} cm^2).

Level J	E_{el}=5.8 keV (C)	E_{el}=5.8 keV (Yu)
Sum (J=0)	3,59	3,20
$3p_{3/2}3d_{5/2}$ 1	4,28	3,81
$3p_{1/2}3d_{3/2}$ 1	2,75	2,48

As the analysis of calculation cross-sections for different levels of the Ba ion shown , the difference between results of calculations with using the Coulombic-type and Yukawa-type potentials reaches ~ 5-15%, that is an evidence of the inportance the shielding effects in hot laser plasma for X-ray lasing. The experimental information about the electron-collisional cross-sections for high-charged Ar-like ions is absent, so our results can be considered as first ones.

References

1. Eds. Aumar F. and Winter H. 1997 Photonic, Electronic and Atomic Collisions. (Singapore: World Sci.); Koshelev K.N., Sidelnikov Y.V., Vikhrov V.V., Ivanov V.I. 1991 Spectroscopy of multicharged ions, Ed. Safronova U.I. (Moscow: Nauka) p.163
2. Klimontovich Yu.L. 1982 Kinetic theory of non-ideal gases and non-ideal plasmas (N. — Y.: Pergamon Press); Kremp D., Semkat D. and Bonitz M. 2003 Progress in Nonequilibrium Green's Functions, Ed. Bonitz M. (Singapore: World. Sci.) p.34.
3. Okutsu H., Sako T., Yamanouchi K., Diercksen G.H.F., Electronic structure of atyoms in laser plasmas: a Debae shielding approach// J.Phys.B. — 2005. — Vol.38. — P.917-927.
4. Rosmej F.B., Hoffman D.H., Geissel M. et al, Advanced X-ray diagnostics based on an observation of high-energy Rydberg transitions from autoionizing levels in dense laser-produced plasmas// Phys. Rev.A. — 2001-Vol.63. — P.063409-063418.
5. Chenais-Popovics C., Rancu O., Renaudin P., Gauthier J.C. X-ray Spectroscopy of Laser-Produced Hot Dense Plasmas// Phys.Scripta. — 1996. — Vol.65,N1. — 163-168.
6. Glushkov A.Deuterium lines spectra analysis in Tokamak// Proc.24th Europ. Conf. on Thermonucl. Fusion and Plasma Physics (Garching, Germany). — 1996.
7. Gurnitskaya E.P., Sensing fontenau-aux-roses tokamak plasma parameters by means x-ray theoretical spectroscopy method: new scheme//Sensor Electr.&Microsys.Tech. — 2005. — N4. — P.43-46.
8. Ivanova E.P., Ivanov L.N. Modern Trends in Spectroscopy of Multicharged Ions// Physics Rep. — 1991. — Vol.166,N6. — P.315-390.
9. Glushkov A.V., Ivanov L.N., Ivanova E.P. Radiation decay of Atomic States: generalized Energy Approach// Autoionization Phenomena in Atoms. — M.: Moscow Univ. — 1986.
10. Ivanov L.N., Ivanova E.P., Knight L. Energy Approach to consistent QED theory for calculation of electron-collision strengths//Phys.Rev.A. — 1993. — Vol.48,N6. — P.4365-4374
11. Glushkov A.V., Malinovskaya S.V., Loboda A.V., Shpinareva I.M., Gurnitskaya E.P., Korchevsky D.A., Diagnostics of the collisionally pumped plasma and search of the optimal plasma parameters of x-ray lasing: Calculation of electron-collision strengths and rate coefficients for Ne-like plasma// J.Phys.CS. — 2005. — Vol.11. — P.188-198.
12. Glushkov A.V., Ambrosov S.V., Ignatenko A.V., Korchevsky D.A., DC Strong Field Stark Effect for Non-hydrogenic Atoms: Consistent Quantum Mechanical Approach // Int.Journ.Quant.Chem. — 2004. — Vol.99,N5. — P.936-939.
13. Glushkov A.V., Gurnitskaya E.P., Ambrosov S.V., Loboda A.V., Prepelitsa G.P., Consistent QED approach to calculation of electron-collision excitation cross-sections and strengths: Ne-like ions // Int. Journ.Quant.Chem. — 2005. — Vol.104, N4 . — P. 562-569.
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. Negative Ions of Inert Gases// JETP Lett. — 1992. — Vol.55, N2- C.95-98.
16. Glushkov A.V., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., Khetselius O.Yu., QED calculation of heavy multicharged ions with account for the correlation, radiative and nuclear effects// Progress of Theor. Phys. and Chem. — 2005. — Vol.41. — P.315-324.
17. Gurnitskaya E.P., Korchevsky D.A., Loboda A.V., Sensing the optimal plasma parameters for x-ray lasing: calculation of electron-collision excitation cross-sections for Ar-like plasma ions//Sensor Electr. and Microsyst. Techn. — 2006. — N1. — P.21-25.