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SENSING THE OPTIMAL PLASMA PARAMETERS FOR X-RAY LASING: CALCULATION OF ELECTRON-COLLISION EXCITATION CROSS-SECTIONS FOR AR-LIKE PLASMA IONS

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Abstract

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

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A new advanved high-accuracy theoretical spectroscopy scheme is used for sensing the optimal collisionally pumped plasma parameters of X-ray lasing. Within the uniform energy approach, it is carried out calculation of electron collision strengths and cross-sections of electron-collisional excitation for ions of Ba in Ar-plasma.

Key words: sensing plasma parameters, X-ray lasing, 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

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

Нова високоточна теоретична схема використана у задачі детектування оптимальних параметрів колізійно накачуємої плазми для лазерного ефекту у рентгенівському діапазоні. Вперше отримані дані про сили електронних зіткнень, перерізи електронного збудження за рахунок зіткнень для іонів Ba в аргоновій плазмі.

Ключові слова: детектування параметрів плазми, лазерний ефект у рентгенівському діапазоні, 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 высокоточная теоретическая схема использована в задаче детектирования и диагностики параметров стокновительно накачиваемой плазмы и поиске оптимальных плазменных параметров для лазерного эффекта в рентгеновском диапазоне. Впервые получены данные о силах электронных столкновений, сечениях электронно-столкновительного возбуждения для ионов Ba в аргоновой плазме.

Ключевые слова:детектирование параметров плазмы, лазерный эффект в рентгеновском диапазоне, сечение электрон-столкновительного возбуждения.

In last years it is of a great interest the experimental and theoretical studies concerning sensing and diagnostics of the parameters of collisionally pumped plasma and search of the optimal plasma parameters for lasing (c.f. [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. There is a hope to find lasing effects on the transitions in the Ne-, Cl-, Ar-, Ni-like 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 the parameters of collisionally pumped plasma and search of the optimal plasma parameters of X-ray lasing, in particular, within the uniform energy approach we have defined the electron collision strengths and cross-sections of electron-collisional excitation for ions of Ba in Ar-plasma.

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 relatifictic functions basis's [15,16] and using the Green's function method for accounting of the complex exchange-correlation, radiation and others corrections. Our version allows to take into account the QED, radiative effects (c.f.[17]). Let us also note that, for example, methods [2,3,7,8] do not allow to account in the entire degree the correlation effects and the QED effects.

In the theory of the non-relativistic atom a convenient field procedure is known for calculating the energy shifts ΔE of degenerate states. This procedure is connected with the secular matrix M diagonalization. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used. A similar approach, using the Gell-Mann and Low formula with the QED scattering matrix, is applicable in the relativistic atom theory (c.f.[9-12]). In contrast to the non-relativistic case, the secular matrix elements are already complex in the second order of the perturbation theory (PT) (first order of the inter-electron interaction). Their imaginary parts are connected with the radiation decay (radiation) possibility. The total energy shift of the state is usually presented in the form:

$$\Delta E = \mathrm{Re}\Delta E + \mathrm{i}\ \mathrm{Im}\Delta E \quad \mathrm{Im}\ \Delta E = -\Gamma/2 \qquad (1)$$

where Γ is interpreted as the level width, and the decay possibility $P = \Gamma$. 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. To start with the QED Gell-Mann and Low formula one must choose the zero-order approximation. 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 or (what is the same) for the basis of one-electron functions which represents such a Hamiltonian. The min-

imization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels is proposed in [15] as "ab initio" optimization principle (see below). In our calculations of different characteristics we dealt with atoms and ions having one, two or three quasiparticles (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-quasiparticle (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 second order of the QED PT the energy shift is expressed in terms of two-electron matrix elements

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

Here Q_λ^{Qul} is corresponding to the Coulomb inter-electron interaction:

$$Q_\lambda^{\mathrm{Qul}} = \{R_\lambda(1243)S_\lambda(1243) + \\ +R_\lambda(\tilde{1}243\tilde{)}S_\lambda(\tilde{1}243\tilde{)} + R_\lambda(1\tilde{2}4\tilde{3})S_\lambda(1\tilde{2}4\tilde{3}) \\ +R_\lambda(\tilde{1}\tilde{2}4\tilde{3}\tilde{)}S_\lambda(\tilde{1}\tilde{2}4\tilde{3}\tilde{)}\}. \qquad (3)$$

where $R\lambda(1,2;4,3)$ is the radial integral of the Coulomb inter-electron interaction with large radial components; the tilde denotes a small component; S is the angular multiplier (see expressions in ref.[11,12]). Expession for the Breit inter- electron interaction part is simnmilar to (3) and presented also in ref.[11,12].

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 ImδE 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 $\rho_C(r)$ in a standard way [15,16]. Moreover, all the results of the approximate calculations are the functionals of the density $\rho_C(r)$. The minimization of the density functional $Im\,\Delta E_{ninv}$ leads to the integral differential equation for the ρ_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: $((3j_{iv})^{-1}4j_{ie}[J_iM_i],\ \varepsilon_{in}) \rightarrow (\Phi_o, \varepsilon_{sc})$. Here Φ_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 ε_{in} and ε_{sc} are the incident and scattered energies, respectively to the incident and scattered electrons. Further 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:

$$|F> = a_{sc}^{+}\Phi_o . \qquad (5)$$

where Φ_o is the state of an ion with closed electron shells (ground state of ne-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* ΔE appears first in the second order of the atomic perturbation theory (fourth order of the QED perturbation theory) in the form of integral over the scattered electron energy ε_{sc}:

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

with $$Im\Delta E=\pi\ G(\varepsilon_{iv},\varepsilon_{ie},\varepsilon_{in},\varepsilon_{sc}) \quad (6)$$

Here G is a definite squired combination of the two-electron matrix elements (2). The value σ=*-2 Im*ΔE 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 δ function.

The collisional strength $\Omega(I \to F)$ is connected with the collisional cross section σ by expression (c.f. [10,11]):

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

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:

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

Here $B^{IK}_{ie,iv}$ 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:

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

In (15) values Q^{Qul}_λ and Q^{Br}_λ are defined by the expressions (3) and (5). For the collisional excitations from the ground state (inverse process) one must consider $a^+_{in}\Phi_0$ as the initial state and

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

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

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

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 [12]. 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 some Ar -like ions are presented in table 1.

Summation over j_{in},j_{sc} in (11) spreads over the range 1/2-23/2. The convergence of this sum has been numerically investigated. It should be noted that the higher partial-wave contribution is less than 0,8% for all states considered. 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. In table 1 we present measured electron-collisional excitation cross-sections σ for Ar-like barium for two values of incident electron energy. The next step in order to make sensing the parameters of collisionally pumped plasma and search of the optimal plasma parameters of X-ray lasing includes the kinetics calculation (c.f.[12]0 to determine level populations, inversions, line intensities and gain coefficients etc. at definite plasma parameters and will be considered in a separated paper.

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Table 1

Calculated electron-collisional excitation cross-sections (σ) for Ar-like barium for two values of incident electron energy 5,8keV and 9,5keV (Units are $10^{-21}cm^2$).

Level J	E_{el}=5.8 keV	Level J	E_{el}=9,5 keV
Sum (J=0)	3,59	Sum (J=0)	2,79
$3p_{3/2}3d_{5/2}$ 1	4,28	$3p_{3/2}3d_{5/2}$ 1	3,96
$3p_{1/2}3d_{3/2}$ 1	2,75	$3p_{1/2}3d_{3/2}$ 1	2,58

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