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## SENSING THE ELECTRON-COLLISION EXCITATION CROSS-SECTIONS FOR NE-LIKE IONS OF FE IN A PLASMA IN THE DEBYE SHIELDING APPROXIMATION

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### Abstract

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Within the uniform QED energy approach with using the Debye shielding approximation it is carried out the calculation of cross-sections of electron-collisional excitation for ions of Fe in Ne-like plasma.

**Key words:** sensing, electron-collisional excitation cross-section, QED approach, Debye shielding approximation

### Резюме

ДЕТЕКТУВАННЯ ПЕРЕРІЗІВ ЕЛЕКТРОН-КОЛІЗІЙНОГО ЗБУДЖЕННЯ НЕ-ПОДІБНИХ  
ІОНІВ FE У ПЛАЗМІ У НАБЛИЖЕННІ ДЕБАЄВСЬКОГО ЕКРАНЮВАННЯ

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Отримані дані про перерізи електронного збудження за рахунок зіткнень для іонів Fe у Ne-подібній плазмі на підставі КЕД підходу з використанням наближення дебаєвського екранювання.

**Ключові слова:** переріз збудження за рахунок електронних зіткнень, КЕД підхід, дебаєвське екранювання

### Резюме

ДЕТЕКТИРОВАНИЕ СЕЧЕНИЙ ЭЛЕКТРОН-СТОЛКНОВИТЕЛЬНОГО ВОЗБУЖДЕНИЯ  
НЕ-ПОДОБНЫХ ИОНОВ FE В ПЛАЗМЕ В ПРИБЛИЖЕНИИ ДЕБАЕВСКОГО  
ЭКРАНИРОВАНИЯ

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Получены данные о сечениях электронно-столкновительного возбуждения для ионов Fe в Ne-подобной плазме на основе КЭД подхода с использованием приближения дебаевского экранирования.

**Ключевые слова:** сечение электрон-столкновительного возбуждения, КЭД подход, дебаевское экранирование

In this paper we present the results of calculation of the electron collision strengths and cross-sections for Ne-like ion of iron within earlier developed new uniform energy approach, formally based on the quantum electrodynamics (QED) [1-4]. The key moment is connected with using the Debye shielding approximation (see below). Obtained data can be used in kinetic calculations of the multicharged ions plasma in order to define the optimal parameters for X-ray lasing (c.f.[5-10]). The matter in a fact that in last years the X-ray laser problem has stimulated a great number of papers devoted to the development of theoretical methods for modelling the elementary processes in collisionally pumped plasma (c.f. [13-19]). There is a hope to find lasing effects on the transitions of Li-, Ne-, Ni-like ions.

Two principal theoretical problems must be solved in order to develop a special code adequate to predict the plasma parameters needed to generate a soft-X-ray or extreme ultraviolet amplified spontaneous emission: i). accurate calculation of electron-collisional excitation cross-sections, strengths, rate coefficients for elementary processes in the plasma that are responsible for formation of emission lines spectra; ii). kinetics calculations to determine level populations, inversions, line intensities and gain coefficients at definite plasma parameters. The most elaborate codes for atomic calculations are based on different kinds of approximations to the multi-configuration Dirac-Fock method (c.f. [11]). In our opinion, the most consistent approach to construction of the optimized one-quasi-electron functions must be based on the QED. Namely such an approach is here used in calculating the electron collision strengths and cross-sections on Ne-like ion of Fe. Consider the key ideas of the method following to refs.[1-4,12,15,19].

Their imaginary parts are connected with the radiation decay (radiation) possibility. The total energy shift of the state is usually presented in the form (c.f.[7,8,12]):

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

where  $\Gamma$  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. The minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels is proposed in [12] as “ab initio” optimization principle.

Recent advances in ultra-short laser technologies have shown laser plasmas to 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  $\rho_e=10^{21}-10^{25}\text{cm}^{-3}$  can be achieved. This suggests that the electronic structure of atoms in plasmas is largely perturbed by a strong interactions with nearby charged particles. Recent studying reports 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 [14-18]. So, the Debye shielding approximation is to be used. In the Debye-Huckel theory of plasmas the interaction potential between two-charged particles in plasmas is modelled by a Yukawa-type potential [16]:

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

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  $\mu$  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  $\mu = (e^2 n / \epsilon_0 k_B T)^{1/2}$ , 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  $T \sim 1\text{keV}$  and  $n \sim 10^{22}\text{cm}^{-3}$ , the  $\mu$  parameter is of the order 0,1 in atomic units. This is our case. Since  $\mu$  parameter is scaled by the square-root of the ratio  $n/T$ , both of a hot-dense plasma and a low-density warm plasma can be characterized by  $\mu$ . By introducing the Yukawa-type electron-nuclear attraction and electron-electron repulsion potentials, the electronic Hamiltonian for an  $N$ -electron atom in a plasma is thus given in atomic units as:

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

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  $1s^2 2s^2 2p^5 nl$  of the Ne-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.  $1s 2s^2 2p^6$ ,  $1s^2 2s 2p^6$ ,  $1s^2 2s^2 2p^5$  states of the F-like ion and  $1s^2 2s^2 2p^6 nl$  states of Na-like ions, with the same nucleus. The individual quasi-particle eigen-functions and eigen-energies satisfy the one-quasi-particle Dirac equation with model potential. Further, this potential is used as a bare potential in the PT of states with any number of quasi-particles outside the same core. To avoid accounting for the 1QP effects twice we omit the real parts of contributions of 1QP Feynman diagrams in orders of PT, thus the theoretical consistency is preserved. The method provides the reliable level structure in the zero-order PT at least for the 2QP and 3QP systems (c.f.[4,6,7,9]). In the second order of the QED PT the energy shift is expressed in terms of two-electron matrix elements [12]:

$$V(1,2;4,3) = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)} \times (-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \times \sum_{\lambda,\mu} (-1)^\mu \begin{bmatrix} j_1 \dots j_3 \dots \lambda \\ m_1 \dots m_3 \dots \mu \end{bmatrix} \begin{bmatrix} j_2 \dots j_4 \dots \lambda \\ m_2 \dots m_4 \dots \mu \end{bmatrix} \times (Q_\lambda^{Qu} + Q_\lambda^{Br}) \quad (3)$$

Here  $Q_\lambda^{Qu}$  is corresponding to the matrix elements of the Coulomb-Yukawa-type interaction and  $Q_\lambda^{Br}$  - the Breit interaction part. To calculate all necessary matrix elements one must use the basis's of the 1QP relativistic functions.. In ref. [12] it has been proposed "ab initio" optimization principle for construction of cited basis's. The details of procedure can be found in [1,12].

When studying the Stark effect, electron-positron pair production in nuclear collisions and el-

ementary processes responsible for emission-lines formation in plasmas, the energy approach has been generalized to cover the problems of scattering theory (c.f. [1-3,8,12]). Here we briefly outline the main idea using, as an example, the collisional de-excitation of the Ne-like ion:  $((2j_{iv})^{-1} 3j_{ie} [J_i M_i], \varepsilon_{in}) \rightarrow (\Phi_o, \varepsilon_{sc})$ . Here  $\Phi_o$  is the state of the ion with closed shells (ground state of the Ne-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  $\varepsilon_{in}$  and  $\varepsilon_{sc}$  are the incident and scattered energies, respectively to the incident and scattered electrons. The initial state of system "atom plus free electron" can be written as

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

Here  $C_{m_{ie}, m_{iv}}^{J_i, M_i}$  is the Clebsh-Gordan coefficient. Final state is:  $|F\rangle = a_{sc}^+ \Phi_o$ , where  $\Phi_o$  is the state of an ion with closed electron shells (ground state of ne-like ion),  $|I\rangle$  represents three-quasiparticle (3QP) state, and  $|F\rangle$  represents the one-quasiparticle (1QP) state. The justification of the energy approach in the scattering problem is in details described in refs. [1-3,8,12]. For the state (1) the scattered part of energy shift  $Im \Delta E$  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  $\varepsilon_{sc}$ :

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

with  $Im \Delta E = \pi G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc})$ . Here  $G$  is a definite squared combination of the two-electron matrix elements (2). The value  $\sigma = -2 Im \Delta E$  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  $\delta$  function. The collisional strength  $\Omega(I \rightarrow F)$  is connected with the collisional cross section  $\sigma$  by expression:

$$\sigma(I \rightarrow F) = \Omega(I \rightarrow F) \cdot \pi / \{(2J_i + 1) \varepsilon_{in} [(\alpha Z)^2 \varepsilon_{in} + 2]\} \quad (6)$$

Here and below the Coulomb units are used; 1 C.u.  $\approx 27,054 Z^2$  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:

$$\sigma(IK \rightarrow 0) = 2\pi \sum_{j_{in}, j_{sc}} (2j_{sc} + 1) \times \left\{ \sum_{j_{ie}, j_{iv}} \langle 0 | j_{in}, j_{sc} | j_{ie}, j_{iv}, J_i \rangle B_{ie, iv}^{IK} \right\}^2 \quad (7)$$

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 (7) has the following form:

$$\begin{aligned} & \langle 0 | j_{in}, j_{sc} | j_{ie}, j_{iv}, J_i \rangle = \\ & = \sqrt{(2j_{ie}+1)(2j_{iv}+1)} (-1)^{j_{ie}+1/2} \times \sum_{\lambda} (-1)^{\lambda+J_i} \times \\ & \quad \times \{ \delta_{\lambda, J_i} / (2J_i + 1) Q_{\lambda}(sc, ie; iv, in) + \\ & \quad + \left[ \begin{matrix} j_{in} \dots j_{sc} \dots J_i \\ j_{ie} \dots j_{iv} \dots \lambda \end{matrix} \right] Q_{\lambda}(ie; in; iv, sc) \} \quad (8) \end{aligned}$$

For the collisional excitations from the ground state (inverse process) the analogous expressions can be derived (c.f.[1,2]). The details of the whole numerical procedure are in [1-5,12,15,19].

We applied our approach to estimate of the electron collisional excitation cross-sections and strengths for Ne-like ion of iron and compare the obtained results with other calculation and experiment. We do not present here the results of our calculations of energy levels for Ne-like ions. The practically coincide with the same results, presented in [1,8]. There the one-electron basis of PT was calibrated on experimental one-electron energies. Here we use ab initio one-electron basis. The first or-

der PT correction is calculated exactly, the high-order contributions are taken into account effectively: polarization interaction of two above-core quasi-particles and the effect of their mutual screening (c.f.[12]). It should be noted that strong compensation of different PT terms is a characteristic feature of the states with vacancies in the core. This is one of the main reasons for the fact that the accuracy of conventional a priori calculations of such states does not always satisfy the requirements arising in many applications. Comparison with experimental energies (c.f.[1,2]) 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 Ne-like iron are presented in table 1. The whole table of data will be published separately. Summation over  $j_{in} j_{sc}$  in (7) 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 incident electron energy is  $E_{el}=1,0454\text{keV}$ . Our results are presented in two approximations: i) purely Coulomb approximation; ii). the Debye shielding approximation. Analysis shows that difference between data in both approximations can reach 5-15%.

Table 1

Electron-collision strengths for excitation from the ground state of Ne-like iron ( $E_i=1,0454\text{keV}$ ) in two approximations: i) purely Coulomb approximation; ii). the Debye shielding approximation. The numbers in brackets denote multiplicative powers of ten.

Transition	Level	J	Present theory (ii)	Present theory (i)
1-2	2s 2p	0	1,125[-03]	1,022[-03]
3	2p <sub>3/2</sub> 3s <sub>1/2</sub>	1	2,671[-03]	2,342[-03]
4	2p <sub>1/2</sub> 3s <sub>1/2</sub>	0	2,169[-04]	2,008[-04]
5	2p <sub>1/2</sub> 3s <sub>1/2</sub>	1	2,234[-03]	1,013[-03]
6	2p <sub>3/2</sub> 3p <sub>3/2</sub>	1	2,831[-03]	23462[-03]
7	2p <sub>3/2</sub> 3p <sub>3/2</sub>	3	3,115[-03]	2,806[-03]
8	2p <sub>3/2</sub> 3p <sub>1/2</sub>	2	2,998[-03]	2,828[-03]
9	2p <sub>3/2</sub> 3p <sub>1/2</sub>	1	1,102[-03]	1,053[-03]
10	2p <sub>3/2</sub> 3p <sub>3/2</sub>	2	2,659[-03]	2,332[-03]
11	2p <sub>1/2</sub> 3p <sub>1/2</sub>	1	2,758[-03]	2,554[-03]
12	2p <sub>1/2</sub> 3p <sub>1/2</sub>	0	1,171[-03]	1,104[-03]
13	2p <sub>1/2</sub> 3p <sub>3/2</sub>	2	1,239[-03]	1,158[-03]

It should be noted that the experimental information about the electron-collisional cross-sections for high-charged Ne-like ions is very scarce and is extracted from indirect observations. Our results are at the lower margin of experimental error as the corresponding data (c.f.[1,2]). But one must understand that extraction of the cross section from the experiment is very complicated procedure. In

any case we have physically reasonable agreement between theory and experiment (see more detailed comparison in [1-3]). It is important to note that inclusion into consideration of Rydberg and autoionization Rydberg states of ions of the previous ionization stage will definitely increase collisional cross-sections. The method, which allows treatment of these states on an equal basis with the ad-

acent continua has been elaborated in the scattering theory [1,2]. The numerical calculations on this subject are in the progress.

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