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

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Abstract. The problem of diagnostics for the collisionally pumped plasma and search of the optimal plasma parameters of X-ray lasing are studied. We present the uniform energy approach, formally based on the quantum electrodynamics with using gauge invariant scheme of generation of the optimal one-electron representation, for the calculation of electron collision strengths and rate coefficients for electron-collisional excitation. The aim is to study, in a uniform manner, elementary processes responsible for emission-line formation in plasmas. The electron collision excitation cross-sections and rate coefficients for some Ne-like ions (Fe, Ba) are calculated. To test the results of calculations we compare them with other authors calculations and with available experimental data.

1. Introduction
Calculation of emission spectra of the plasma ions based in high-precision quantum-electrodynamics techniques is practical tool, which may be used instead of very expensive sophisticated experiments. Given systematic data about intensities of spectral lines and respective gins, one can establish basic rules of plasma motion in phase space. An important application of the theory of atomic spectra in plasma is search of the optimum plasma excitation condition for lasing and discovery of new pumping approaches. In addition, these investigations are important to understand the plasma processes themselves. The history of plasma spectrum modeling extends for decades, starting with the simplest models (see, e.g., [1–5]). Different atomic levels are populated in laboratory plasma by different physical processes. This results in a different dependence of each line intensity on the plasma parameters. It had been understood for a long time that this phenomenon could be used for plasma diagnostics. The general principles of such a diagnostic for the simple H-like and He-like ions have been formulated (c.f. [1–4]). These diagnostic principles have proven to be useful for understanding the physics of the system and for planning new experiments.

In recent 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. [1–23]). There is a hope to find lasing effects on the transitions of Li-,...
Ne-, Ni-like ions. Very shocking example is a scheme for accomplishing tabletop X-ray lasing
in Li-like ion of Ne at 98 Å in optically ionized plasma during recombination in the transient
regime [2]. Saturation effects and parametric heating processes by stimulated Raman scattering
are analyzed and found to allow energy efficiencies in excess of $10^{-5}$ for a 100-fsec duration,
0.25-µm laser driver of intensity $10^{17}$ W cm$^{-2}$. Significant improvement in efficiency is possible
for shorter laser pulse lengths. However, low temperature plasma sources are more efficient
and less expensive devices. They show promise for producing lasing in the vacuum ultraviolet
and soft X-ray region. Preliminary investigations of capillary spark discharge were made (c.f.
[2–5]), which show the possibility of their use as effective plasma sources for the generation of a
soft-X-ray or extreme ultraviolet amplified spontaneous emission.

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 and rate coefficients for elementary processes in the plasma that are responsible for
the formation of emission lines spectra (c.f. [1, 3, 10]); ii). kinetics calculations to determine
level populations, inversions, line intensities and gain coefficients at definite plasma parameters
(c.f. [3, 10, 24]). Under steady-state plasma conditions two dominating elementary processes
should be included: i). electron-collisional excitation and de-excitation; ii). radiative relaxation
of excited states. We consider the inclusion of the highly-lying Rydberg and autoionization
Rydberg states of the ions of the previous ionization stage into kinetic scheme to be one of the
most important refinement of the usually used models. Another principal refinement is connected
with using optimized basis’s of atomic wave functions in calculation scheme. It is well known that
a search of the optimal one-quasi-electron representation is a traditional problem of quantum
chemistry during last several decades. The most elaborate codes for atomic calculations are
based on different kinds of approximations to the multi-configuration Dirac-Fock procedure (c.f.
[5]). Alternative solutions are known as the method of natural orbitals and the density-functional
approach [6, 7]. In our opinion, the most consistent approach to construction of the optimized
one-quasi-electron functions must be based on the quantum electrodynamics (QED). In ref.
[11] the problem of the construction of the optimal one-electron representation in the theory of
the multi-electron atom is reduced to the minimization of the gauge dependent multielectron
contribution to the radiation widths of atomic levels. The procedure is based on the well-known
Gell-Mann and Low adiabatic formalism for energy shift with electrodynamics scattering matrix
(the energy approach).

In this paper we consider a problem of diagnostics for the collisionally pumped plasma
and search of the optimal plasma parameters of X-ray lasing. We present the uniform energy
approach, formally based on the QED theory with using gauge invariant scheme of generation
of the optimal one-electron representation, for the calculation of electron collision strengths,
cross-sections and rate coefficients [3]. The aim is to study, in a uniform manner, elementary
processes responsible for emission-line formation in plasmas. The electron collision excitation
cross-sections, strengths and rate coefficients for some Ne-like ions are calculated. To test the
results of calculations we compare them with other authors’ calculations and with available
experimental data.

2. Energy approach in the theory of decaying atomic states
Following to ref. [3, 10, 11] we remind the key aspects of applying energy approach in the
theory of decaying atomic states. In the theory of the non-relativistic atom a convenient field
procedure is known for calculating the energy shifts $\Delta E$ of degenerate states. This procedure
is connected with the secular matrix $M$ diagonalization [17]. In constructing $M$, the Gell-Mann
and Low adiabatic formula for $\Delta E$ is used. A similar approach, using the Gell-Mann and Low
formula with the QED scattering matrix, is applicable in the relativistic atom theory [8–11, 15,
The method is a consistently electrodynamics one, allowing for the uniform consideration of a variety of induced and spontaneous processes different by their physical nature and with any number of photons. The energy approach had been applied previously in the study of the purely electronic, electron-nuclear processes in atoms and meso-atomic systems, in the problem of the collisional electron-positron pair production [8–18]. 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) [15, 16, 18]. Their imaginary parts are connected with the radiation decay (radiation) possibility. The total energy shift of the state is usually presented in the form:

\[ \Delta E = \text{Re} \Delta E + i \text{Im} \Delta E \quad \text{Im} \Delta E = -\Gamma/2 , \]

(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 \( M \). In the papers of different authors, the calculation procedure for \( \text{Re} \Delta E \) has been generalised for the case of nearly degenerate states, whose levels form a more or less compact group. One of these variants has been previously used by us [15] for a system with a dense energy spectrum, a group of nearly degenerate states is extracted and their matrix \( M \) is calculated and diagonalized. If the states are well separated in energy, the matrix \( M \) reduces to one term, equal to \( \Delta E \). 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. Here one should mention the method of natural orbitals of Davidson [7]. The diagonalization of the ‘exact’ one-electron density matrix of the many-electron systems is accepted as the optimization principle in this method. Another famous solution is known as the density functional method [6]. The minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels is proposed in [11] as \textit{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 \( 1s^22s^22p^{nl} \) 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. \( 1s^2s^2p^6, 1s^22s2p^6, 1s^22s^22p^5 \) states of the F-like ion and \( 1s^22s^22p^{6nl} \) states of Na-like ions, with the same nucleus. Usually the experimental one-quasi-particle eigen-energies are used for determination of parameters of the model potential (c.f. [8–10, 15, 16]). The individual quasi-particle eigen-functions and eigen-energies satisfy the one-quasi-particle Dirac equation with model potential [8–10]. 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 consistence is preserved. The method provides the reliable level structure in the zero-order PT at least for the 2QP and 3QP systems (c.f. [8–10, 15–18]). In the second order of the QED PT the energy shift is expressed in terms of two-electron matrix elements.
\[ V(1, 2; 4, 3) = \sqrt{(2j_1 + 1)(2j_2 + 1)(2j_3 + 1)(2j_4 + 1)}(-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \times \]
\[ \times \sum_{\lambda, \mu} (-1)^\mu \left( \begin{array}{ccc} j_1 & j_3 & \lambda \\ m_1 & -m_3 & \mu \end{array} \right) \left( \begin{array}{ccc} j_2 & j_4 & \lambda \\ m_2 & -m_4 & \mu \end{array} \right) (Q_\lambda^{Qul} + Q_\lambda^{Br}). \]  

Here \( Q_\lambda^{Qul} \) is corresponding to the Coulomb inter-electron interaction:

\[ Q_\lambda^{Qul} = \{ R_\lambda(1243)S_\lambda(1243) + R_\lambda(\bar{1}24\bar{3})S_\lambda(\bar{1}24\bar{3}) + R_\lambda(\bar{1}\bar{2}4\bar{3})S_\lambda(\bar{1}\bar{2}4\bar{3}) + R_\lambda(\bar{1}\bar{2}\bar{4}\bar{3})S_\lambda(\bar{1}\bar{2}\bar{4}\bar{3}) \} . \]  

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. The angular multiplier in (3) is as follows [15]:

\[ S_\lambda(1243) = \{ \lambda l_1 l_3 \} \{ \lambda l_2 l_4 \} \left( \begin{array}{ccc} j_1 & j_3 & \lambda \\ 1/2 & -1/2 & 0 \end{array} \right) \left( \begin{array}{ccc} j_2 & j_4 & \lambda \\ 1/2 & -1/2 & 0 \end{array} \right) , \]

with factorized angular part \( S(1243) \):

\[ Q_\lambda^{Br} = \{ R_\lambda(1\bar{2}4\bar{3})S_\lambda'(1\bar{2}4\bar{3}) + R_\lambda(\bar{1}\bar{2}4\bar{3})S_\lambda'(\bar{1}\bar{2}4\bar{3}) + R_\lambda(\bar{1}\bar{2}\bar{4}\bar{3})S_\lambda'(\bar{1}\bar{2}\bar{4}\bar{3}) + R_\lambda(\bar{1}\bar{2}\bar{4}\bar{3})S_\lambda'(\bar{1}\bar{2}\bar{4}\bar{3}) \} . \]

The highest-order corrections are usually accounted for through the modification of the bare potential and the interaction of quasi-particles with each other, thus preserving the analytic form of the lowest-order corrections [15, 16].

3. Construction of the optimal one-quasi-electron representation

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 of wave functions. In ref. [11] it has been proposed \textit{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 [11]. Here we briefly describe the key moments. In the fourth order of QED PT there appear diagrams, whose contribution into the $\text{Im}\Delta E$ 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 $\rho_C(r)$. Here, the lowest order multi-electron effects, in particular, the gauge dependent radiative contribution for a certain class of photon propagator calibration is treated. This value is considered to a typical electron correlation effect, whose minimization is a reasonable criterion in search for the optimal one-electron basis of PT. All the gauge non-invariant terms are multielectron by their nature (the particular case of the gauge non-invariance manifestation is non-coincidence of the oscillator strengths values, obtained in the approximate calculations with the ‘length’ and ‘velocity’ transition operator forms). Quite complicated calculation of contribution of the QED PT fourth order polarization diagrams into $\text{Im}\Delta E$ gives the following result [11]:

$$\text{Im}\Delta E_{\text{inv}}(\alpha - s; b) = -C \int \int \int \int dr_1 dr_2 dr_3 dr_4 \sum_{n \geq f} \sum_{m \leq f} \left( \frac{1}{\omega_{mn} + \omega_{ns}} + \frac{1}{\omega_{mn} - \omega_{ns}} \right) \psi_+^+(r_1) \times$$

$$\times \psi_m^+(r_2) \psi_s^+(r_4) \psi_n^+(r_3) \frac{1 - \alpha_1 \alpha_2}{r_{12}} \left( \left( \alpha_3 \alpha_4 - \alpha_3 \alpha_4 \alpha_2 \alpha_4 \right) / r_{14} \right) \sin (\omega_{an}(r_{12} + r_{34})) +$$

$$+ \omega_{an} \sin (\omega_{an}(r_{12} + r_{34})) + (1 + \alpha_3 \alpha_4 \alpha_2 \alpha_4) \psi_m(r_3) \psi_n(r_4) \psi_s(r_1).$$

Here, $C$ is a gauge constant, $f$ is the boundary of the closed shells; $n \geq f$ indicating the unoccupied bound and the upper continuum electron states; $m \leq f$ indicates the finite number of states in the core and the states of the negative continuum (accounting for the electron vacuum polarization). All the vacuum polarization and the self-energy corrections to the sought for values are omitted (due to the obvious numerical smallness compared with the other relativistic corrections). The minimization of the density functional $\text{Im}\Delta E_{\text{inv}}$ leads to the integral differential equation for the $\rho_C$, 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 [10, 12, 18] and give main formulas.

4. Energy approach in scattering theory

When studying the Stark effect, electron-positron pair production in nuclear collisions and elementary processes responsible for emission-lines formation in plasmas, the energy approach has been generalized to cover the problems of scattering theory (c.f. [10, 11, 14, 18]). 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. 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

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

(8)
Here $C^{j_i,m_{f,v}}_{m_{i,e},m_{i,v}}$ is the Clebsh-Gordan coefficient. Final state is:

$$|F⟩ = a^+_scΦ_o,$$

(9)

where $|I⟩$ represents three-quasiparticle (3QP) state, and $|F⟩$ represents the one-quasiparticle (1QP) state. The justification of the energy approach in the scattering problem is in details described in refs. [10, 12, 18]. For the state (1) the scattered part of energy shift $\text{Im} ΔE$ 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 $ε_{sc}$ [10, 18]:

$$\int dε_{sc}(ε_{ie},ε_{ie},ε_{in})/(ε_{sc} - ε_{iv} - ε_{ie} - ε_{in} - i0)$$

(10)

with

$$\text{Im} ΔE = πG(ε_{iv},ε_{ie},ε_{in},ε_{sc}).$$

(11)

Here $G$ is a definite squared combination of the two-electron matrix elements (2). The value

$$σ = -2\text{Im} ΔE$$

(12)

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 $Ω(I → F)$ is connected with the collisional cross section $σ$ by expression (c.f. [10, 11]):

$$σ(I → F) = Ω(I → F)π/ ((2J_i + 1)ε_{in} ((αZ)^2ε_{in} + 2)).$$

(13)

Here and below the Coulomb units are used: 1 C.u.≈27.054Z^2 eV, for energy; 1 C.u.≈ 0.529·10^{-8}/Z cm, for length; 1 C.u.≈ 2.419·10^{-17}/Z^2 sec for time.

The collisional de-excitation cross section is defined as follows [10, 18]:

$$σ(IK → 0) = -π \sum_{j_{in},j_{sc}} (2j_{sc} + 1)\left( \sum_{j_{iv},j_{iv}} δ_{j_{in},j_{sc}; j_{iv},j_{iv}} B_{k_{i,e},k_{i,v}}^{IK} \right)^2.$$ (14)

Here $B_{k_{i,e},k_{i,v}}^{IK}$ is a real matrix of eigen-vectors coefficients, which is obtained after diagonalization of the secular energy matrix. The amplitude like combination in (14) has the following form:

$$⟨j_{in},j_{sc};j_{ie},j_{iv},J_i⟩ = sqrt{(2j_{ie} + 1)(2j_{iv} + 1)(-1)^{j_{ie} + 1/2}} \sum_{λ} (-1)^{λ + J_i} \times$$

$$× \left( \delta_{λ,λ_i}/(2J_i + 1)Q_λ(sc,ie;iv,in) + \left( j_{in} j_{sc} j_{ie} j_{iv} \right) Q_λ(ie,in;iv,sc) \right).$$

(15)

In (15) values $Q_λ^{Q_{ul}}$ and $Q_λ^{Q_{Br}}$ are defined by the expressions (3) and (5). For the collisional excitations from the ground state (inverse process) one must consider $a^+_scΦ_o$ as the initial state and

$$|F⟩ = a^+_sc \sum_{m_{j,e},m_{j,v}} a^+_fJ_fΦ_oC^{j_f,M_f}_{m_{j,e},m_{j,v}}.$$

(16)
as a final state. The cross-section is as follows:

$$\sigma(0 \rightarrow IF) = 2\pi(2J_f + 1) \sum_{j_{in}, j_{sc}} (2j_{sc} + 1) \left( \sum_{j_{fe}, j_{fv}} B_{fe,fv}^{FK} \langle j_{fe}, j_{fv}, J_f | j_{in}, j_{sc} | 0 \rangle \right)^2$$

(17)

with

$$\langle j_{fe}, j_{fv}, J_f | j_{in}, j_{sc} | 0 \rangle = \sqrt{(2j_{fe} + 1)(2j_{fv} + 1)}(-1)^{j_{fe}+1/2} \sum_{\lambda} (-1)^{\lambda + J_f} \times$$

$$\times \left( \delta_{\lambda, j_f} \langle 1/(2J_f + 1) \rangle Q_{\lambda}(sc, ie; iv, in) \left( \begin{array}{ccc} j_{in} & j_{sc} & J_f \\ j_{fe} & j_{fv} & \lambda \end{array} \right) Q_{\lambda}(fe, sc; fv, in) \right).$$

(18)

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 (17). The expression for the cross-section of the collisional excited-excited \(IK - IF\) transition can be found in [10, 18]. The details of the whole numerical procedure of calculation of the collisional cross-section and strength can be found in [8–18]. It is worthwhile to indicate that the energy approach with using the optimal one-electron basis of PT first is used for description of elementary electron processes in collisionally pumped plasma.

5. Results and discussion

We applied our approach to estimate of the electron collisional excitation cross-sections, strengths and rate coefficients for electron-collisional excitation for Ne- and Ar-like ions. To test our theory we compare our calculations on collisional cross-sections for Ne-like iron with known calculations [10, 20, 21]. 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 refs. [10, 15, 16]. Let us remind that in refs. [10, 15, 16] one-electron basis of PT was calibrated on experimental one-electron energies. Her we use ab initio one-electron basis. The first order 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. [10, 15, 16]). 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 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.

| Level | Our Calculation | Ref. [10] | Ref. [22] | Ref. [23] |
|-------|-----------------|-----------|-----------|-----------|
| 1/2   | 0.125           | 0.15      | 0.10      | 0.20      |
| 3/2   | 0.250           | 0.20      | 0.25      | 0.30      |

Table 1: Comparison of theoretical and experimental electron collision strengths for Ne-like iron.

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.
Table 1. Electron-collision strengths for excitation from the ground state of Ne-like iron (incident electron energy 1.0454 keV). Two approximations are given: (i) first order of the PT; (ii) first order of the PT plus effective accounting for the high PT orders corrections. The numbers in brackets denote multiplicative powers of ten.

| Transition | Level | $J$  | Theory ref. [22] | Theory ref. [10] | Present theory (i) | Present theory (ii) |
|------------|-------|------|-----------------|-----------------|-------------------|-------------------|
| 1-2        | 2s2p  | 0    | 1.351 [-03]    | 1.073 [-03]     | 1.151 [-03]       | 1.125 [-03]       |
| 3          | 2p_{3/2}3s_{1/2} | 1    | 2.439 [-03]    | 2.603 [-03]     | 1.222 [-03]       | 2.671 [-03]       |
| 4          | 2p_{1/2}3s_{1/2} | 0    | 2.730 [-04]    | 2.118 [-04]     | 2.303 [-04]       | 2.169 [-04]       |
| 5          | 2p_{1/2}3s_{1/2} | 1    | 2.266 [-03]    | 2.227 [-03]     | 1.158 [-03]       | 2.234 [-03]       |
| 6          | 2p_{3/2}3p_{3/2} | 1    | 3.550 [-03]    | 2.772 [-03]     | 3.381 [-03]       | 2.831 [-03]       |
| 7          | 2p_{3/2}3p_{3/2} | 3    | 3.581 [-03]    | 3.032 [-03]     | 2.816 [-03]       | 3.115 [-03]       |
| 8          | 2p_{3/2}3p_{1/2} | 2    | 2.898 [-03]    | 2.966 [-03]     | 3.446 [-03]       | 2.998 [-03]       |
| 9          | 2p_{3/2}3p_{1/2} | 1    | 1.375 [-03]    | 1.033 [-03]     | 1.308 [-03]       | 1.102 [-03]       |
| 10         | 2p_{3/2}3p_{3/2} | 2    | 3.178 [-03]    | 2.572 [-03]     | 2.276 [-03]       | 2.659 [-03]       |
| 11         | 2p_{1/2}3p_{1/2} | 1    | 3.142 [-03]    | 2.683 [-03]     | 2.810 [-03]       | 2.758 [-03]       |
| 12         | 2p_{1/2}3p_{1/2} | 1    | 1.466 [-03]    | 1.144 [-03]     | 1.375 [-03]       | 1.171 [-03]       |
| 13         | 2p_{1/2}3p_{3/2} | 2    | 3.826 [-03]    | 1.154 [-03]     | 1.504 [-03]       | 1.239 [-03]       |
| 14         | 2p_{1/2}3p_{3/2} | 1    | 3.826 [-03]    | 3.057 [-03]     | 2.692 [-03]       | 3.163 [-03]       |
| 15         | 2p_{2/2}3p_{3/2} | 0    | 4.567 [-02]    | 4.099 [-02]     | 5.042 [-02]       | 4.112 [-02]       |
| 16         | 2p_{3/2}3d_{3/2} | 0    | 1.661 [-03]    | 1.417 [-03]     | 1.462 [-03]       | 1.448 [-03]       |
| 17         | 2p_{3/2}3d_{3/2} | 1    | 5.030 [-03]    | 4.464 [-03]     | 4.339 [-03]       | 4.541 [-03]       |
| 18         | 2p_{3/2}3d_{5/2} | 2    | 6.449 [-03]    | 5.530 [-03]     | 5.424 [-03]       | 5.648 [-03]       |
| 19         | 2p_{3/2}3d_{5/2} | 4    | 6.593 [-03]    | 4.744 [-03]     | 4.905 [-03]       | 4.839 [-03]       |
| 20         | 2p_{3/2}3d_{5/2} | 3    | 4.317 [-03]    | 3.692 [-03]     | 3.528 [-03]       | 3.785 [-03]       |
| 21         | 2p_{3/2}3d_{5/2} | 2    | 2.313 [-03]    | 1.865 [-03]     | 1.996 [-03]       | 1.974 [-03]       |
| 22         | 2p_{3/2}3d_{5/2} | 3    | 3.165 [-03]    | 2.694 [-03]     | 2.572 [-03]       | 2.801 [-03]       |
| 23         | 2p_{3/2}3d_{5/2} | 1    | 2.517 [-02]    | 2.778 [-02]     | 2.471 [-02]       | 2.829 [-02]       |
| 24         | 2p_{1/2}3d_{3/2} | 2    | 2.682 [-03]    | 2.201 [-03]     | 2.344 [-03]       | 2.305 [-03]       |
| 25         | 2p_{1/2}3d_{3/2} | 3    | 3.517 [-03]    | 2.930 [-03]     | 3.058 [-03]       | 3.012 [-03]       |
| 26         | 2p_{1/2}3d_{5/2} | 2    | 3.834 [-03]    | 3.207 [-03]     | 3.064 [-03]       | 3.311 [-03]       |
| 27         | 2p_{1/2}3d_{5/2} | 1    | 1.058 [-01]    | 1.042 [-01]     | 7.162 [-02]       | 1.058 [-02]       |
| 28         | 2s_{1/2}3s_{1/2} | 1    | 9.570 [-04]    | 8.179 [-04]     | 9.768 [-04]       | 8.265 [-04]       |
| 29         | 2s_{1/2}3s_{1/2} | 0    | 1.590 [-02]    | 1.596 [-02]     | 1.908 [-02]       | 1.640 [-02]       |
| 30         | 2s_{1/2}3p_{1/2} | 0    | 2.500 [-04]    | 2.059 [-04]     | 2.116 [-04]       | 2.152 [-04]       |
| 31         | 2s_{1/2}3p_{1/2} | 1    | 9.190 [-04]    | 8.833 [-04]     | 6.538 [-04]       | 8.936 [-04]       |
| 32         | 2s_{1/2}3p_{1/2} | 2    | 1.278 [-03]    | 1.019 [-03]     | 1.103 [-03]       | 1.116 [-03]       |
| 33         | 2s_{1/2}3p_{3/2} | 1    | 2.070 [-03]    | 2.514 [-03]     | 8.006 [-04]       | 2.557 [-03]       |
| 34         | 2s_{1/2}3d_{3/2} | 1    | 1.773 [-03]    | 1.519 [-03]     | 1.662 [-03]       | 1.613 [-03]       |
| 35         | 2s_{1/2}3d_{5/2} | 2    | 3.004 [-03]    | 2.574 [-03]     | 2.671 [-03]       | 2.678 [-03]       |
| 36         | 2s_{1/2}3d_{5/2} | 3    | 4.139 [-03]    | 3.570 [-03]     | 3.688 [-03]       | 3.685 [-03]       |
| 37         | 2s_{1/2}3d_{5/2} | 2    | 1.428 [-02]    | 1.398 [-02]     | 1.059 [-02]       | 1.442 [-02]       |
Table 2. Comparison of measured [19] and calculated electron-collisional excitation cross-sections (σ) for Ne-like barium for two values of incident electron energy 5.69 keV and 8.20 keV (Units are $10^{-21}$ cm$^2$).

| Level     | $J$ | Measured Marrs et al. [19] | Calculated Ivanov et al. [10] | Calculated Zhang et al. [20] | Calculated Reed [21] | Calculated present paper |
|-----------|-----|-----------------------------|-------------------------------|-----------------------------|---------------------|-------------------------|
| Sum       | $J=0$ | 2.50±0.35                  | 2.48                         | 2.58                        | 2.60                | 2.51                    |
| 2p$_{3/2}$3d$_{5/2}$ | 1    | 3.98±0.56                  | 3.20                         | 3.44                        | 3.56                | 3.25                    |
| 2p$_{1/2}$3d$_{3/2}$ | 1    | 2.12±0.30                  | 1.78                         | 2.42                        | 2.00                | 1.84                    |
| Sum       | $J=0$ | 2.27±0.32                  | 1.83                         | 1.89                        | 1.94                | 1.86                    |
| 2p$_{3/2}$3d$_{5/2}$ | 1    | 3.30±0.46                  | 2.87                         | 2.99                        | 3.23                | 2.93                    |
| 2p$_{1/2}$3d$_{3/2}$ | 1    | 1.82±0.25                  | 1.64                         | 2.10                        | 1.82                | 1.64                    |

Such experimental information for a few collisional excitations of the Ne-like barium ground state had been obtained in Ref. [19]. In table 2 we present measured electron-collisional excitation cross-sections σ for Ne-like barium for two values of incident electron energy 5.69 keV and 8.20 keV [19]. First of all, no obvious discrepancies for the considered states are found. Our results are at the lower margin of experimental error as the corresponding data of ref. [10] with one exception: for the state 2p$_{3/2}$3d$_{5/2}$ ($J = 1$) our cross-section at collisional energy 5.69 keV is a few percent lower. But one must understand that extraction of the cross section from the experiment is the most ambiguous for this level. In any case one can see that there is physically reasonable agreement between theory and experiment. The collisional strengths have been calculated for several values of the incident electron energy and then approximated by a simple analytical formula with exact asymptotics. The latter have been used in the convolution relativistic formula for rate coefficients. The comparison of our collisional rate coefficients for iron with those from refs. [10, 23] is shown in Fig.1.

Their dependence on the electron temperature is shown for three different transitions. Like the cross-sections, our rate coefficients are typically less than those of Ref. [23] and more than those of Ref. [10]. 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 adjacent continua has been elaborated in the scattering theory [18]. The numerical calculations on this subject are in the progress. We are calculating the spectra of plasma, containing Ne- and Na-Like Ions, with consistent account for Rydberg and autoionizing Rydberg series in the balance equations, following to methodic of Ivanov-Ivanova [10]. The inclusion of Na-like states, accounting for diffusion-like processes, can increase the population inversion for the ‘lasing candidates’ by at least a factor of two for a wide range of plasma conditions. This is important for the ionization equilibrium too. Besides, we are calculating the functions $N_{el}$, which describe the population distribution within each Rydberg series dependent on the Rydberg electron energy. These functions bear diagnostic information. Detailed calculations will be done for the homogeneous steady-state Maxwellian plasma. The role of transient processes in the population inversion creation is also under studying. The details of kinetics calculation [24] to determine level populations, inversions, line intensities and gain coefficients etc. at definite plasma parameters will be considered in a future paper.
In conclusion let us note that in any case our calculation encourages us to believe that using the optimal one-electron basis of PT is more consistent and effective procedure from the point of view of the theory correctness and results exactness. This fact was surely confirmed by calculations of the oscillator strengths, radiative widths in atoms and multicharged ions (c.f. [11, 14]). Our \textit{ab initio} approach can be used in calculations of the cross sections of other collisional processes and, in general speaking, other systems (c.f. [14, 18]). When the experimental information about the corresponding characteristics and systems is very scarce we believe that its use is especially perspective.

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