Generalized energy approach in an electron-collisional spectroscopy of multicharged ions in plasma in the Debye approximation

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Abstract. The generalized relativistic energy approach is used for the studying the spectra of plasma of the multicharged ions and calculation of electron-ion collision strengths, cross-sections in Ne-like ions. The approach is based on the Debye shielding model relativistic Dirac Hamiltonian for electron-nuclear and electron-electron potentials and energy approach. The relativistic many-body perturbation theory with using gauge-invariant scheme of generation of the optimal one-electron representation is used. The measured and calculated electron-collisional excitation cross-sections for Ne-like barium for value of incident electron energy 8.20keV and the effective collision strengths of the Ne-like krypton excitation states for temperature T=5×10^6 K and electron density n_e=10^{14} cm^{-3} are presented and analysed.

1. Introduction
The properties of laser-produced hot and dense plasmas, known as laser plasma, have drawn considerable attention over the last two decades through the recent laser-fusion studies [1,2]. 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. 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. [1-25]). The laser effects have been discovered on the transitions of Li-, Ne-, Ni-like and other ions. Very useful data on the X-lasers problem are firstly received and collected in the papers by Ivanova et al [2,13-16]. Calculation of emission spectra of the plasma ions based in the precise theoretical techniques is practical tool, which may be used instead of very expensive sophisticated experiments. 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. 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. 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. There are constructed first lasers with using plasma of Li-, Ne-, Ni-like ions as an active medium. 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 VUV lasing: i). accurate calculation of electron-collisional strengths and rate coefficients for processes in plasma; ii). kinetics calculations to determine level inversions, intensities, gain coefficients at definite plasma parameters.
In this paper the generalized relativistic energy approach is used for the studying the spectra of plasma of the multicharged ions and calculation of electron-ion collision strengths, cross-sections in Ne-like ions. The approach is based on the Debye shielding model relativistic Dirac Hamiltonian for electron-nuclear and electron-electron potentials and energy approach [2,3,6-8,22]. The relativistic many-body perturbation theory (PT) with using the gauge-invariant scheme of generation of the optimal one-electron representation is used. The measured and calculated electron-collisional excitation cross-sections for Ne-like barium for value of incident electron energy 8.20keV and the effective collision strengths of the Kr\textsuperscript{26+} Ne-like ion excitation states for temperature T=5×10\textsuperscript{6}K and electron density n\textsubscript{e}=10\textsuperscript{14}cm\textsuperscript{-3} are presented and analysed.

2. Energy approach in scattering theory

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 [2,3,16]. 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 [2-6]. In contrast to the non-relativistic case, the secular matrix elements are already complex in the PT second order (the first order of the inter-electron interaction). Their imaginary parts are connected with the radiation decay possibility. The total energy shift of the state is usually presented in the form:

\[
\Delta E = \text{Re}\Delta E + i \text{Im}\Delta E
\]

(1a)

\[
\text{Im} \Delta E = -\Gamma/2
\]

(1b)

where \(\Gamma\) is interpreted as the level width.

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 \(M\) and definition of matrix of the coefficients with eigen state vectors \(B_{ie,iv}^{\epsilon_i}\) [2-5]. 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. [3] 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. In the fourth order of QED PT there appear diagrams, whose contribution into the \(\text{Im}\Delta E\) accounts for the polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution \(\Delta E_{\text{inv}}\)). The minimization of the functional \(\text{Im} \Delta E_{\text{inv}}\) leads to the integral differential equation, that is numerically solved. In result one can get the optimal one-electron basis of the PT [2,5,6].

The energy approach has been generalized to cover the problems of scattering theory (c.f.[2-5]). Here we briefly outline the main idea considering the collisional de-excitation of the Ne-like ion:

\[
(2j_{iv})^13j_{ie}[J,M_J], \epsilon_{iv,\epsilon_ie} \rightarrow (\Phi_{\epsilon_ie},\epsilon_{ie}).
\]

Here \(\Phi_{\epsilon_ie}\) is the state of the ion with closed shells (ground state of the Ne-like ion); \(J\) is the total angular moment of the initial target state; indices \(iv, ie\) are related to the initial states of vacancy and electron; indices \(\epsilon_{iv}\) and \(\epsilon_{ie}\) are the incident and scattered energies, respectively to the incident and scattered electrons. The initial state of the system “atom plus free electron” can be written as

\[
| I \rangle = a_{iv}^{+} \sum_{m_{iv},m_{ie}} a_{ie}^{+} \Phi_{\epsilon_i,\epsilon_{iv}} C_{m_{ie},m_{iv}}^{J_i,M_i}.
\]

(2)
Here \( C_{m_i,m_{iv}}^{J_i,M_i} \) is the Clebsh-Gordan coefficient. Final state is as follows: \( |F>| = a_{\Phi}^{+} \Phi \), where \( \Phi \) is the state of an ion with closed electron shells (ground state of Ne-like ion), \( |lF>| \) represents three-quasiparticle (3QP) state, and \( |lF>| \) represents the one-quasiparticle (1QP) state. The justification of the energy approach in the scattering problem is in details described in refs. [2,3,5,15]. For the state (2) the scattered part of energy shift \( \text{Im} \Delta E \) appears first in the second order of the atomic perturbation theory.

The collisional de-excitation cross section is defined as follows [2,5]:

\[
\sigma(IK \rightarrow 0) = 2\pi \sum_{j_{1w},j_{2w}} (2j_{1w} + 1)(\sum_{j_{1w},j_{2w}} < 0 | j_{in} , j_{sc} | j_{ie}, j_{iv}, J_i > | B_{w,n}^{ik} |^2)
\]

The amplitude like combination in (3) has the following form:

\[
< 0 | j_{in} , j_{sc} | j_{ie}, j_{iv}, J_i > \propto \sqrt{(2j_{ie} + 1)(2j_{iv} + 1)}(-1)^{j_{ie} + 1/2} \prod_{\lambda} (-1)^{\lambda + J_i} \times \\
\times \{ \delta_{\lambda,J_i} / (2J_i + 1) Q_{\lambda}(sc;ie;iv,in) + \sum_{j_{ie},j_{iv}} J_i \} Q_{\lambda}(ie;in;iv,sc),
\]

where \( Q_{\lambda} = Q_{\lambda}^{\text{Coul}} + Q_{\lambda}^{\text{Bre}} \) is, as a rule, the sum of the Coulomb and Breit matrix elements. The details of their calculating can be found in [2-4,13-15,19,20].

3. The Debye shielding model

As it is well known (c.f.[17,22] and refs. therein) in the classical theory of plasmas developed by Debye and Hückel, the interaction potential between two charged particles in a plasma is modelled by a Yukawa-type potential as follows:

\[
V(r_i, r_j) = \left( Z_a Z_b / r_{ij} \right) \exp(-\mu r_{ij})
\]

where \( r_{ij} = r_{iw} - r_{jw} \) represent respectively the spatial coordinates of particles A and B and \( Z_a, Z_b \) denote their charges. A difference between the Yukawa type potential and standard Coulomb potential is in account for the effect of plasma, which is modeled by the shielding parameter \( \mu \) [17]. In fact, this parameter describes the shape of the long-rang potential. The parameter \( \mu \) is connected with the plasma parameters such as the temperature \( T \) and the charge density \( n \) as follows:

\[
\mu \sim \sqrt{e^2 n / k_B T}
\]

Here, as usually, \( e \) is the electron charge and \( k_B \) is the Boltzman constant. The density \( n \) is given as a sum of the electron density \( N_e \) and the ion density \( N_k \) of the \( k \)-th ion species having the nuclear charge \( q_k \):

\[
n = N_e + \sum_k q_k^2 N_k
\]

Under typical laser plasma conditions of \( T \approx 1 \text{keV} \) and \( n \approx 10^{22} \text{cm}^{-3} \) the parameter \( \mu \) is of the order of 0.1 in atomic units [17]. By introducing the Yukawa-type electron-nuclear attraction and electron-
electron repulsion potentials, the electronic Hamiltonian for a N-electron multicharged ion in a plasma is given in atomic units as follows:

\[
H = \sum_i \left[ \alpha_r c - \beta m e^2 - Z \exp(-\mu r_i) / r_i \right] + \sum_{i>j} \left( \frac{l - \alpha_i \alpha_j}{r_{ij}} \right) \exp(-\mu r_{ij})
\]  

(8)

A difference between our model Hamiltonian (8) and analogous model Hamiltonian with the Yukawa potential of ref. [17] (c.f. refs there too) is in using the relativistic approximation, which is obviously necessary for adequate description of such relativistic systems as the multicharged ions of the neon isoelectronic sequence.(c.f. details in refs. [13,14]). Further in the calculation procedure we introduce also the model electron-core potential of Ivanova et al [13,15] with parameter, calibrated within the special ab initio procedure within the relativistic energy approach [3].

4. Results

We applied our approach to calculate the electron collisional excitation cross-sections, strengths and rate coefficients for electron-collisional excitation for some Ne-like ions. To test our theory we compare our calculations results on the collisional cross-sections for Ne-like iron with the known theoretical data [2,5,6,11,12,21]. In tables 1 and 2 we present the measured (plasma) electron-collisional excitation cross-sections \( \sigma \) for Ne-like barium for two values of incident electron energy 5.69keV and 8.20 keV [11] and the theoretical data: our calculation data and results of four other theoretical papers [2,5,6,12,13,22]. 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. Such experimental information for a few collisional excitations of the Ne-like barium ground state has been presented in Ref.[11]. Let us note that in ref. [2] one-electron basis of PT was calibrated using the experimental one-electron energies. Here we use ab initio one-electron basis. The PT first order correction is calculated exactly, the high-order contributions are taken into account for effectively: polarization interaction of two above-core quasi-particles and an effect of their mutual screening (internal correlation effects) [13-16].

Table 1. Comparison of measured and calculated electron-collisional excitation cross-sections for Ne-like barium for incident electron energy 5.69 keV (units are \( 10^{-21} \text{cm}^2 \)).

| Level     | J    | Measured Marrs et al [11] | Calculated Ivanov et al [2,13] | Calculated Zhang et al [12] | Calculated Reed [21] | Calculated Glushkov et al [5] | Our paper |
|-----------|------|-------------------------|-------------------------------|-----------------------------|---------------------|-----------------------------|-----------|
| Sum (J=0) |      | 2.50±0.35               | 2.48                          | 2.58                        | 2.60                | 2.51                        | 2.63      |
| 2p3/23d5/2 | 1    | 3.98±0.56               | 3.20                          | 3.44                        | 3.56                | 3.25                        | 3.61      |
| 2p1/23d3/2 | 1    | 2.12±0.30               | 1.78                          | 2.42                        | 2.00                | 1.84                        | 2.02      |

Table 2. Comparison of measured and calculated electron-collisional excitation cross-sections for Ne-like barium for incident electron energy 8.20 keV (units are \( 10^{-21} \text{cm}^2 \)).

| Level     | J    | Measured Marrs et al [11] | Calculated Ivanov et al [2,13] | Calculated Zhang et al [12] | Calculated Reed [21] | Calculated Glushkov et al [5] | Our paper |
|-----------|------|-------------------------|-------------------------------|-----------------------------|---------------------|-----------------------------|-----------|
| Sum (J=0) |      | 2.27±0.32               | 1.83                          | 1.89                        | 1.94                | 1.86                        | 1.97      |
| 2p3/23d5/2 | 1    | 3.30±0.46               | 2.87                          | 2.99                        | 3.23                | 2.93                        | 3.27      |
| 2p1/23d3/2 | 1    | 1.82±0.25               | 1.64                          | 2.10                        | 1.82                | 1.69                        | 1.84      |
In table 3 we present the theoretical data on the effective collision strengths of the Kr$^{26+}$ Ne-like ion excitation states for the temperature T=$5\cdot10^6$ K and the electron density $n_e=10^{14}$ cm$^{-3}$ (the typical electron density of the tokamak plasma). The R-matrix data by DF Griffin et al (RM) [23] are listed for comparison too. 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. Summation over $j_{m_{j_{sc}}}$ in (18) 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. For some levels the corrections due the correlation effects change the results by a factor of 2-3.5. Our final electron-collisional excitation cross-sections appear to be typically larger than those of Ref.[2,5,12,21], where the plasma shielding effects are not directly included. But, in whole there is physically reasonable agreement between theory and experiment.

| Term | RM [23] | Our paper |
|------|----------|-----------|
| $2p^5s\, (3/2,1/2)_2$ | $8.29(-3)$ | $8.13(-3)$ |
| $2p^5s\, (3/2,1/2)_1$ | $9.36(-3)$ | $9.19(-3)$ |
| $2p^5p\, (3/2,1/2)_1$ | $3.49(-3)$ | $3.38(-3)$ |
| $2p^5p\, (3/2,1/2)_2$ | $4.30(-3)$ | $4.18(-3)$ |
| $2p^5s\, (1/2,1/2)_0$ | $1.32(-3)$ | $1.21(-3)$ |
| $2p^5s\, (1/2,1/2)_1$ | $7.69(-3)$ | $7.56(-3)$ |
| $2p^5p\, (3/2,3/2)_1$ | $4.03(-3)$ | $3.89(-3)$ |
| $2p^5p\, (3/2,3/2)_2$ | $3.14(-3)$ | $3.01(-3)$ |
| $2p^5p\, (3/2,3/2)_3$ | $3.36(-3)$ | $3.12(-3)$ |
| $2p^5p\, (3/2,3/2)_0$ | $8.67(-3)$ | $8.49(-3)$ |
| $2p^5p\, (1/2,1/2)_1$ | $2.69(-3)$ | $2.54(-3)$ |
| $2p^5p\, (1/2,3/2)_1$ | $2.80(-3)$ | $2.72(-3)$ |
| $2p^5p\, (1/2,3/2)_2$ | $3.27(-3)$ | $3.16(-3)$ |
| $2p^5d\, (3/2,3/2)_1$ | $1.24(-3)$ | $1.13(-3)$ |
| $2p^5p\, (1/2,1/2)_0$ | $1.71(-2)$ | $1.58(-2)$ |
| $2p^5d\, (3/2,3/2)_2$ | $3.45(-3)$ | $3.31(-3)$ |
| $2p^5d\, (3/2,3/2)_1$ | $3.80(-3)$ | $3.67(-3)$ |
| $2p^5d\, (3/2,5/2)_1$ | $4.13(-3)$ | $3.96(-3)$ |

Using of the Debye shielding approach and an account for the highly-lying excited states is quantitatively important for the adequate description of the collision cross-sections. In conclusion let us note that in any case our calculation encourages us to believe that using QED energy approach with the optimal one-electron PT basis and Debye shielding model block is quite consistent and effective one 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, hyperfine structure constants in atoms, multicharged ions (c.f. [3,19,20]). Our ab initio approach can be used in calculations of the cross sections of other collisional processes and, in general speaking, other systems [24,25]. Its using is especially perspective when the experimental information about corresponding properties and systems is very scarce.

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