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ELECTRON-COLLISIONAL SPECTROSCOPY OF ATOMS AND MULTICHARGED IONS IN PLASMA: Ne ATOM AND Be-LIKE IONS

The generalized relativistic energy approach with using the Debye shielding model is used for studying spectra of plasma of the multicharged ions and determination of electron-impact cross-sections and other spectral parameters for Ne-atom and Be-, Ne-like ions.

1. **Introduction**

Optics and spectroscopy of laser-produced hot and dense plasmas, known as laser plasma, has drawn considerable attention over the last two decades through the recent laser-fusion studies [1-24]. Similar interest is also stimulated by importance of these data for correct description of parameters 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 (see [1-16] and Refs. therein). There are constructed first lasers with using plasma of Li-, Ne-like ions as an active medium. The laser effects have been discovered on the transitions of Ni-like and other ions. 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 a plasma by different physical processes. This results in a different dependence of the each line intensity on the plasma parameters. In most plasma environments the properties are determined by the electrons and the ions, and the interactions between them. The electron-ion collisions play a major role in the energy balance of plasmas. For this reason, modelers and diagnosticians require absolute cross sections for these processes. Cross sections for electron-impact excitation are needed to interpret spectroscopic measurements and for simulations of plasmas using collisional-radiative models.

In many papers the calculations of various atomic systems embedded in Debye plasmas have been performed (as example, see [13-19]). Different theoretical methods have been employed along with the Debye screening to study plasma environments. Two principal theoretical problems must be solved in order to develop a code adequate to predict the plasma parameters for many applications, i.e. accurate estimate of electron-collisional parameters for processes in plasma and kinetics calculations to find level inversions, gain coefficients at definite plasma parameters. Earlier [19-25] we developed a new generalized relativistic energy approach combined with the relativistic many-body perturbation theory (RMBPT) for multi-quasiparticle (QP) atomic systems for studying spectra of plasma of the multicharged ions and electron-ion collisional parameters. The method is based on the Debye shielding model and energy approach [4-8,21-25]. Here some new results on oscillator strengths and energy shifts due to the plasma environment effect, collisional excitation cross-sections for atom of neon and some Be, Ne-like ions are presented for different plasma parameters.

2. **Energy approach in scattering theory and the Debye shielding model**

The generalized relativistic energy approach combined with the RMBPT has been in details described in Refs. [21-24]. It generalizes earlier developed energy approach by Ivanov-Ivanova et al [4-8]. Here we briefly present the key moments of our method. Namely, the key idea is in calculating the energy shifts DE of degenerate states that is connected with the secular matrix M diagonalization [4-6]. To construct M, one should use the Gell-Mann and Low adiabatic formula for DE. The secular matrix elements are already complex in the PT second order (the first order on the inter-electron interaction). The whole calculation is reduced to calculation and diagonalization of the complex matrix M .and definition of matrix of the coefficients with eigen state vectors $B^{K}_{ie,iv}$ [4-6,19]. To calculate all necessary matrix elements one must use the basis's of the 1QP relativistic functions. In many calculations of the atomic elementary process parameters it has been shown that their adequate description requires using the optimized basis's of wave functions. In [6] 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 ImdE accounts for the polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution dE_{ninv}). The minimization of functional $ImdE_{ninv}$ leads to an integral differential equation, that is numerically solved. In result one can get the optimal one-electron basis of the PT [21-23]. As an example, consider the collisional de-excitation of the Ne-atom:

$$((2j_{iv})^{-1}3j_{ie}[J_iM_i],\ \varepsilon_{in})\rightarrow(\Phi_o,\ \varepsilon_{sc}). \qquad (1)$$

Here Φ_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 initial target state; indices iv, ie are related to initial states of vacancy and electron; indices ε_{in}, ε_{sc} are the incident and scattered energies respectively to incident and scattered electrons. The initial state of the system «atom plus free electron» can be written as

$$|I>=a^{+}_{in}\sum_{m_{iv},m_{ie}} a^{+}_{ie}a_{iv}\Phi_o C^{J_i,M_i}_{m_{ie},m_{iv}} \qquad (2)$$

Here $C^{J_i,M_i}_{m_{ie},m_{iv}}$ is the Clebsh-Gordan coefficient. Final state is as follows: where Φ_o is the state of an ion with closed electron shells (ground state of Ne-like ion), $|I>$ represents the 3QP state, and $|F>$ represents the 1QP state. The justification of the energy approach in the scattering problem is in details described in [4-6,21-23]. For the state (2) a scattered part of energy shift ImdE appears first in the second order of the atomic perturbation theory. The collisional de-excitation cross section is defined as follows:

$$\sigma(IK\rightarrow 0)=2\pi\sum_{j_{in},j_{sc}}(2j_{sc}+1)$$
$$\{\sum_{j_{ie},j_{iv}}<0|\,j_{in},j_{sc}\,|\,j_{ie},j_{iv},J_i>B^{IK}_{ie,iv}\}^2 \qquad (3)$$

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

$$<0|\,j_{in},j_{sc}\,|\,j_{ie},j_{iv},J_i>=\sqrt{(2j_{ie}+1)(2j_{iv}+1)}$$
$$(-1)^{j_{ie}+1/2}\times\sum_{\lambda}(-1)^{\lambda+J_i}\times \qquad (4)$$
$$\times\{\delta_{\lambda,J_i}/(2J_i+1)Q_\lambda(sc,ie;iv,in)+$$
$$+\begin{bmatrix} j_{in}\cdots j_{sc}\cdots J_i \\ j_{ie}\cdots j_{iv}\cdots\cdots\lambda \end{bmatrix}Q_\lambda(ie;in;iv,sc)\},$$

where $Q_\lambda = Q_\lambda^{\mathrm{Qul}} + Q_\lambda^{\mathrm{Br}}$ is, as a rule, the sum of the Coulomb and Breit matrix elements.

Further consider the Debye shielding model. It is known (see [10-14,19] and refs. therein) in the classical theory of plasmas developed by Debye and Hückel, the interaction potential between two charged particles is modelled by a Yukawa - type potential as follows:

$$V(r_i, r_j) = (Z_aZ_b/|r_a-r_b|\}exp\,(-\mu|r_a-r_b|), \qquad (5)$$

where r_a, r_b 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 μ [1]. The parameter μ is connected with the plasma parameters such as the temperature T and the charge density n as follows: $\mu\sim\sqrt{e^2n/k_BT}$. Here, as usually, e is the electron charge and κ_B is the

Boltzman constant. The density n is given as a sum of the electron density N_e and 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~1keV and n~10^{22} cm^{-3} the parameter μ is of the order of 0.1 in atomic units [13,14]. If the Debye radius limits to 0, or a parameter μ becomes very large, the Debye approximation doesn't be true. If the parameter μ becomes very small, the plasma screening effect on the plasma-embedded atomic systems is not significant. But, even in this case it is practically useful to apply the formulas of the Debye shielding model. By introducing the Yukawa-type e-N and e-e interaction potentials, an electronic Hamiltonian for N-electron multicharged ion in a plasma is in atomic units as follows [19]:

$$H = \sum_i [\alpha c p - \beta m c^2 - Z \exp(-\mu r_i)/r_i] + \sum_{i>j} \frac{(1 - \alpha_i \alpha_j)}{r_{ij}} \exp(-\mu r_{ij}) \tag{6}$$

A difference between our model Hamiltonian (6) and analogous model Hamiltonian with the Yukawa potential of Refs. [13,14] is in using the relativistic approximation, which is obviously necessary for adequate description of such relativistic systems as the high-Z multicharged ions. To describe the electron-ionic core interaction we use the optimized Dirac-Fock potential (for Be-like ions) or optimized model potential by Ivanova et al (for Ne-like ions) with one parameter [8], which calibrated within the special ab initio procedure within the relativistic energy approach [6]. The modified PC numerical code 'Superatom" is used in all calculations. Other details can be found in Refs. [4-8, 19-24].

3. **Results**

We applied our approach to calculate the radiative and collisional characteristics (energy shifts, oscillator strengths, electron-ion cross-sections and collision strengths) for the neon atom and Be-, Ne-like ions embedded to the plasma environment. Firstly, we present our results on energy shifts and oscillator strengths for transitions $2s^2$-$2s_{1/2}2p_{1/2,3/2}$ in spectra of the Be-like Ni and Kr. The corresponding plasma parameters are as follows: $n_e=10^{22}$-$10^{24}cm^{-3}$, T=0.5-2 keV (i.e. m~0.01-0.3). In table 1 and 2 we list the results of calculation of the energy shifts DE (cm^{-1}) for $2s^2$-$[2s_{1/2}2p_{1/2,3/3}]_1$ transitions and oscillator strengths changes for different plasma parameters (the electron density and temperature). There are also listed the available data by Li etal and Saha-Frische: the multiconfiguration Dirac-Fock (DF) calculation results and ionic sphere (I-S) model simulation data (from [13,19] and refs. therein). The analysis shows that the presented data are in physically reasonable agreement, however, some difference can be explained by using different relativistic orbital basises and different models for accounting of the plasma screening effect. From the physical point of view, the behavior of the energy shift is naturally explained, i.e by increasing blue shift of the line because of the increasing the plasmas screening effect. The electron-ion collisional characteristics of the Be-like ions are of a great importance for such applications as diagnostics of astrophysical, thermonuclear plasma and also EBIT plasma [1-13]. In the last case the characteristic values of electron density are significantly lower as the considered above on several orders. In [16,17] it is performed the MEIBEL (merged electron-ion beams energy-loss) experiment. The experimental data (dots) are listed for Be-like ion of oxygen in figure 1, where the cross-section of electron-impact excitation of [$2s^2$ ^1S-(2s2p ^1P)] transition for Be-like oxygen is presented. In figure 1 there are also presented the theoretical results for the cross-section (in 10^{-16} cm^3), obtained by calculation on the basis of the 3-configuration R-matrix theory and our data [16,25]. The analysis shows that for energies lower 20eV there is a physically reasonable agreement between data of both theories and experiment. For energies higher 20eV there is a large disagreement of our data and R-matrix data.

It is provided by different degree of accounting for the correlation effects (configuration interaction) and different basises of relativistic wave functions. In table 3 there are listed our theoretical results and experimental data by Khakoo et al [23] for integral electron-impact cross-sections (in $10^{-19}cm^2$) of excitation of the neon atom to the $2p^5 3s[3/2]^o_2$, $2p^5 3s[1/2]^o_0$ states of the $2p^53s$ configuration. The full data for neutral Ne are in Ref. [25]. Further we present results of studying collisional parameters of ions in collisionally pumping plasma of the Ne-like ions with parameters T_e= 20-40eV and density n_e= 10^{19-20} cm^{-3}. This system is of a great interest for generation of laser radiation in the short-wave range of spectrum [4].

Table 1. Energy shifts DE (cm^{-1}) for $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in spectra of the Be-like Ni and Kr for different values of the n_e (см$^{-3}$) and T (in eV) (see explanations in text)

	n_e	10^{22}	10^{23}	10^{24}	10^{22}	10^{23}	10^{24}
Z	kT	Li et al	Li et al	Li et al	Our data	Our data	Our data
NiXXV	500	31.3	292.8	2639.6	33.8	300.4	2655.4
	1000	23.4	221.6	2030.6	25.7	229.1	2046.1
	2000	18.0	172.0	1597.1	20.1	179.8	1612.5
	I-S	8.3	86.6	870.9			
KrXXXIII	500	21.3	197.9	2191.9	27.2	215.4	2236.4
	1000	15.5	150.5	1659.6	21.3	169.1	1705.1
	2000	11.5	113.5	1268.0	16.9	128.3	1303.8

Table 2. Oscillator strengths gf for $2s^2$-$[2s_{1/2}2p_{3/2}]_1$ transition in Be-like Ni and Kr for different values of the n_e (см$^{-3}$) and T (in eV) (gf_0–the gf value for free ion)

n_e		10^{22}	10^{23}	10^{24}		10^{22}	10^{23}	10^{24}
kT	Li etal	Li etal	Li etal	Li etal	gf_o-our	our data	our data	our data
500	0.1477	0.1477	0.1478	0.1487	0.1480	0.1480	0.1483	0.1495
1000		0.1477	0.1477	0.1482		0.1480	0.1483	0.1495
2000		0.1477	0.1477	0.1481		0.1479	0.1482	0.1493
I-S		0.1477	0.1477	0.1479				

Figure 1. Cross-section of electron-impact excitation of $[2s^2\,{}^1S$ -$(2s2p\,{}^1P)]$ transition for Be-like oxygen with the MEIBEL experiment data (dots); theory — R-matrix theory (continuous line) [16,17]; our theory (dotted line).

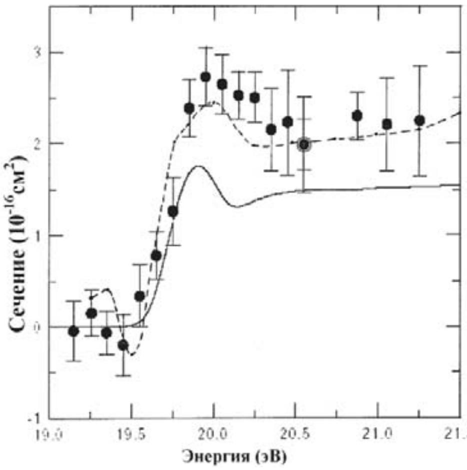

Table 3. Theoretical (Th.; our) and experimental (Exp.) data by Khakoo et al [23] for integral electron-impact cross-sections (in 10^{-19}cm^2) of excitation of neon atom to the $2p^53s[3/2]^o_2$, $2p^53s[1/2]^o_0$ states of the $2p^53s$ configuration. (E_0,eV) [10,11,19]

E_0	Exp.- $2p^53s[3/2]^o_2$	Exp.- $2p^53s[1/2]^o_0$	Th. - $2p^53s[3/2]^o_2$	Th.- $2p^53s[1/2]^o_0$
20	14.6	2.7	14.9	2.9
30	9.7	1.7	9.9	1.8
40	4.9	1.1	5.1	1.15
50	4.0	0.9	3.9	0.8
100	0.5	0.1	0.4	0.13

It is obviously more complicated case in comparison with previous one. Here an accurate account of the excited, Rydberg, autoionization and continuum states plays a critical role. In table 4 we present the theoretical values of the collisional excitation rates (CER) and collisional de-excitation rates (CDR) for Ne-like argon transition between the Rydberg states and from the Rydberg states to the continuum states (see details in [5,19]). Speech is about the Rydberg states which converge to the corresponding lower boundary of continuum $-e_0$ (figure 2). As it is indicated in [5,19], the parameter $-e_0$ is the third parameter of the plasma environment (together with electron density and temperature). In fact it defines the thermalized energy zone of the Rydberg and autoionization states which converge to the ionization threshold for each ion in a plasma. Usually value e_0 can be barely estimated from simple relation: $e_0=0.1\times T_e$. In the consistent theory the final results must not be dependent on the model parameters, so the concrete value of e_0 is usually chosen in such way that an effect of its variation in the limits $[0.01\times T_e, 0.1\times T_e]$ (for Ne-like ions) doesn't influence on the final results. Usually few subzones can be separated in the zone of Rydberg states (figure 2) [5]. In tables 4 and 5 we list the theoretical collisional excitation (CER) and de-excitation (CDR) rates for Ne-like Ar in plasma with $n_e=10^{19\text{-}20}$cm^{-3}, T_e =20eV (table 4) and 40 eV (table 5). For comparison there are listed data by Ivanov etal (RMPPT without shielding effect [4,5]).

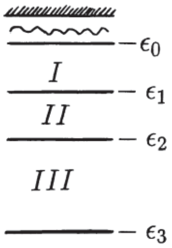

Figure 2. Rydberg states zones (Ne-like ion: [Ne,i],nl); e_0 is a boundary of thermalized zone, neighboring to continuum; e_3 -ionization potential for states nl=3s; $e_2=(e_0+e_3)/2$, $e_1=(e_0+e_2)/2$

This effect plays an important role for Debye plasma. An account for exchange-correlation effects and superposition of the highly-lying excited states are quantitatively important for adequate description of the collision parameters. In our scheme the optimal 1-QP basis is used. The PT first order correction is calculated exactly, the high-order contributions are taken into account for effectively: polarization interaction of the above-core QPs and effect of their mutual screening (correlation effects). The calculations encourage us to believe that using energy approach combined with the optimized relativistic Debye-model many-body PT is quite consistent and effective tool from point of view of the theory correctness and exactness. Obviously, the presented approach can be used in theory of other collisional processes and, in general speaking, other systems (see [24] and refs. therein). Its using is very perspective when the experimental data on corresponding properties and systems are very scarce or absent.

Table 4. The collisional excitation (CER) and de-excitation (CDR) rates (in cm^3/s) for Ne-like argon in plasma with parameters: $n_e= 10^{19\text{-}20}$ cm^{-3} and temperature T_e =20eV.

		RMPPT			Our data		
Parameters	n_e, cm^{-3}	T_e = 20eV	T_e = 20eV	T_e = 20eV	T_e = 20eV	T_e = 20eV	T_e= 20eV
Transition		1→2	1→3	2→3	1→2	1→3	2→3
CDR (i→i ;k)	1.0+19	5.35-10	1.64-10	1.13-09	5.77-10	1.92-10	1.28-09
	1.0+20	5.51-10	1.60-10	1.12-09	5.94-10	1.78-10	1.25-09
Transition		2→1	3→1	3→2	2→1	3→1	3→2
CER (i→i ;k)	1.0+19	5.43-10	5.39-12	2.26-11	5.79-10	1.88-12	2.64-11
	1.0+20	3.70-10	8.32-12	2.30-11	4.85-10	1.13-11	2.78-11

Table 5. Collisional excitation (CER) and de-excitation (CDR) rates (in cm^3/s) for Ne-like argon in plasma with parameters: $n_e= 10^{19\text{-}20}$ cm^{-3} and temperature T_e =40eV (our data)

Parameters	n_e, cm^{-3}	T_e =40 eV	T_e =40 eV	T_e =40 eV
Transition		1→2	1→3	2→3
CDR (i→i ;k)	1.0+19	3.18-10	8.45-11	6.81-10
	1.0+20	5.02-10	1.56-10	4.99-10
Transition		2→1	3→1	3→2
CER (i→i ;k)	1.0+19	5.33-10	5.63-11	7.11-11
	1.0+20	7.67-10	6.94-11	8.93-11

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Abstract. The generalized relativistic energy approach with using the Debye shielding model is used for studying spectra of plasma of the multicharged ions and determination of electron-impact cross-sections and other spectral parameters for Ne-atom and Be-, Ne-like ions.

Key words: electron-collisional spectroscopy, relativistic energy approach

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ЭЛЕКТРОН-СТОЛКНОВИТЕЛЬНАЯ СПЕКТРОСКОПИЯ АТОМОВ И МНОГОЗАРЯДНЫХ ИОНОВ В ПЛАЗМЕ: АТОМ Ne, Be-ПОДОБНЫЕ ИОНЫ

Резюме. На основе обобщенного релятивистского энергетического подхода с использованием модели экранирования Дебая выполнено изучение спектра плазмы многозарядных ионов и рассчитаны столкновительные сечения возбуждения и другие параметры для атома неона и Be-, Ne-подобных ионов.

Ключевые слова: электрон-столкновительная спектроскопия, энергетический подход

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СПЕКТРОСКОПІЯ ЗА РАХУНОК ЕЛЕКТРОННИХ ЗІТКНЕНЬ АТОМІВ ТА БАГАТОЗАРЯДНИХ ІОНІВ У ПЛАЗМІ: АТОМ Ne, Be-ПОДІБНІ ІОНИ

Резюме. На основі узагальненого релятивістського енергетичного підходу з використанням моделі экранювання Дебая виконано вивчення спектру плазми багатозарядних іонів і розраховані перерізи збудження за рахунок зіткнень і інші спектральні параметри для атома неону і Be- ,Ne-подібних іонів.

Ключові слова:електронна спектроскопія за рахунок зіткнень, енергетичний підхід