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NEW RELATIVISTIC APPROACH TO COMPUTING SPECTRAL PARAMETERS OF MULTICHARGED IONS IN PLASMAS

It is presented a new relativistic approach to computing the spectral parameters of multicharged ions in plasmas for different values of the plasmas screening (Debye) parameter (respectively, electron density, temperature). The approach used is based on the generalized relativistic energy approach combined with the optimized relativistic many-body perturbation theory (RMBPT) with the Dirac-Debye shielding model as zeroth approximation, adapted for application to study the spectral parameters of ions in plasmas. An electronic Hamiltonian for N-electron ion in plasmas is added by the Yukawa-type electron-electron and nuclear interaction potential. The special exchange potential as well as the electron density with dependence upon the temperature are used.

1. Introduction

An accurate data about spectra, radiative decay widths and probabilities, oscillator strengths, electron-collision strengths, collisional excitation and de-excitation rates for atoms and especially ions are of a great interest for different applications, namely, astrophysical analysis, laboratory, thermonuclear plasma diagnostics, fusion research, laser physics etc [1–44]. It is also very important for studying energy, spectral and radiative characteristics of a laser-produced hot and dense plasmas [1,2,9, 10].

Above other stimulating factors to studying electron-collisional spectroscopy of ions one should mention the X-ray laser problem, which has stimulated a great number of papers, devoted to modelling the elementary processes in laser, collisionally pumped plasma (see [1,2] and Refs. therein) and construction of the first VUV and X-ray lasers with using plasma of Li-, Ne-like ions as an active medium. Very useful data on the X-lasers problem are firstly received and collected in the papers by Ivanova et al (see [2] and Refs. therein]. From the other side, studying spectra of ions in plasmas remains very actual in order to understand the plasma processes themselves. 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 of ions are needed to interpret spectroscopic measurements and for simulations of plasmas using collisional-radiative models. At present time a considerable interest has been encapsulated to studying elementary atomic processes in plasma environments (for example, see [1,9-18] and Refs. therein) because of the plasma screening effect on the plasma-embedded atomic systems. In many papers the calculations of various atomic and ionic systems embedded in Debye plasmas have been performed [1,9-15]). Different theoretical methods have been employed along with the Debye screening to study plasma environments. 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. Nevertheless, there are known principal theoretical problems to be solved in order to receive the correct description of the elementary atomic processes in laser, collisionally pumped plasma. First of all, speech is about development of the advanced quantum-mechanical models for the further accurate computing oscillator strengths, electron-collisional strengths and rate coefficients for atomic ions in plasmas, including the Debye plasmas. As usually, a correct accounting for the relativ-

istic, exchange-correlation, plasma environment effects is of a great importance. To say strictly, solving of the whole problem requires a development of the quantum-electrodynamical approach as the most consistent one to problem of the Coulomb many-body system.

In this paper, which goes on our work [15-20], we present a new relativistic approach to computing the spectral parameters of multicharged ions in plasmas for different values of the plasmas screening (Debye) parameter (respectively, electron density, temperature). The approach used is based on the generalized relativistic energy approach combined with the optimized RMBPT with the Dirac-Debye shielding model as zeroth approximation, adapted for application to study the spectral parameters of ions in plasmas. An electronic Hamiltonian for N-electron ion in plasmas is added by the Yukawa-type electron-electron and nuclear interaction potential. The special exchange potential as well as the electron density with dependence upon the temperature is used.

2. Optimized relativistic perturbation theory formalism for ions in plasmas

Some fundamental aspects of the approach developed were earlier presented (see, for example, Refs. [15-20]). Therefore, below we are limited only by the key and as a rule new points of a theory.

The generalized relativistic energy approach combined with the RMBPT has been in detail described in Refs. [6,24-29]. It generalizes earlier developed energy approach. The key idea is in calculating the energy shifts ΔE of degenerate states that is connected with the secular matrix M diagonalization [6,24,25]. To construct M, one should use the Gell-Mann and Low adiabatic formula for ΔE. The secular matrix elements are already complex in the PT second order. 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 $B_{ie,iv}^{IK}$ [6,25]. To calculate all necessary matrix elements one must use the bases of the 1QP relativistic functions.

Within an energy approach the total energy shift of the state is usually presented as [24]:

$$\Delta E = Re\Delta E + i\ \Gamma/2 \qquad (1)$$

where Γ is interpreted as the level width and decay (transition) possibility $P = \Gamma$. Let us start our consideration from formulation relativistic many-body PT with the Debye shielding model Dirac Hamiltonian for electron-nuclear and electron-electron systems. Formally, a multielectron atomic systems (multielectron atom or multicharged ion) is described by the relativistic Dirac Hamiltonian (the atomic units are used) as follows:

$$H = \sum_i h(r_i) + \sum_{i>j} V(r_i r_j). \qquad (1)$$

Here, $h(r)$ is one-particle Dirac Hamiltonian for electron in a field of a nucleus and V is potential of the inter-electron interaction. According to Refs. [6] it is useful to determine the interelectron potential with accounting for the retarding effect and magnetic interaction in the lowest order on parameter α^2 (α is the fine structure constant) as follows:

$$V(r_i r_j) = exp(i\omega_{ij} r_{ij}) \cdot \frac{(1 - \alpha_i \alpha_j)}{r_{ij}}, \qquad (2)$$

where ω_{ij} is the transition frequency; α_i, α_j are the Dirac matrices.

In order to take into account the plasmas environment effects already in the PT zeroth approximation we use the known Yukawa-type potential of the following form:

$$V(r_i, r_j) = (Z_a Z_b / |r_a - r_b|) exp(-\mu \cdot |r_a - r_b|) \qquad (3)$$

where r_a, r_b represent respectively the spatial coordinates of particles, say, A and B and Z_a, Z_b denote their charges.

The potential (3) is well known (look, for example, [1,12,15] and Refs there) well known, for example, in the classical Debye-Hückel, theory of plasmas. The plasmas environment effect is modelled by the shielding parameter μ, which describes a shape of the

long-rang potential. The parameter μ is connected with the plasma parameters such as the temperature θ and the charge density n as follows:

$$\mu \sim \sqrt{e^2 n / k_B T} \qquad (4)$$

Here 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 with the nuclear charge q_k : $n = N_e + \sum_k q_k^2 N_k$ .It is very useful to remind the simple estimates for the shielding parameter.

For example, under typical laser plasma conditions of $T \sim 1$keV and n~ 10^{23} cm^{-3} the parameter μ is of the order of 0,1 in atomic units. By introducing the Yukawa-type electron-nuclear attraction and electron-electron repulsion potentials, the Debye shielding model Dirac Hamiltonian for electron-nuclear and electron-electron subsystems is given in atomic units as follows [15]:

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

$$(5)$$

where c is the velocity of light and Z is a charge of the atomic ion nucleus.

The formalism of the relativistic many-body PT is further constructed in the same way as the PT formalism in Refs. [16-26]. In the PT zeroth approximation one should use a mean-field potential, which includes the Yukawa-type potential (insist of the pure Coulomb one) plus exchange potential and additionally the correlation potential (for example, the Lundqvist-Gunnarson potential with the optimization parameter b can be used) as in Refs. [16-18,23,24]. As alternative one could use an optimized model potential by Ivanova-Ivanov (for Ne-like ions) [6], which is calibrated within the special ab initio procedure within the relativistic energy approach [8,16].

Let us concretize the corresponding mean-field potential. In particular, one of the possible versions U(r) is as follows (sum of the Coulomb or Yukawa-type potential plus exchange potential:

$$U(r) = U_{Coul-Yuk\pi}(r) + U_{ex}(r), \qquad (6)$$

With the exchange potential as follows:

$$U_{o6m}(r) =$$
$$\frac{4\pi}{T} \rho(r) \left[1 + 6 \frac{\rho(r)}{T^{3/2}} + \frac{\pi^4}{3} \left(\frac{\rho(r)}{T^{3/2}} \right)^2 \right]^{-1/3}, \qquad (7)$$

where $\rho(r)$ is an electron density.
The electron density can be presented as a sum of the following terms:

$$\rho(r) = \rho_1(r) + \rho_2(r), \qquad (8)$$

$$\rho_1(r) \sim \sum_{n,l} | \Psi_{nl}(r) |^2 \qquad (9)$$

$$\rho_1(r) = \frac{\sqrt{2} T^{3/2}}{\pi^2} \int \sqrt{y} \left[1 + \exp \left(y - \frac{U(r)}{T} + \eta \right) \right]^{-1} dy, \qquad (10)$$

$$y > \frac{1}{T} (U(r) + E_0), \qquad (11)$$

where $\eta = -\frac{\mu}{T}$, μ is a chemical potential and E_0 is a boundary between state of discrete spectrum and continuum.
The averaged numbers of fulfilling electron states can be determined on the basis of the Fermi-Dirac expression:

$$N_{nl} = 2(2l + 1) \left[1 + \exp \left(\frac{1}{T} (E_{nl} + \mu) \right) \right]^{-1} \qquad (12)$$

In order to determine a chemical potential μ one should use the condition electroneutrality of the atomic corel

The point of accounting for the many-body exchange-correlation corrections within

a presented theory can be treated as in an usual perturbation theory for free multicharged ions. As usually, in the PT second order, there are two kinds of the exchange and correlation diagrams: polarization and ladder ones. The polarization diagrams take into account the quasiparticle interaction through the polarizable core, and the ladder diagrams account for the immediate quasiparticle interaction. An effective procedure of their accounting are in details described in Refs. [6-9,20-24]. The modified PC numerical code 'Superatom' is used in all calculations. Other details can be found in Refs. [15-20,22,23,38].

3. Results and conclusion

In Tables 1 and 2 we list the numerical variations in the lifetimes of the $2p_{1/2}$, $3s_{1/2}$, $3p_{1/2}$, $3d_{3/2}$, and $4s_{1/2}$ states in Ca XVIII for different μ values.

Table 1.

The dependence of the lifetimes (ps) of the $2p_{1/2}$ state in the Ca XVIII spectrum upon the screening parameter μ: RCC - relativistic coupled-cluster (RCC) method [3]; This - this work

μ	$2p_{1/2}$	$2p_{1/2}$
	RCC	This
0.133	741	740
0.667	494	493
1.000	334	333
1.250	242	242
1.429	192	191
0.60	140	139

Table 2.

The dependence of the lifetimes (ps) of the 3lj,4lj states in the Ca XVIII spectrum upon the parameter μ (this work)

μ	$3s_{1/2}$	$3p_{1/2}$	$3d_{3/2}$	$4s_{1/2}$
0.133	1.09	0.45	0.16	1.64
0.667	1.28	0.54	0.88	2.56
1.000	1.55	0.68	0.22	4.83
1.250	1.87	0.86	0.28	12.6
1.429	2.22	1.08	0.35	82.9

The analysis shows that the presented data are in physically reasonable agreement with the NIST experimental data and theoretical results by relativistic coupled-cluster (RCC) method calculation [3]. However, some difference between the corresponding results can be explained by using different relativistic orbital bases and by difference in the model of accounting for the screening effect as well as some numerical differences..

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Summary. It is presented a new relativistic approach to computing the spectral parameters of multicharged ions in plasmas for different values of the plasmas screening (Debye) parameter (respectively, electron density, temperature). The approach used is based on the generalized relativistic energy approach combined with the optimized RMBPT with the Dirac-Debye shielding model as zeroth approximation, adapted for application to study the spectral parameters of ions in plasmas. An electronic Hamiltonian for N-electron ion in plasmas is added by the Yukawa-type electron-electron and nuclear interaction potential. The special exchange potential as well as the electron density with dependence upon the temperature are used.

Key words: spectroscopy of ions in plasmas, relativistic energy approach, new relativistic quantum mechanical model

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НОВЫЙ РЕЛЯТИВИСТСКИЙ ПОДХОД К РАСЧЕТУ СПЕКТРАЛЬНЫХ ПАРАМЕТРОВ МНОГОЗАРЯДНЫХ ИОНОВ В ПЛАЗМЕ

Резюме. Представлен новый релятивистский подход к расчету спектральных параметров многозарядных ионов в плазме для различных значений параметра экранирования плазмы (дебаевского) (соответственно электронной плотности, температуры).Подход основан на обобщенном релятивистском энергетическом подходе, совмещенном с формализмом оптимизированной релятивистской многочастичной теории возмущений с приближением Дирака-Дебая в качестве нулевого приближения, адаптированной для применения при изучении спектральных параметров ионов в плазме. Электронный гамильтониан для иона N-электронов в плазме добавляется потенциалом электрон-электронного и ядерного взаимодействия типа Юкавы. Используются специальный обменный потенциал, а также плотность электронов с фиксацией явной зависимости от температуры.

Ключевые слова: спектроскопия ионов в плазме, энергетический подход, новая релятивистская квантово-механическая модель

Терновський Є В., Михайлов О.Л.

НОВИЙ РЕЛЯТИВІСТСЬКИЙ ПІДХІД ДО РОЗРАХУНКУ СПЕКТРАЛЬНИХ ПАРАМЕТРІВ БАГАТОЗАРЯДНИХ ІОНІВ В ПЛАЗМІ

Резюме. Представлений новий релятивістський підхід до розрахунку спектральних параметрів багатозарядних іонів в плазмі для різних значень параметра екранування плазми (дебаєвсього) (відповідно електронної щільності, температури). Підхід ґрунтується на узагальненому релятивістському енергетичному підході, поєднаному з формалізмом оптимізованої релятивістської багаточастинкової теорії збурень з наближенням Дірака-Дебая в якості нульового наближення, адаптованого для застосування при вивченні спектральних параметрів іонів у плазмі. Електронний гамільтоніан для іона N-електронів в плазмі додається потенціалом електрон-електронного та ядерного взаємодії типу Юкави. Використовуються спеціальний обмінний потенціал, а також щільність електронів з фіксацією явної залежності від температури.

Ключові слова: спектроскопія іонів в плазмі, енергетичний підхід, нова релятивістська квантово-механічна модель.