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RELATIVISTIC APPROACH TO COMPUTING WAVELENGTHS OF TRANSITIONS IN SPECTRA OF ATOMIC SYSTEMS IN PLASMAS

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) is presented. The presented approach is based on the generalized relativistic energy approach combined with the optimized relativistic many-body perturbation theory with the Dirac-Debye screening hamiltonian as a zeroth approximation, adapted for application to study the energy and spectral parameters of atoms and ions in plasmas. The special exchange potential as well as the electron density with dependence upon the temperature are used. The wavelengths for a number of transitions, including (A): E(1s2p $^1P_1$)-E(1s^2 ^1S); (B) E(1s3p $^1P_1$)_E(1s^2 ^1S); (C)AK: E(1s2p $^3P_1$)_E(1s2s ^3S); (D): E(1s3p $^3P_1$)_E(1s2s ^3S) of the helium in plasmas for various Debye lengths are calculated and compared with the corresponding data by Kar-Ho.

1. **Introduction.**

The properties of laboratory, thermonuclear (tokamak), laser-produced, astrophysical plasmas have drawn considerable attention over the last decades [1-5]. It is known that multicharged ions play an important role in the diagnostics of a wide variety of plasmas [1-23]. 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. It has stimulated a great number of papers, devoted to modelling the elementary processes in laser, collisionally pumped plasmas and construction of the first VUV and X-ray lasers with using plasmas of Li-, Ne-like ions as an active medium.

Such well-known atomic methods as the multi-configuration Dirac–Fock, R-, T-matrix, relativistic distorted-wave methods, coupled-cluster theories, and more simplified approaches such as the quantum defect and Coulomb approximations, pseudo- and model potential methods, the classical and quasiclassical models and others have been intensively applied to problems considered. At present time a considerable interest has been encapsulated to studying elementary atomic processes in plasmas environments because of the plasmas screening effect on the plasmas-embedded atomic systems. In many papers the calculations of various atomic and ionic systems embedded in the Debye plasmas have been performed [1-28]; a development of the advanced computational quantum methods and models for the further accurate computing wavelengths and oscillator strengths for the atomic systems in plasmas, including the Debye plasmas, remained a very actual and difficult problem (for example, see [1-42] and Refs. therein) . 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.

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 relativistic, 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 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) is presented. The presented approach is based on the generalized relativistic energy approach combined with the optimized relativistic many-body perturbation theory with the Dirac-Debye screening hamiltonian as a zeroth approximation, adapted for application to study the energy and spectral parameters of atoms and ions in plasmas. The special exchange potential as well as the electron density with dependence upon the temperature are used.

2. **Theoretical Approach.**

Some fundamental aspects of the approach developed were earlier presented (see, for example, Refs. [20-26]). Therefore, below we are limited only by the key and as a rule new points of a theory, following to Refs. [20-23]. 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:

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

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:

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

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:

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

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, [1-4,24] 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:

$$\mu \sim \sqrt{e^2 n / k_B T} \tag{4}$$

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* ~ 1keV 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 [20-22]:

$$H = \sum_i [\alpha c p - \beta m c^2 - Z \exp(-\mu r_i)/r_i] + \\ + \sum_{i>j} \frac{(1-\alpha_i\alpha_j)}{r_{ij}} \exp(-\mu r_{ij}) \tag{5}$$

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. [20,24-32]. 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. [24-26]. As alternative one could use an optimized model potential by Ivanova-Ivanov (for Ne-like ions) [1,30], which is calibrated within the special ab initio procedure within the relativistic energy approach [24-27].

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:

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

With the exchange potential as follows:

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

where $\rho(r)$ is an electron density.

The electron density can be presented as a sum of the following terms:

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

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

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

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

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:

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

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" [24-32] is used in all calculations. Other details can be found in Refs. [33-40].

3. Results and conclusions.

Below we will present our data on the wavelengths for a number of transitions, including (A): E(1s2p $^1P_1$)-E(1s^2 ^1S); (B) E(1s3p $^1P_1$)_E(1s^2 ^1S); (C)AK: E(1s2p $^3P_1$)_E(1s2s ^3S); (D): E(1s3p $^3P_1$)_E(1s2s ^3S) of the helium in plasmas for various Debye lengths and compare with the corresponding data by Kar-Ho [2]. It should be noted that Kar-Ho [2] have used the highly correlated basis functions for singly excited S, P, D states and CI-type basis functions for doubly excited meta-stable D states, and the plasmas effect has been taken into account by using a screened Coulomb (Yukawa) potential obtained from the Debye model that admits a variety of plasma conditions. The analysis shows that the presented data are in physically reasonable agreement with the theoretical data [2].

However, some difference between the corresponding results can be explained by using different relativistic orbital bases and by differences in the numerical realization of model for accounting for the screening effect as well as some numerical differences

Table 1. Transition wavelengths (in A °) of helium atom below the He+(1S) threshold for different Debye lengths (A): E(1s2p $^1P_1$)-E(1s^2 ^1S); (B) E(1s3p $^1P_1$)_E(1s^2 ^1S); (C)AK: E(1s2p $^3P_1$)_E(1s2s ^3S); (D): E(1s3p $^3P_1$)_E(1s2s ^3S); See text

$1/\mu$	[2]	(A)-this	(B)- this
$\propto$	584.234	584.236	536.940
100	584.388	584.389	537.296
50	584.838	584.840	538.307
20	587.829	587.831	544.707
10	597.826	597.828	565.208
8	605.098	605.099	580.696
$1/\mu$	(B)- this	(C)-this	(D)-this
$\propto$	536.940	10831.59	3889.372
100	537.296	10834.584	3901.312
50	538.307	10843.193	3935.133
20	544.707	10901.684	4155.382
10	565.208	11136.233	4985.283
8	580.696	11351.615	5831.351

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Summary. 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) is presented. The presented approach is based on the generalized relativistic energy approach combined with the optimized relativistic many-body perturbation theory with the Dirac-Debye screening hamiltonian as a zeroth approximation, adapted for application to study the energy and spectral parameters of atoms and ions in plasmas. The special exchange potential as well as the electron density with dependence upon the temperature are used. The wavelengths for a number of transitions, including (A): E(1s2p $^1P_1$)-E(1s^2 ^1S); (B) E(1s3p $^1P_1$)_E(1s^2 ^1S); (C)AK: E(1s2p $^3P_1$)_E(1s2s ^3S); (D): E(1s3p $^3P_1$)_E(1s2s ^3S) of the helium in plasmas for various Debye lengths are calculated and compared with the corresponding data by Kar-Ho.

Key words: atomic spectroscopy, plasmas, energy approach, relativistic theory

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РЕЛЯТИВІСТСЬКИЙ ПІДХІД ДО ОБЧИСЛЕННЯ ДОВЖИН ХВИЛЬ ПЕРЕХОДІВ У СПЕКТРАХ АТОМНИХ СИСТЕМ У ПЛАЗМІ

Резюме. Представлено новий релятивістський підхід до обчислення спектральних параметрів атомних систем у плазмі для різних значень параметра екранування (Дебая) плазми (відповідно, електронної густини, температури). Представлений підхід базується на узагальненому релятивістському енергетичному підході в поєднанні з оптимізованою релятивістською багаточастинковою теорією збурень з модельним гамільтоніаном Дірака-Дебая як нульовим наближенням теорії збурень, адаптованим для дослідження енергетичних та спектральних параметрів атомів та іонів у плазмі. Використовується спеціальний обмінний потенціал, а також електронна густина в залежності від температури. Довжини хвиль для ряду переходів, включаючи (A) E(1s2p $^1P_1$)-E(1s^2 ^1S); (B) E(1s3p $^1P_1$)_E(1s^2 ^1S); (C)AK: E(1s2p $^3P_1$)_E(1s2s ^3S); (D): E(1s3p $^3P_1$)_E(1s2s ^3S) гелію в плазмі для різних довжин Дебая обчислюються та порівнюються з відповідними даними Кар-Хо.

Ключові слова: атомна спектроскопія, плазма, енергетичний підхід, релятивістська теорія

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