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RELATIVISTIC SPECTROSCOPY OF MULTICHARGED IONS IN PLASMAS: Li-LIKE IONS

The transition probabilities and lifetimes for different excited states in spectrum of the Li-like calcium are computed within the consistent relativistic many-body approach for different values of the plasmas screening parameter (correspondingly, electron density and temperature) and compared with available alternative data. The approach is based on the generalized relativistic energy approach combined with the optimized relativistic many-body perturbation theory with the Dirac-Debye shielding model as zeroth approximation, adapted for application to study of 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.

1. Introduction

The properties of laboratory, thermonuclear (tokamak), laser-produced, astrophysical plasmas have drawn considerable attention over the last decades [1-14]. It is known that multicharged ions play an important role in the diagnostics of a wide variety of plasmas [1-10]. Electron-ion collisions involving multiply charged ions, as well as various radiation and radiation-collisional processes, predetermine the quantitative characteristics of the energy balance of the plasmas [1-6,15-20]. For this reason, the plasmas modelers and diagnosticians require absolute cross sections for these processes. The cross sections for electron-impact excitation of ions are needed to interpret spectroscopic measurements and for simulations of plasmas using collisional-radiative models. The electron-ion collisions play a major role in the energy balance of plasmas. ([1-6]). Different theoretical methods were employed along with the Debye screening to study plasma medium. Earlier we have developed a new version of a relativistic energy approach combined with the many-body perturbation theory (RMBPT) for multi-quasiparticle (QP) systems to study spectra of plasma of the multicharged ions, electron-ion collisional parameters [15-20]. The method is based on the Debye shielding model and energy approach [21-23]. A new element of this paper is in using the effective optimized Dirac-Kohn-Sham method in general relativistic energy approach to collision processes in the Debye plasmas.

In this paper, which goes on our work [15-20], we present the results of computing the transition probabilities and lifetimes for different excited states in spectrum of the Li-like calcium for different values of the plasmas screening (Debye) parameter (respectively, electron density, temperature) and compared with available alternative spectroscopic data. 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.

2. Optimized relativistic perturbation theory formalism for ions in plasmas

The detailed description of our approach was earlier presented (see, for example, Refs. [15-20]). Therefore, below we are limited only by the key points. 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 $B^K_{k,i}$ [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]:

$$\Delta E = \mathrm{Re}\Delta E + i\,\Gamma/2 \qquad (1)$$

where Γ is interpreted as the level width and decay (transition) possibility $P = \Gamma$. The imaginary part of electron energy of the system, which is defined in the lowest PT order as [6]:

$$\mathrm{Im}\,\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \qquad (2)$$

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega| r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (3)$$

where $\sum_{\alpha>n>f}$ for electron and $\sum_{\alpha<n\le f}$ for vacancy. The separated terms of the sum in (2) represent the contributions of different channels.

According to the definition, a lifetime of some excited state f is defined as follows (included all possible transition channels):

$$\tau_f = 1/\sum_{A,i} P^A_{f-i} \qquad (4)$$

for the transition rate P^A_{f-i} due to a radiative operator A. The transition rates via various multipole channels are determined as follows:

$$P^{E1}_{f-i} = \frac{2.02613\cdot 10^{18}}{\lambda^3 (2J_f+1)} S^{E1}_{f-i} \qquad (5a)$$

$$P^{M1}_{f-i} = \frac{2.69735\cdot 10^{13}}{\lambda^3 (2J_f+1)} S^{M1}_{f-i} \qquad (5b)$$

$$P^{E2}_{f-i} = \frac{1.11995\cdot 10^{18}}{\lambda^5 (2J_f+1)} S^{E2}_{f-i} \qquad (5c)$$

where λ is the wavelength (Å), J_f is the total angular momentum of the f state, $S^A_{f-i} \sim \mathrm{Im}\Delta E$ is a line strength due to the corresponding transition operator A (the decay channels E1, M1 and E2 represent the electric dipole, magnetic dipole, and electric quadrupole transition channels respectively). It is known [3,4,25] that the matrix elements computed with using the length gauge expressions converge faster than the velocity ones with respect to the configuration space of the orbital bases; the authors [3] considered the length gauge expressions for evaluating the foregoing transition properties.

This fact is directly linked with correct accounting for the correlation effects and using the optimized basis of wave functions. In [25] it has been proposed "ab initio" optimization principle for construction of cited basis. It uses a minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution δE_{ninv}). The minimization of $\mathrm{Im}\delta E_{ninv}$ leads to integral differential equation, that is numerically solved. In result one can get the optimal one-electron basis of the PT [24-26]. It is worth to note that this approach was used while solving multiple problems of modern atomic, nuclear and molecular physics (see [30-38]).

Further let us firstly consider the Debye shielding model according to Refs. [15,16]. What is known from the classical theory of plasmas developed by Debye-Hückel, the interaction potential between two charged particles is modeled by the Yukawa-type potential, which contains the shielding parameter μ. The parameter μ is connected with the plasma parameters such as

the temperature T and the charge density n as follows: $\mu \sim \sqrt{e^2(1+Z)n_e / k_B T_e}$. 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

$$q_k : n = N_e + \sum_k q_k^2 N_k . \qquad (6)$$

It is very useful to remind the simple estimates for the shielding parameter. For example, under typical laser plasmas conditions of T~ 1keV and n~ 10^{22} cm^{-3} the parameter μ is of the order of 0.1 in atomic units; in the EBIT plasmas T~ 0.05keV, n~10^{18} cm^{-3} and μ~10^{-3}. We are interested in studying the spectral parameters of ions in plasmas with the temperature T~ 0.1-1keV (10^6-10^7K) and n~10^{14}-10^{26} cm^{-3} (μ~10^{-5}-10^0). It should be noted that indeed the Debye screening for the atomic electrons in the Coulomb field of nuclear charge is well understood due to the presence of the surrounding plasma electrons with high mobility. On the other hand, the contribution due to the Debye screening between electrons would be of smaller magnitude orders. Majority of the previous works on the spectroscopy study have considered the screening effect only in the electron-nucleus potential where the electron-electron interaction potential is truncated at its first term of the standard exponential expansion for its dominant contribution [3]. However, it is also important to take into account the screening in the electron- electron interactions for large plasma strengths to achieve more realistic results in the search for stability of the atomic structure in the plasma environment.

By introducing the Yukawa-type e-N and e-e interaction potentials, an electronic Hamiltonian for N-electron ion in a plasma is in atomic units as follows [15,16]:

$$H = \sum_i [\alpha cp - \beta mc^2 - Z\exp(-\mu r_i)/r_i] + \sum_{i>j} \frac{(1-\alpha_i\alpha_j)}{r_{ij}} \exp(-\mu r_{ij}) \qquad (7)$$

To generate the wave functions basis we use the optimized Dirac-Kohn-Sham potential with one parameter [15], which is calibrated within the special ab initio procedure within the relativistic energy approach [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

Firstly, we present our results on the transition probabilities and lifetimes for some excited states of the Li-like ion of calcium. The spectroscopic properties for plasma-isolated ion with μ=0 have been considered. In Tables 1 and 2 there are listed probabilities values for transitions (E1, M1, and E2 channels) from the excited states to the low-lying states of Ca XVIII. Using these values, one could calculate the corresponding lifetimes of the excited states.

Table 1.

The transition probabilities (P) for some transitions in spectrum of Ca XVIII: RCC - relativistic coupled-cluster (RCC) method [3]; This - this work

Transition	$P_{f\to i}$	$P_{f\to i}$
f-i	RCC	This
$2p_{1/2}$-(E1)-$2s_{1/2}$	1.31[9]	1.33[9]
$2p_{3/2}$-(E1)-$2s_{1/2}$	2.00[9]	2.02[9]
-(M1)-$2p_{1/2}$	7.00[2]	7.03[2]
-(E2)-$2p_{1/2}$	2.54[-2]	2.57[-2]
$3s_{1/2}$- M1 -$2s_{1/2}$	2.04[4]	2.06[4]
-(E1)-$2p_{1/2}$	3.01[11]	3.02[11]
-(E1)-$2p_{3/2}$	6.22[11]	6.24[11]

The analysis shows that the presented data are in physically reasonable agreement with the NIST experimental data and theoretical

Table 2.

The transition probabilities (P) for some transitions in spectrum of Ca XVIII (our data)

Transition	$P_{f\to i}$
f-i	This
$3p_{1/2}$ - E1-$2s_{1/2}$	2.37[12]
- M1-$2p_{1/2}$	1.48[3]
- M1-$2p_{3/2}$	6.78[4]
- E2-$2p_{3/2}$	8.45[8]
- E1-$3s_{1/2}$	1.72[8]
$3p_{3/2}$ - E1-$2s_{1/2}$	2.32[12]
- M1-$2p_{1/2}$	1.24[4]
- E2-$2p_{3/2}$	4.25[8]
- M1-$2p_{3/2}$	2.78[4]
- E2-$2p_{3/2}$	4.22[8]
- E1-$3s_{1/2}$	2.66[8]
- M1-$3p_{1/2}$	1.83[1]
- E2-$3p_{1/2}$	2.13[-3]

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. In Tables 3 and 4 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. It is worth to note that our computing oscillator strengths within energy

Table 3.

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	738
0.667	494	492
1.000	334	332
1.250	242	241
1.429	192	190
0.60	140	138

Table 4.

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	1.07	0.428	0.143	1.62
0.667	1.26	0.518	0.688	2.54
1.000	1.53	0.658	0.206	4.81
1.250	1.85	0.849	0.262	12.48
1.429	2.20	1.072	0.336	82.77

approach with different forms of transition operator (i.e. using the photon propagators in the form of Coulomb, Feynman or Babushkin) gives very close results.

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Summary. The transition probabilities and lifetimes for different excited states in spectrum of the Li-like calcium are computed within the consistent relativistic many-body approach for different values of the plasmas screening parameter (correspondingly, electron density and temperature) and compared with available alternative data. The approach is based on the generalized relativistic energy approach combined with the optimized relativistic many-body perturbation theory with the Dirac-Debye shielding model as zeroth approximation, adapted for application to study of 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.

Key words: spectroscopy of ions in plasmas, relativistic energy approach, radiative transition probabilities

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РЕЛЯТИВИСТСКАЯ СПЕКТРОСКОПИЯ МНОГОЗАРЯДНЫХ ИОНОВ В ПЛАЗМЕ: Li-ПОДОБНЫЕ ИОНЫ

Резюме. Вероятности переходов и времена жизни для различных возбужденных состояний в спектре Li-подобного кальция вычисляются в рамках последовательного релятивистского многочастичного подхода для различных значений параметра экранирования плазмы (соответственно, электронной плотности и температуры) и сравниваются с имеющимися альтернативными данными. 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.

Ключевые слова: спектроскопия ионов в плазме, энергетический подход, вероятности радиационных переходов

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РЕЛЯТИВІСТСЬКА СПЕКТРОСКОПІЯ БАГАТОЗАРЯДНИХ ІОНІВ В ПЛАЗМІ: Li-ПОДІБНІ ІОНИ

Резюме. Ймовірності переходів і часи життя для різних збуджених станів в спектрі Li-подібного кальцію обчислюються в рамках послідовного релятивістського багаточастинко-

вого підходу для різних значень параметра екранування плазми (відповідно, електронної щільності і температури) і порівнюються з наявними альтернативними даними. 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.

Ключові слова: спектроскопія іонів в плазмі, енергетичний підхід, ймовірності радіаційних переходів