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SPECTROSCOPY IN Ne-LIKE PLASMAS. Z-DEPENDENCE OF THE ATOMIC DATA USED IN A COLLISIONAL-RADIATIVE MODEL

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RESUME

Les expériences Laser X à Livermore en 1984 ont montré l'existence d'inversions de population 3p-3s au sein d'un plasma collisionnel de Sélénium ($Z=34$) correspondant à des gains significatifs (5 cm^{-1}). Nous avons concentré nos efforts sur le comportement de ces gains en fonction de la charge nucléaire Z de l'élément cible. Cette étude implique la détermination de la dépendance en Z des coefficients de taux de tous les processus atomiques mis en cause : excitation collisionnelle (C), décroissance radiative (A) et recombinaison diélectronique (α_d). Pour cela, nous avons utilisé les codes de structure atomique et de collision électron-ion suivants : SUPERSTRUCTURE, Distorted-Waves, AUTOLSJ et JJOM. Les calculs ont été faits pour un vaste échantillon d'ions, de l'Argon à l'Argent, et, pour un schéma de structure fine, comprenant des effets relativistes. La dépendance en Z des différents résultats numériques est exprimée sous forme polynomiale ou rationnelle.

ABSTRACT

The Livermore X-ray Laser experiments in 1984 have shown the existence of Ne-like 3p-3s population inversions in a collisional Se plasma ($Z=34$) with significant gains (5 cm^{-1}). We have focused our efforts on the behavior of the gains along the target neon isoelectronic sequence. This study implies the determination of the Z -dependence of the rate coefficients of all the involved atomic processes : collisional excitation (C), radiative decay (A) and dielectronic recombination (α_d). Thus we use atomic structure and electron-ion collisional codes (SUPERSTRUCTURE, Distorted Waves, AUTOLSJ and JJOM). The different calculations have been done on a large selection of ions, from Ar to Ag. They include relativistic effects in a fine structure scheme. The Z -dependence of the numerical results is expressed as polynomial or rational forms.

ENERGIES AND DECAY RATES : SUPERSTRUCTURE

The wavefunctions, energy levels, wavelengths and decay rates are calculated using the SUPERSTRUCTURE computer code (1). In a first step this code determines a set of non-relativistic wavefunctions, by diagonalisation of the non-relativistic Hamiltonian, using orbitals calculated in a Thomas-Fermi-Dirac potential. For this potential, the scaling parameters λ_l ($l=0, 1, 2, \dots$) are determined by energy minimization of the terms corresponding to a set of chosen configurations. In a second step, the code diagonalizes the Breit-Pauli Hamiltonian on this basis. Thus, the multi-configurational wavefunctions obtained contain the relativistic effects in the configuration mixing coefficients.

For Ne-like studied ions :

Fe XVII, Ge XXIII, Se XXV, Mo XXXIII, Ag XXXVIII

the scaling parameters λ_l ($l=0, 1, 2$) are determined by energy minimization of all the terms of the configurations $1s^2 2s^2 2p^6$, $1s^2 2s^2 2p^5 3l$ ($l=0, 1, 2$)

The potentials corresponding to these scaling parameters have been used for the larger following set of configurations :

$(1s^2 2s^2) 2p^6$, $2p^5 3l$, $2p^5 4l$ ($l=0, 1, 2$; $l=0, 1, 2, 3$) for $l=3$, $\lambda_3 = \lambda_2$

to calculate all the corresponding energies and decay rates. The Selenium levels are labeled by increasing energy and the same designation is then retained for the levels of all values of Z . For some selected levels a comparison between our calculations and those presented in (2-4) has been done. It shows a very satisfactory energy separation between the levels (lower than $5/1000$). The Z -dependence of energies and radiative de-excitation rates, for levels and transitions of interest in X-ray laser experiments have been calculated.

COLLISION STRENGTHS : DISTORTED WAVES

The collision strengths are calculated by three computer codes : Distorted Waves (5), JJOM (6) and Coulomb-Bethe. The first one (D.W.) is a non-relativistic code based upon the distorted waves approximation. It is the logical extension of the multi-configurational method with a central potential (SUPERSTRUCTURE) to calculate the continuum wavefunction. This potential $V\lambda(r)$ is chosen to be a scaled Thomas-Fermi-Dirac one which contains a scaling parameter for each set of radial orbitals λ_l for a given angular momentum l . The set-up of the D.W. code is very similar to the set-up of SUPERSTRUCTURE, but more sophisticated, because it is necessary to separate the target from the projectile in the angular couplings. The first part of the computer code is related to the target and is similar to the non-relativistic part of SUPERSTRUCTURE, but do not contain the energy minimization procedure. In the second part the target and the projectile are coupled and the transition matrix elements are calculated, thus it is possible to obtain the non-relativistic collision strengths. The relativistic ones are obtained by the second computer code : JJOM.

COLLISION STRENGTHS : JJOM

This code uses scattering data obtained in LS coupling by D.W., but provides the possibility of transforming these data so as to allow the intermediate coupling of the target, the transformation coefficients being obtained by SUPERSTRUCTURE; that represents the solution of the Breit-Pauli Hamiltonian for the target by an expansion over the wavefunctions, for the non-relativistic target. These "term coupling coefficients" are supplied as inputs to JJOM which uses them to transform the transition matrix from which the relativistic collision strengths are obtained.

COLLISION STRENGTHS : COULOMB-BETHE

For large values of l for the colliding electron D.W. and JJOM become very tedious. In this case the collision strengths are calculated by using a code based upon the Coulomb-Bethe approximation (CBe) (7). For a large angular momentum, the colliding electron radial function is very small inside the target and begins to oscillate outside the target. This allows us to simplify the Slater radial integrals required to calculate the transition matrix elements in the D.W. approximation. The only important corresponding case is the electric dipole transitions in the target. Furthermore, assuming very small transition matrix elements, we can directly relate the collision strengths to the radiative line strengths.

We have calculated the collision strengths Ω , for all the transitions between the 65 Ne-like levels, for Fe XVII, Ge XXIII, Se XXV, Mo XXXIII, Ag XXXVIII with the D.W. approximation for $l=0$ up to $l=19$ (Ω_{DW}) and with the CBE approximation for $l=20$ up to $l=50$ (Ω_{CBE}) (l is related to the colliding electron). Then, the collision strengths Ω are the sum of Ω_{DW} and Ω_{CBe} . The matching at $l=19$ has been checked carefully.

Different incident electron energies for Selenium have been computed and allow us to exhibit a E -dependence (E being the incident electron energy) according to :

$$\Omega_{ij}(E) = a + b/u + c/u^2$$
 where, for the transition from the level j to level $i - |j| -$, E_{ij} is the transition energy ($E_{ij} = E(j) - E(i)$) and u the reduced incident electron energy ($u = E/E_{ij}$).

The computation of five Ne-like ions gave us the Z -dependence of the collision strengths

$$\Omega_{ij}(E, Z) = \frac{1}{(Z + a + b/Z)^2} (c_0 + c_1/u + c_2/u^2)$$

the so introduced parameters only depending on the transition definition.

DIELECTRONIC RECOMBINATION : AUTOLSJ

The autoionization probabilities and the line factors are calculated by using the AUTOLSJ code (8). The spirit of this code is very similar to JJOM one. The "term coupling coefficients" for N and $N+1$ electronic systems are calculated by SUPERSTRUCTURE and are supplied as inputs to AUTOLSJ. The transition matrix elements (bound-free) are obtained in the D.W. approximation. As JJOM, AUTOLSJ calculates the recoupling coefficients and afterwards the autoionization probabilities. The radiative de-excitation probabilities are given by SUPERSTRUCTURE. Thus the line factors F^*_{ij} are derived, according to

$$F^*_{ij} = g_j/g_i \frac{A_a A_r}{\sum A_a + \sum A_r}$$

where g_j and g_i are respectively the statistical weights of the upper (doubly-excited) and lower (singly-excited) levels, A_a and A_r the corresponding autoionization and radiative probabilities.

For a large set of ions - from Ar to Ag -, we have calculated the dielectronic recombination rate coefficient α_d from $1s^2 2s^2 2p^6 \ ^1S_0$ (the Ne-like ground state) to $1s^2 2s^2 2p^6 3l$ ($l=0, 1, 2$) (the four first Na-like excited states and the ground state) via the set of doubly-excited states $1s^2 2s^2 2p^5 3l 3l'$ ($l=0, 1, 2; l'=0, 1, 2$)

$$\alpha_d(i) = 1.65 \cdot 10^{-22} \sum_{\delta} F_{i\delta}^* \exp\left(-\frac{E_{ion} + \bar{E}(i)}{T_e}\right) T_e^{-3/2}$$

T_e being the electronic temperature of the plasma (in eV), E_{ion} the ionization energy of the Na-like involved ion (in eV - as all the energies) and the rate coefficient α_d expressed in cm^3/s .

We approximate $\alpha_d(i)$

$$\alpha_d(i) = 1.65 \cdot 10^{-22} F_S^*(i) \exp\left(-\frac{\bar{E} + E(i)}{T_e}\right) T_e^{-3/2}$$

The total dielectronic recombination rate coefficient α_d^{tot} can be written :

$$\alpha_d^{\text{tot}}(Z, T_e) = \sum_i \alpha_d(i) \\ = A \exp\left(-\beta / T_r\right) T_r^{-3/2}$$

where $T_r = T_e / Z^2$.

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