

# Complex Atoms Modelling for Plasma Diagnostics

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The spectra of high  $Z$  elements in fusion reactor are complex and thus their calculation requires a much larger quantity of atomic data. In the present work we report fundamental atomic data and related quantities for tungsten ions as related to the modeling of high temperature plasmas. In our calculations we used the atomic structure code of Cowan for the parent ion terms and a new perturbative methods for quasi-continuum ion states of tungsten Hf-like ion.

## 1. Introduction

High particle and energy fluxes in future fusion experiments demand the investigation of materials for plasma facing components. A promising alternative to the present frequently used low- $Z$  materials carbon and beryllium is tungsten. Partially ionized ions of elements such as tungsten and tantalum in the second long period, however, have two problems, an atomic structure which increasingly should be described in intermediate coupling and a consequent description of their emitted spectrum lines into very many separated levels from many transition arrays often associated with partially inner shells. The spectral emission may appear as a quasi-continuum.

The main contribution to the quasi-continuum is emitted from tungsten ions around the silver-like  $W^{27+}$  ion. This was confirmed by the dependence of the quasi-continuum intensity on the plasma temperature[1] belonging to tungsten ions with open 4d and 4f subshells.

In this work we report atomic data calculations for tungsten ions with two electrons outside closed shell of type Ca-like, Zn-like, Sr-like, Ba-like or Hf-like. Our method is based on the atomic structure code of Cowan [2] for parent ion states and a new perturbative approach for quasi-continuum states [3].

## 2. Method of calculation

In our work we consider the perturbative approach for doubly excited level position as suggested by Poirier[3]. The atomic system is described by a closed-shell core and two active electrons, named valence with coordinates referred through index 2, and Rydberg electron the coordinates of which are referred through index 1. For example, Ba-like  $W^{18+}$

has configuration  $[Xe] 6s^2$ , Sr-like  $W^{36+}$  has  $[Kr]5s^2$  Hf-like  $W^{2+}$  has  $[Xe] 4f^{14}5d^26s^2$ , etc. These configurations can be written as  $[Xe] n_2l_2j_2n_1l_1$ , for Ba-like and in a similar form for the others. The quasi-continuum states are of type  $5d_{5/2}nf$  ( $J=5$ ) or  $6p_{3/2}nh$  in Ba-like  $W^{36+}$  with decay channel  $5d_{5/2}nl \rightarrow 5d_{3/2}\epsilon'l$  and a such spectra may be grass-like in their complexity. To account theoretically for such transitions, one has to consider the quadrupolar term in the electronic structure.

The proper description of a system is the intermediate pair-coupling scheme,  $jk$ . Then, in a single configuration description, the Rydberg electron is assumed to evolve from a bound hydrogenic state  $(n_1l_1)$  to a continuum state  $(\epsilon l)$  while the valence electron falls from the excited ionic state  $(n_2 l_2 j_2)$  to a lower state  $(n_0 l_0 j_0)$ . The valence electron strongly interacts with the core; hence the spin-orbit effect for this electron dominates all other interactions. The electronic repulsion  $1/r_{12}$  is generally stronger than spin-orbit effects for the Rydberg electron. Finally, a  $jk$  or  $jl$ -coupling scheme is more appropriate for a system. The only thing which changes when different iso-electronic sequences are considered are the Slater integrals and parent ion term

This parent term energy has been calculated by using the atomic structure code of Cowan which allows us to consider  $LS$  or intermediate coupling scheme.

In the perturbation expansion, the solution of the considered Hamiltonian has been written in the form:  $E = E^{(0)} + E^{(1)} + E^{(2)}$  where,  $E^{(0)}$  is unperturbed energy:

$$E^{(0)} = E(n_2 l_2 j_2, n_1 l_1) = E_{n_2 l_2 j_2} - \frac{\xi^2}{2n_1^2} E_{n_2 l_2 j_2}$$

being the parent-ion energy; the first order shift  $E^{(1)}$  is obtained after multipolar expansion of  $V = 1/r_{12} - 1/r_1$  (i.e.(first-order) configuration mixing) and the second order shift implies a sum over the principal quantum numbers of the perturbing state  $(n_0, \ell)$  including the discrete and continuum part of the spectrum. However, the sum over  $n_0$  may usually be restricted to a discrete and even finite one.

$E^{(1)}$  includes the interaction of the valence electron with the core polarized by the inner electrons. The core polarization will give rise to an additional term in energy shift; if there are quasi-degenerate states, the non-diagonal matrix elements are taken into account.

### 3. Results

In the present work we report calculations for  $W^{72+}$  Hf-like ions and preliminary results for Sr-like  $W^{36+}$ .

We studied the following electronic configurations for  $W^{72+}$  :  $4f^{14}5d^26s^2$  ,  $4f^{14}5d5f6s^2$  and  $4f^{14}5d5g6s^2$  with two electrons outside closed shell. Fourteen orthogonal one-electron orbitals  $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 5s, 5p, 4f, 5d, 6s$  were used in our work. An initial structure calculation was carried out for  $W^{72+}$  to determine the lowest thirteen states. The atomic structure code of Cowan has been apply to output values of energy levels in  $jk$  coupling. The Hamiltonian matrix elements were obtained in  $LS$  coupling scheme by including the relativistic Drawin correction term.

The corresponding  $jk$  partial waves imply 600 odd terms, giving rise to  $J=1, J=2, J=4, J=3/2$  and  $J=5/2$ . The analysis of the autoionizing state positions and electron-electron correlation effects on the energy level position will be given in terms of Slater integrals involved into the calculations. The numerical methods consists of following steps:

- (i) the calculation of the bound radial wave functions of the parent ion  $R_{ijk}$  taking account core polarization;
- (ii) the calculation of the continuum wave function  $R_{el}$  on the basis of Seaton's method for the regular Coulomb wave function;
- (iii) the calculation of the bound Coulomb wave function for  $n_1 l_1$ ; since the outer electron wave function is assumed to be hydrogenic, this function is efficiently

computed using the  $l$  downward recursion relation and analytic formulas;

- (iv) the calculation of the Slater integrals corresponding to exchange term in the expression of energy shift.

### References

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- [3] M. Poirier, Phys.Rev. **A38**(1988)3484

