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# Analysis of magnetic-dipole transitions in tungsten plasmas using detailed and configuration-average descriptions

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ABSTRACT

This paper is devoted to the analysis of transition arrays of magnetic-dipole ($M_1$) type in highly charged ions. Such transitions play a significant role in highly ionized plasmas, for instance in the tungsten plasma present in tokamak devices. Using formulas recently published and their implementation in the Flexible Atomic Code for $M_1$-transition array shifts and widths, absorption and emission spectra arising from transitions inside the $3^*n$ complex of highly-charged tungsten ions are analyzed. A comparison of magnetic-dipole transitions with electric-dipole ($E_1$) transitions shows that, while the latter are better described by transition array formulas, $M_1$ absorption and emission structures reveal some insufficiency of these formulas. It is demonstrated that the detailed spectra account for significantly richer structures than those predicted by the transition array formalism. This is due to the fact that $M_1$ transitions may occur between levels inside the same relativistic configuration, while such inner configuration transitions are not accounted for by the currently available averaging expression. In addition, because of configuration interaction, transition processes involving more than one electron jump, such as $3p_{1/2}3d_{5/2} \rightarrow 3p_{3/2}3d_{3/2}$, are possible but not accounted for in the transition array formulas. These missing transitions are collected in pseudo-arrays using a post-processing method described in this paper. The relative influence of inner- and inter-configuration transitions is carefully analyzed in cases of tungsten ions with net charge around 50. The need for an additional theoretical development is emphasized.



## 1. Introduction

Since the first observation of unresolved transition arrays (UTA) in atomic spectroscopy tracing back to the 40s [1] and the pioneering analysis by Moszkowski [2], a special attention has been paid to averaging procedures devoted to the analysis of complex spectra such as those occurring in warm dense plasmas. Noticeably Bauche et al. have obtained formulas for the shift and variance of energies of transitions between two given configurations [3,4], avoiding the very costly procedure of computing spectra involving thousands of levels and millions of lines in a detailed way. When considering highly charged ions, spin-orbit effect becomes dominant and the observed transition arrays connect pairs of *relativistic* configurations and are named Spin-Orbit-Split Arrays (SOSA) [5]. The averaging procedure has been even more generalized by gathering configurations into super-configurations which leads one to consider super-transition arrays (STA) [6].

While most of this theoretical effort has been devoted to electric-dipole ($E_1$) transitions, Bar-Shalom et al. [7] provided formulas for the array widths involving the electric ($E_n$) and magnetic ($M_n$) multipole moments at any order, and Pain et al. [8] provided expressions for $E_2$ arrays. Recently it was pointed out by Krief and Feigel [9] that formulas from Ref. [7] needed to be corrected. Furthermore, these newly derived expressions have been implemented by the same authors in the Flexible Atomic Code (FAC) [10]. Widely used by the community of atomic physics in plasmas, this fully relativistic code is well adapted to the analysis of highly-charged ions of heavy elements, for instance tungsten (W, $Z = 74$), element chosen as plasma facing material in fusion devices [11]. Large radiative losses in tungsten could drastically impact the tokamak operation, therefore their accurate calculation, including $M_1$ effects, is essential [12]. Radtke et al. have studied the complex N-shell band structure in W using an electron-beam ion trap [13]. Several $M_1$ line ratios involving highly-charged tungsten ion with an open $3d$ subshell provide reliable diagnostics for determining temperature and density in hot fusion devices [14].

Owing to the availability of $M_1$-transition array formulas in FAC, we have studied absorption and emission spectra of W ions with a net charge of about 50, comparing detailed and statistical approaches. Our analysis of these sample cases shows that $M_1$ transition array formulas, though accurate for the main peaks in opacity or emissivity spectra, poorly reproduce the wing structures. This paper aims at investigating the origin of this discrepancy, using a

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"constructed-UTA" method based on numerical treatment of detailed transitions.

The present paper is organized as follows. In Section 2, we present the basic formalism used in analysis of absorption and emission in plasmas involving electric- or magnetic-dipole transitions. We then propose several examples of tungsten spectra showing that the standard unresolved transition array analysis may be insufficient to describe $M_1$-type transitions. Two effects may explain this inconsistency. On the one hand the standard theory only involves the first two moments, while higher-order moments may significantly impact the spectral distribution, which is analyzed in Section 3. On the other hand, as studied in Section 4, the UTA/SOSA description may be "incomplete", meaning that certain transitions accounted for in the detailed description are not included in the FAC computation. Conclusions and perspectives are finally proposed.

## 2. Absorption and emission spectra in detailed or averaged approaches

The interest of magnetic dipole transitions can be emphasized considering transition rates. For $E_1$ lines the transition rate from level $b$ to level $a$ is [15]

$$A_{ba}(E_1) = \frac{4\alpha a_0^2 E_{ab}^3}{3\hbar^3 c^2 g_b} (aJ_a \parallel D \parallel bJ_b)^2 \tag{2.1a}$$

where $\alpha$ is the fine-structure constant, $a_0$ is the Bohr radius, $E_{ab}$ the transition energy, $\hbar$ the quantum of angular momentum, $c$ the speed of light, $g_b$ the statistical weight of the upper level and $(aJ_a||D||bJ_b)$ the dimensionless reduced matrix element of the electric dipole vector in atomic units, such as

$$(aJ_a \parallel D \parallel bJ_b)^2 = \sum_{M_a M_b Q} \left\langle aJ_a M_a \left| D_Q^{(1)} \right| bJ_b M_b \right\rangle^2, \tag{2.1b}$$

$D_Q^{(1)}$ $(Q = 0, \pm 1)$ being the standard tensorial components of the electric dipole. Accordingly, the magnetic-dipole rate is [16]

$$A_{ba}(M_1) = \frac{\alpha^3 a_0^2 E_{ab}^3}{3\hbar^3 c^2 g_b} (aJ_a \parallel M \parallel bJ_b)^2 \tag{2.2}$$

where $(aJ_a||M||bJ_b)$ is the reduced matrix element of the vector $\mathbf{M} = \mathbf{L} + 2\mathbf{S}$, $\mathbf{L}$ (resp. $\mathbf{S}$) being the total orbital (resp. spin) angular momentum. In a H-like picture the squared element (2.1b) scales as $Z^{-2}$ if $Z$ is the nucleus charge, while the magnetic moment is $Z$-independent. This shows that $M_1/E_1$ rates scale as $Z^2\alpha^2$, assuming analogous transition energies and "ordinary" matrix elements. For non-hydrogenic ions with an effective charge $Z_c$ acting on outer electrons, this ratio is expected to be $\sim Z_c^2\alpha^2$. Therefore, the higher the average charge is, the more important $M_1$ transitions are.

Such rates play a central role in the absorption and emission properties of a plasma. The spectral opacity at energy $E$, directly connected to the absorption coefficient, is given by $\kappa(E) = \mathscr{N}_{\mathrm{Av}}\sigma(E)/A = \sigma(E)/M$ where $\mathscr{N}_{\mathrm{Av}}$ the Avogadro number, $\sigma(E)$ the absorption cross-section, $A$ the molar mass, and $M$ the ion mass. The bound-bound contribution to this cross-section $\sigma_{\mathrm{b-b}}$ involves a sum over transitions $a \to b$

$$\sigma_{\mathrm{b-b}} = \pi^2\hbar^3 c^2 \sum_{ab} p_a \frac{g_b A_{ba}}{g_a E_{ab}^2} \mathscr{S}_{ab}(E) = 2\pi^2\alpha^2\hbar c a_0 \sum_{ab} p_a f_{ab} \mathscr{S}_{ab}(E), \tag{2.3}$$

where $f_{ab}$ is the absorption oscillator strength, $p_a$ the level-$a$ population such as $\sum_a p_a = 1$, and $\mathscr{S}_{ab}(E)$ the lineshape, normalized according to $\int dE\ \mathscr{S}_{ab}(E) = 1$. The spectral emission assuming a point-like source, i.e. with a plasma size much less than the absorption length — or 0-dimensional emission — so that opacity effects can be ignored, is given for its bound-bound part by

$$\mathscr{E}_{\mathrm{b-b}}^{0d}(E) = N_{\mathrm{ions}} \sum_{ab} p_b A_{ba} E_{ab} \mathscr{S}_{ab}(E). \tag{2.4}$$

The bound-free contribution should be added to these expressions. However in the examples considered below, the ionization thresholds lie above 4 keV, which is significantly higher than the analyzed range, so this contribution is not needed here.

In most of the cases considered the lineshape $\mathscr{S}_{ab}(E)$ is given by a Doppler profile with a variance given by $\sigma_{\mathrm{D}}^2 = E_{ab}^2 k_{\mathrm{B}} T/(Mc^2)$, where $k_{\mathrm{B}}$ is the Boltzmann constant and $T$ the ion temperature. When unresolved transition arrays (UTA) are considered, their variance $\sigma_{\mathrm{UTA}}^2$, given by the theory [4,17] or by the atomic code [9,10] adds up to the Doppler variance, leading to the profile

$$\mathscr{S}_{ab}(E) = \frac{1}{(2\pi)^{1/2}\sigma} \exp\left(-\frac{(E - E_{ab})^2}{2\sigma^2}\right) \text{ with } \sigma^2 = \sigma_{\mathrm{D}}^2 + \sigma_{\mathrm{UTA}}^2. \tag{2.5}$$

If we account for natural broadening, this Gaussian profile has to be convolved with the natural Lorentzian profile, giving rise to Voigt profile. The distinction between Voigt and Gaussian profiles is discussed in Appendix A. In this work the "UTA" considered are groups of transitions between pairs of *relativistic* configurations, which are more often refered to as Spin-Orbit-Split Arrays (SOSA) in the literature [4,5]. However we use the term UTA because this acronym is standard in FAC documentation.

In order to illustrate the above considerations, we present in Fig. 1a and b sample computations of the opacity of a tungsten plasma with an effective temperature of 180 eV, which intends to simulate the non-LTE charge distribution of a tokamak plasma, as explained in Appendix B. The inner K and L shells are filled, as in all other examples in this paper. Detailed and UTA computations are plotted on the same graphs. Lineshapes are assumed to be given by Voigt profiles, the natural broadening effect arising from bound-bound emission. The very narrow structures observed on the UTA opacity correspond to transition arrays consisting of only one line, with therefore no UTA broadening. To make the detailed-UTA comparison easier, the detailed spectra have been convolved with a Gaussian response function of 10-eV FWHM using standard fast-Fourier transform (FFT) techniques [18] and a 131072-point grid. As seen in Fig. 1a, except in the 800-eV wing and to a lesser extent close to 500 eV, the UTA formulas reproduce correctly the spectral opacity originating from $E_1$ transitions. Conversely considering the $M_1$ contribution shown in Fig. 1b, it turns out that the UTA formulas, though reproducing correctly the main structures around 90 eV and 330 eV, are orders of magnitude off when considering the far wings of these structures, e.g. around 650 eV. Accordingly, we show *0-d-emission* spectra arising from $M_1$ transitions in tungsten plasma in Fig. 2. Four different charge states are plotted to show that the detailed-UTA discrepancy occurs independently of the ion considered. The next two sections of this paper are devoted to explaining the origin for this discrepancy between the detailed and the unresolved-transition array descriptions, which may arise from two different effects: influence of high-order moments, and missing lines in the UTA method.

## 3. Spectrum analysis using constructed transition arrays

In order to check the hypothesis that moments of order above 2 may play a role, we have designed a "constructed" or pseudo-UTA computation in the following way. The various detailed transitions are sorted so that all lines connecting a pair of given relativistic configurations ($\alpha$, $\beta$) are collected in this pseudo-UTA structure. Since the oscillator strengths are known from the detailed transition list, we may compute the average energies and centered moments for each pair of relativistic configurations $\alpha$, $\beta$ using the relations

$$E_{\alpha\beta} = \sum_{\substack{a\in\alpha \\ b\in\beta}} g_a f_{ab} E_{ab} \Big/ \sum_{\substack{a\in\alpha \\ b\in\beta}} g_a f_{ab} \tag{3.1a}$$