Configuration interaction effect on open M shell Fe and Ni LTE spectral opacities, Rosseland and Planck means

D Gilles¹, M Busquet², F Gilleron³, M Klapisch⁴ and J-C Pain³

¹CEA, DSM, IRFU, F-91191 Gif-sur-Yvette, Cedex, France
²Research Support Instruments, Lanham, MD 20706, USA
³CEA, DAM, DIF, F-91297 Arpajon, France
⁴Berkeley Research Associates, Beltsville, MD 21042, USA

E-mail: dominique.gilles@cea.fr

Abstract. We have recently shown that iron and nickel open M-shell opacity spectra, up to \(\Delta n = 2\) are very sensitive to Configuration Interaction (CI) treatments at temperature around 15 eV and for various densities. To do so we had compared extensive CI calculations obtained with two opacity codes HULLAC-v9 and SCO-RCG. In this work we extend these comparisons to a first evaluation of CI effects on Rosseland and Planck means.

1. Introduction

HULLAC-v9 [1, 2] and SCO-RCG [3, 4] detailed opacity codes can now provide precise spectral opacities for many applications like comparisons with experimental spectra and astrophysical studies [4, 5]. We shall discuss in this work an example of low temperature (\(kT = 15.3\) eV) - low density (\(n_e = 3 \times 10^{-17}\) cm\(^{-3}\)) plasma condition typical of stellar envelopes [5]. In such example a precise evaluation of the spectrum, and of the associated Rosseland (\(K_R\)) and Planck (\(K_P\)) means, supposes a careful evaluation of the billion of open M-shell transitions together with full Configuration Interaction treatment [6]. This is impossible in practise and only partial CI is included in recent improved opacity tables [7]. In a previous work we explored CI effect using HULLAC-v9 until convergence over the set of configurations [6]. We have shown that full CI treatment is really important for the first open M-shell transitions (\(n = 3, \Delta n = 0, 1, 2\)) by comparing "full CI" and "CI in one Non Relativistic Configuration (NRC)". But it is not practically possible to include higher excited levels (\(n > 5\)) using full CI treatment. A complete detailed description of the spectrum and of CI effect on the associated \(K_R\) and \(K_P\) requires mixed CI treatments and validation of the results are ongoing.

In this work we have taken advantage of interplaying comparisons [6] between the large possibilities and complementarities of HULLAC-v9 and SCO-RCG codes to discuss full CI influence on \(K_R\) and \(K_P\) means. The latter code is able to produce complete and precise LTE spectra, Rosseland and Planck means assuming CI in one NRC and the former can evaluate main full CI effects on the first M-shell transitions. On the example chosen above, we shall discuss and validate a method to provide corrections to \(K_R\) (and \(K_P\)) by using comparisons between HULLAC-v9 full CI and CIinNRC results and SCO-RCG ones. The Stark broadening of ion lines is now implemented using simple Dimitrijevic


2. Main features of the des opacity codes

2.1. The SCO-RCG code. The detailed opacity code SCO-RCG [3, 4, 6] is devoted to the diagnostics and interpretation of spectroscopy experiments in LTE plasmas. The data required for the calculation of the detailed transition arrays (Slater, spin-orbit and dipolar integrals) are obtained from the super-configuration code SCO, providing in this way a consistent description of the plasma screening effects on the wave functions. Then, the level energies and the lines (position and strength) are computed by an adapted RCG routine of Cowan. The extended list of configurations or super-configurations is generated automatically according to several criterions (on Boltzmann probability, number of successive excitations,...). DLA calculations are performed only for pairs of configurations giving rise to less than 800,000 lines. In other cases, transition arrays are represented statistically by Gaussian profiles in the UTA or SOSA formalisms. The strength of the hybrid approach is that we take into account many satellite lines and highly excited states, using an extension of the PRTA (Partially Resolved Transition Array) model, which enables us to replace many statistical transition arrays by small-scale DLA calculations. The SCO-RCG code, which includes many satellite lines and highly excited states, provides precise opacities, required for astrophysics, inertial confinement fusion, and for the interpretation of laser and Z-pinch experimental spectra. SCO-RCG iron spectral opacity is illustrated in Fig. 1, corresponding to the stellar envelope plasma condition of interest (15.3 eV, 3.2 \text{10}^{17} \text{cm}^{-3}), showing the numerous open M-shell transitions contributing to Rosseland and Planck means for 1 < u = h\nu/kT < 20 (see definitions on Fig. 1). To compute 1/KR we split the spectral range in 3 domains. (a): below u < 0.7 (mainly f-f which gives a small contribution of 5 \times 10^{-5}), (b): 0.7 < u < 10, where K_{bb} is dominant and can be solely used as it contributes to 96% of the integral, (c): above u=10, where line and b-f contributions are negligible (3 \times 10^{-6}). Same decomposition is applied to KP.

Fig 1: Iron SCO-RCG spectral f-f (blue dotted-dashed), b-f (red long dashed) and total opacities (full black line) at 15.3 eV and 3.2 \text{10}^{17} \text{cm}^{-3} (< Z > = 8.5). K_R and K_P means definitions and values are reported on the figure.

2.2. The HULLAC-v9 code. This code is an integrated code for calculating atomic structure and cross sections for collisional and radiative atomic processes, in a jj coupling scheme [1, 2, 6] and references inside). In the Detailed Level description mode it is possible to take into account CI effects inside user defined groups of configurations (GroC). The diagonalization of eigenvectors for all levels of same J
(in one charge state) is performed in each GroC. To be named "full or exact", CI treatment requires
the inclusion of the whole set of fine structure levels in the same GroC, what means there will be one
GroC per charge state. The keyword ClinNRC in the code generates coefficients of the Hamiltonian
only between Relativistic Configurations pertaining to the same parent Non Relativistic Configuration
(RCM), whereas CI lifts this restriction. The size of the matrices to be diagonalized obviously and
dramatically increases with $\Delta n$. Following previous study conclusions our CI comparisons are
performed over most intense and most sensitive to CI $\Delta n \leq 2$ transitions. More details on the validation
are given in [2, 6]. Stark broadening of ion lines is now implemented using [8], together with Doppler
and instrumental gaussian. Fig. 2 shows a comparison and a good agreement between SCO-RCG (all
transitions) and HULLAC-v9 (assuming "CI in one NRC" and only $n = 3$, $\Delta n \leq 2$ transitions) over all
the energy range of interest. This is true also for nickel (not illustrated) for same conditions.

Fig. 2: Good agreement between SCO-RCG (all transitions) and HULLAC-v9 (assuming "CI in one
NRC" $n = 3$, $\Delta n \leq 2$ transitions) spectral opacity for $0.7 < u < 13$ and same conditions as Fig. 1. A
Gaussian broadening of 0.01 eV is applied to make the figure readable.

3. Evaluation of CI effect using HULLAC-v9 code.

In preceding sections we have shown that $\Delta n \leq 2$ b-b contributions are sensitive to CI and mainly
contribute to $K_R$ (and $K_P$) changes. Thus we can now continue and restrict our comparisons to
HULLAC full CI and HULLAC ClinNRC b-b $\Delta n \leq 2$ contributions (Fig. 3 a, b). As we assume LTE,
total opacity is just the opacity of different ionic species contributions, weighted by the populations.
For our case we get: Fe VIII (0.03), Fe IX (0.41), Fe X (0.52), Fe XI (0.04). On Fig. 3 we have
compared the two calculations for Fe VIII, spectral integrand (3a) and integrated over $\Delta \nu = 0.1$ eV
(3b). Fig. 3b reveals at which energies the integrals are most sensitive to CI. $K_R$ is reduced by 38%
because of CI. To obtain $K_R$ correction for any other density ones just needs to use the appropriated
ionic populations. $K_R$ linear means is less sensitive to CI (19.5%) and present a quite constant
reduction for each individual charge states, 17% (Fe VIII), 19 % (Fe IX), 20 % (Fe X) and 18 % (Fe
XI). Full CI and ClinNRC atomic data (energies, cross sections,...) have been stored for the different
Fe (and Nickel not illustrated here) ions. We shall repeat this work for other temperatures in the range
10-30 eV to obtain quantitative corrections (ion, T, $\rho$) for all stellar envelopes conditions of interest
[5]. For larger T we expect inclusion of more excited transitions to be required. These extensive
studies are ongoing to calculate full CI and ClinNRC spectra using the atomic HULLAC-v9 data already calculated [1] and to characterize \((T, \rho)\) regions of importance.

![Fig. 3 a, b: Comparisons between iron HULLAC full CI and HULLAC ClinNRC b-b \((\Delta n \leq 2)\) \(1/\text{Kr}\) contributions: (a) spectral integrand, (b) same after integration over \(\Delta h\nu = 0.1 \text{ eV}\) for clarity.]

4. Conclusion.

In a CI treatment both the CI effects and the number of configurations play a role, but the difficulty increases with the value of the principal quantum number of the upper shell of the transitions. Thus extensive detailed comparisons between SCO-RCG and HULLAC-v9 (including nickel opacities not illustrated in this paper) have been very instructive and useful for understanding the sensitivity of the opacity to CI, to the inclusion of highly excited transitions and to determine the spectral region of importance in the method proposed here. In this example full CI treatment up to \(\Delta n \leq 2\) transitions is enough and make change in the b-b contribution to Rosseland means of about 38\% (and around 20\% for \(K_p\)). HULLAC-v9 and SCO-RCG have been upgraded to take into account Stark effects. As expected Stark broadening effect is small compared to Doppler effect for low density - low temperature application. After this first comparison on a typical stellar envelope condition, we shall use HULLAC-v9 CI and ClinNRC atomic data [6] to investigate more conditions \((\rho-T)\) in the future and we shall also include Stark broadening in our corrections.

References

[1] Busquet M, Bar-Shalom A, Klapisch, Oreg J 2006 *J. Phys. IV* 133 973.
[2] Busquet M, Klapisch and M Gilles 2013 D *EPJ Web of Conferences* 59 14004;
   Gilles D, Turck-Chièze S, Busquet M & al 2013 *EPJ Web of Conferences* 59 14003.
[3] Pain J-C and Gilleron F 2015 *High Energy Density Phys.* 15 30.
[4] Pain J-C and Gilleron to be published in 9th Ifsa 2015 conference proceedings.
[5] Gilles D, Tuck-Chièze S, G Loisel & al 2011 *High Energy Density Phys.* 7 312;
   Turck-Chièze S, Gilles D, Le Pennec M, Blenski T & al 2013 *High Energy Density Phys.* 9 473.
[6] Gilles D, Busquet M, Klapisch M, Gilleron F, and Pain J-C 2015 *High Energy Density Phys.* 16 1.
[7] New OPLIB (http://aphysics2.lanl.gov/opacity/lanl/); OPAL (https://opalopacity.llnl.gov/).
[8] Dimitrijevic M S and Konjevic N 1980 J. Quant. Spectrosc. Radiat. Transfer 24 451.