

Converged Close-Coupling R-Matrix calculations of Photoionization of Fe XVII in Astrophysical Plasmas: from Convergence to Completeness

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Abstract. Extensive resonance structures are manifest in R-Matrix (RM) calculations. However, there exist a large number of highly excited electronic configurations that may contribute to background non-resonant bound-free opacity in high-temperature plasmas. Since RM calculations are very complex, and not essential for background contributions, the Relativistic Distorted Wave (RDW) method is utilized to complement ("top-up") photoionization cross sections of Fe XVII obtained using Close-Coupling Breit-Pauli R-Matrix (CC-BPRM) method. There is good agreement between RDW and BPRM for background cross sections where resonances are not present, and individual fine structure levels can be correctly matched spectroscopically, though resonances are neglected in the RDW. To ensure completeness, a high energy range up to 500 Ry above the ionization threshold for each level is considered. Interestingly, the hydrogenic Kramer's approximation also shows the same energy behavior as the RDW. Grouping separately, the BPRM configurations consist of 454 bound levels with resonances corresponding to configurations $1s^2 2s^2 2p^4 n l n' l'$ ($n \leq 3$, $n' \leq 10$); including RDW configurations there are 51,558 levels in total. The topup contribution results in ~20% increment, in addition to the 35% enhancement from BPRM calculations over the Opacity Project value for the Rosseland Mean Opacity at the Z-temperature of 2.11×10^6 K (Pradhan & Nahar 2017)..

1. Introduction

Iron opacity at the condition similar to the solar radiation/convection zone boundary was measured in Sandia National lab (Bailey et al. 2015), revealing that the iron opacity is up to 30-400% higher than that predicted by theoretical opacity models. To resolve this discrepancy, extensive Close-Coupling R-Matrix calculations with 60 fine structure levels of the core ion Fe XVIII with $n \leq 3$ (Nahar, et al. 2011), and 99 LS terms with $n \leq 4$ were carried out, showing strong photon absorption due to core excitation and resulting in an increment of 35% in the Rosseland mean opacity over the Opacity Project (OP) data (Nahar & Pradhan 2016, hereafter NP16). Whereas the NP16 work demonstrated that in R-Matrix opacity calculations convergence of the CC wavefunction expansion is a necessary condition for accuracy, sufficiency in terms of completeness of all possible excited configurations at Z plasma temperatures still

requires additional contributions in the high-energy range (Blancard et al. 2016; Nahar & Pradhan 2016; Iglesias & Hansen 2017).

In this paper, we address completeness issue as follows. We consider the 60-level BPRM calculations since (i) fine structure is included and is important, and (ii) the 99LS calculations show background convergence with additional resonances converging on to the $n = 4$ Fe XVIII levels, but do not result in further enhancement of the Fe XVII Rosseland Mean Opacity, most likely owing to neglect of fine structure. The 60 CC BPRM (Nahar, et al. 2011) levels have also been identified (accessible through NORAD Atomic Data (Fe XVII) <http://norad.astronomy.ohio-state.edu/fe17/fe17.en.fs.txt>). In the following sections, the 60CC data included in Nahar, et al. (2011) are displayed, followed by the RDW top-up configurations and transitions calculated using the flexible atomic code (FAC), an open-source software package (Gu 2008). To ensure the correspondence of the data from FAC, comparison of the photoionization cross section from both FAC and BPRM is investigated. Moreover, to also ensure completeness in energy, calculation in the high energy region is extended to 500 Ry using FAC.

2. Configurations in 60 CC BPRM

The 60 CC BPRM calculation of photoionization of Fe XVII is comprehensively studied in Nahar, et al. (2011), and the 454 bound levels as well as the 60 target states are readily available in NORAD Atomic Data (Fe XVII) <http://norad.astronomy.ohio-state.edu/fe17/fe17.en.fs.txt>. The bound and target configurations are in the below (the full K-shell is omitted for simplicity):

- Bound Configurations:
 - $2s^22p^6$
 - $2s^22p^5$ with $3l, 4l, 5l, 6l, 7l, 8l, 9(s-k), 10(s-k)$, where l represents all the subshells in a shell
 - $2s2p^6$ with $3l, 4l, 5s$
- Target Configurations:
 - $2s^22p^5$
 - $2s2p^6$
 - $2s^22p^43l$

In the next section, all the possible top-up transitions do not involve any one appearing in 60 CC BPRM.

3. Top-up Configurations and Transitions

To complement the photoionization cross section of 60 CC BPRM, part of the top-up configurations and transitions are taken from Badnell & Seaton (2003), Badnell et al. (2005) and Iglesias & Hansen (2017). Here are the top-up configurations and transitions in the following below:

- 454-level L-shell photoionization

- The same 454 levels as in 60 CC BPRM, but are considered as L-shell photoionization only, excluding any transition that appears in 60 CC BPRM.
- The other L- and outer-shell photoionization
 - $2s2p^6$ with $5(p - g)$, $6l$, $7l$, $8l$, $9l$ and $10l$.
 - One type of transition is L-shell photoionization, which ionizes one electron in L-shell, leaving the rest intact.
 - The other type of transitions is "outer-shell" photoionization, with any dipole-allowed final states from $2s2p^6$, $2s^22p^5$, $2s^22p^43l$.
- 2-hole Configurations

Each 2-hole configuration can be divided into two parts, inner part and outer part, and the 2-hole configurations included are formed by combining any one in inner part and any one in outer part.

 - Inner Part:
 - * $2p^6$
 - * $2s2p^5$
 - * $2s^22p^4$
 - Outer Part:
 - * $3l^2$, $3l4l'$, $3l5l'$, $3l6l'$
 - * $4l^2$, $4l5l'$, $4l6l'$
 - * $5l^2$, $5l6l'$
 - * $6l^2$

The transitions considered from the 2-hole configurations are: i) in the outer part either of the two electrons is ionized, leaving the inner part intact; ii) one electron is ionized from the L-shell.

Using FAC, it's fairly easy to implement the photoionization calculations compared with the BPRM, resulting in 51,558 initial levels and more pairs of transitions among them. For each level, an individual energy mesh is created according to the ionization thresholds so that the photoionization cross section is well resolved at all energies. The final photoionization cross section for a level is the sum of all the transitions from the level in the same energy mesh, up to 500 Ry above the lowest threshold.

4. Comparison between RDW and BPRM

To top up the photoionization cross section for 454 levels included in 60 CC BPRM (Nahar, et al. 2011) by including additional transitions from the L-shell, energy levels have to be matched between RDW and BPRM. By comparing J, Pi, energy order and some other factors, they are readily matched. To ensure their being matched correctly, RDW calculation is done on the photoionization cross section from the 454 levels to any possible core states included in 60 CC BPRM, i.e. levels in $2s^22p^5$, $2s2p^6$ and $2s^22p^43l$. Generally the RDW matches well with the background of the BPRM result, but misses out all the resonances in BPRM (see Figure 1).

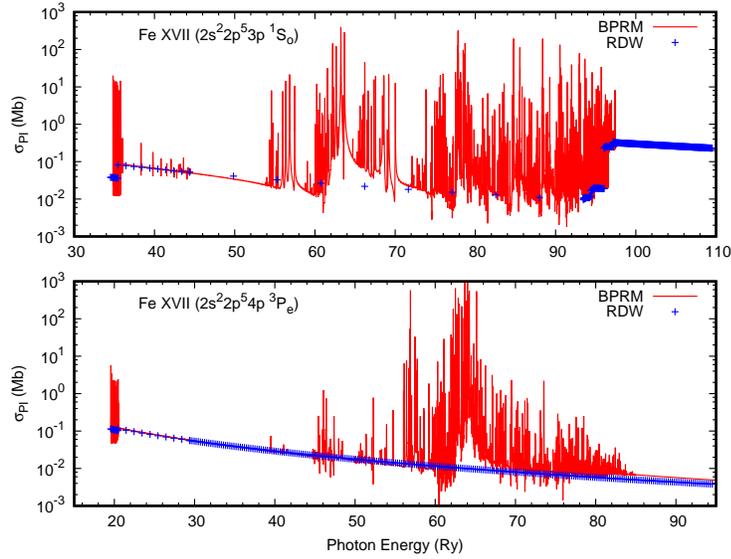


Figure 1. Comparison of the photoionization cross section for two levels using both RDW and BPRM. *Above:* Fe XVII $2s^2 2p^5 3p^1 S_0$. *Below:* Fe XVII $2s^2 2p^5 4p^3 S_e$

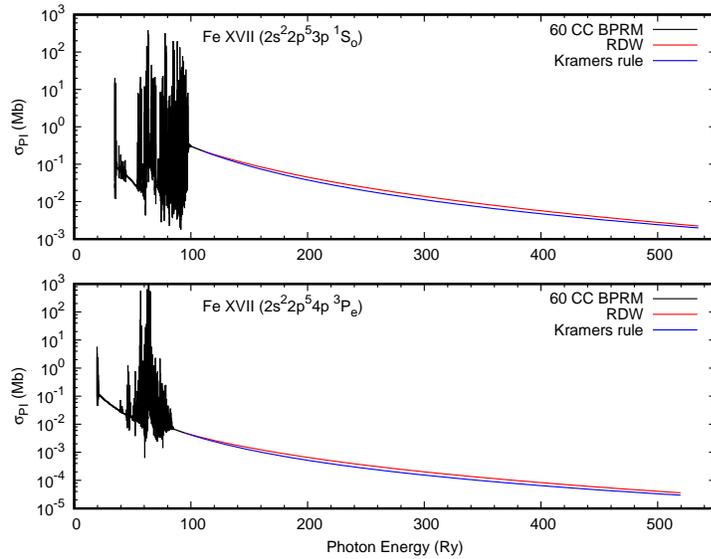


Figure 2. Photoionization cross section in high energy regime using RDW and Kramer's rule. *Above:* Fe XVII $2s^2 2p^5 3p^1 S_0$. *Below:* Fe XVII $2s^2 2p^5 4p^3 S_e$

5. Photoionization Cross section in high energy region

In addition to adding more possible configurations and transitions, energy range in which the calculation is done is extended to 500 Ry above the lowest energy threshold for each level. As the BPRM computation in such a large energy range is expensive,

and also unnecessary, the RDW is used to extend the high-energy "tails" of photoionization cross section for the 454 levels in 60 CC BPRM. The RDW data are rescaled by the ratio of photoionization cross section from BPRM and RDW at the last energy point in BPRM, as the BPRM data should be more accurate. Kramer's rule ($\sigma_\nu = \sigma_1(\nu_1/\nu)^3$) is also applied to extrapolate in the tails region. It turns out that the opacity contribution from the high energy regime is equivalent using RDW and Kramer's rule (see Figure 2).

6. Conclusion

Calculation of photoionization cross section of Fe XVII is completed by including more top-up configurations and transitions, and extending into the high-energy bound-free continuum. We find an additional $\sim 20\%$ enhancement, in addition to the 35% reported in NP16, with the total topped-up result of 1.64 times the OP value for the Rosseland mean opacity at the Z temperature (Pradhan & Nahar 2017). The high-energy topup is thus close to the 16% estimated in (Iglesias & Hansen 2017). However, the actual Fe XVII Rosseland mean opacity might be still larger due to additional fine structure thresholds from the 218-level BPRM calculation in progress including resonances converging on to the $n = 4$ thresholds of Fe XVIII.

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