R-MATRIX CALCULATIONS FOR OPACITIES IV: CONVERGENCE, COMPLETENESS, AND COMPARISON OF RELATIVISTIC R-MATRX AND DISTORTED WAVE CALCULATIONS FOR Fe XVII AND FE XVIII

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R-MATRIX AND DISTORTED WAVE APPROXIMATIONS

CONVERGENCE, COMPLETENESS, AND COMPARISON OF RELATIVISTIC R-MATRIX AND DISTORTED WAVE CALCULATIONS FOR Fe xvii AND Fe xviii

The objective of the series "R-matrix calculations for opacities" is to provide high accuracy opacities obtained using the high accuracy atomic data.

• The R-matrix method is the most powerful method to obtain high accuracy parameters for the two main radiative atomic processes of photo-absorption or opacities:
i) Photo-excitation,
ii) Photo-ionization

• Relativistic Breit-Pauli R-matrix (BPRM) method implements close-coupling (CC) wavefunction expanion that generates very large number oscillator strengths for transitions and resoanances in photoioniza-tioin

• It can accommodate interactions of a large number of configurations that is not possible for an atomic structure calculation. This results in large Hamiltonian matrix, transition matrix elements.

• Hence, solving the Hamiltonian matrix with coupled channels becomes complex and extensive for numerical computation.

Role of R-matrix codes

• For practicability, but still producing largest sets of atomic data, R-matrix method adopts typically to compute

- All radiative transitions with $n \leq 10$ and $l \leq 9$
- All resonancese in photoionization with effective quantum number of the Rydberg series $\nu \leq 10$ and $l \leq 9$
- Computation of photoionization cross sections at energies well beyond all core ion excitations specified in the wavefunction expansion

• HOWEVER, it can include core excitations going to n=2-4, levels, that is, create Rydberg series of resonances with $n \leq 4$ which still requiring extensive computation. Beyond it, computations are too expensive for practical need accuracies.

- Our findings indicate that this limited condition is more than sufficient for most cases since i) no bound states form with higher core excitation and ii) resonances have weakened converging on to the background

• The other issue is R-matrix can not compute the impact on photoionization cross ssections due to ionization of deeper core electrons when crossing their ionization energy thresholds if they are not included in the CC wavefunction. Usually the R-matrix high energy cross sections are extended by extrapolation using Kramers formula.

- The impact of the above issue is typically low unless the energy needs to reach K-shell ionization.

Role of a code with simpler approximation, such as, FAC

• To ensure our goal of convergence and completeness for the opacity calculations, all possible excited configurations with additional contributions in the high-energy region, named as "top-up" contributions, still remained to be ascertained.

- The top-up transitions for bound–bound and bound–free data are obtained from relativistic distorted wave (RDW) calculations using the flexible atomic code (FAC). We carried out the followings:

• Calculated all oscillator strengths with core excitations going to $n \leq 6$.

- Being an atomic structure code, FAC was able to find some missing bound energy levels from R-matrix code. R-matrix code can miss energies which are very closely lying and the energy bin to search them is not fine enough.
- FAC computed many energy levels, bound and in the continuum which are typical for atomic structure codes, and computed extensive sets of oscillator strengths for transitions among them adding contributions for higher excitations.
- Overlapping transitions from FAC were omitted which required spectroscopic indentification of levels.
- To ensure data correspondence from FAC, a procedure for matching the bound levels from BPRM and FAC results was adopted. For

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identification comparison between BPRM and RDW energy levels, careful examination of the level parameters, such as quantum defects and associated bound–bound and bound–free transitions were carried out. The following table illustrates matching of levels.

Table 2. Selected levels of Fe XVII ($J = 3, \pi = 1$) and Fe XVIII ($J = 1/2, \pi = 1$) to be matched (note: the energy is z-scaled, and in units of $10^{-2} Ry$)

	Level index	BPRM	RDW
Fe XVII	12	−3.670 657	−3.679 60
	13	−2.873 930	−2.843 19
	14	−2.868 775	−2.842 38
	15	−2.842 915	−2.837 61
	16	−2.835 625	−2.835 55
	17	−2.774 853	−2.779 98
	Level index	**BPRM**	**RDW**
Fe XVIII	64	−1.275 887	−1.277 03
	65	−1.234 865	−1.241 75
	66	−1.226 084	−1.237 24
	67	−1.136 909	−1.146 91

Selected levels of Fe xvii (J = 3, $\pi = 1$) and Fe xviii (J = 1/2, $\pi = 1$) are matched (note: the energy is z-scaled, and in -2 units of 10 Ry)

- The bound-contrinuum transitions were treated as resonance lines as following general convention, and hence represented Rydberg series of resonances with core excitations beyond $n > 4$.
- Transitions among continuum states were treated as free-free transitions.

• FAC also added the contributions on photoionization cross ssections at very high energies. Although FAC does not compute resonances, its higher orbital wavefunctions could compute the background enhancement at inner core ionization thresholds.

• There are cases where FAC produced cross sections that matched very well with the background cross sections from BPRM method. Figure 2 illustrates such case for Fe XVII.

- In case of lower or higher cross sections from FAC compared to the background cross sections of BPRM method, a multification factor was derived to match FAC cross sections with the BPRM ones. They are illustrated in Figure 3.
- However, discrepancy in matching in the low energy region near ionization threshold remained an issue for many levels. Increment of number of configurations were attempted for the matching and we obtained partial success, as illustrated in Figures 3 and 4.

• We replaced Kramer's extrapolation for the high energy region by the extention of RDW cross section. RDW can include the effect on photoionization due to ionization of deeper core electrons when crossing their ionization energy thresholds.

Matching of RDA photoionization cross sections of Fe XVII and Fe XVIII with the background cross sections from BPRM method.

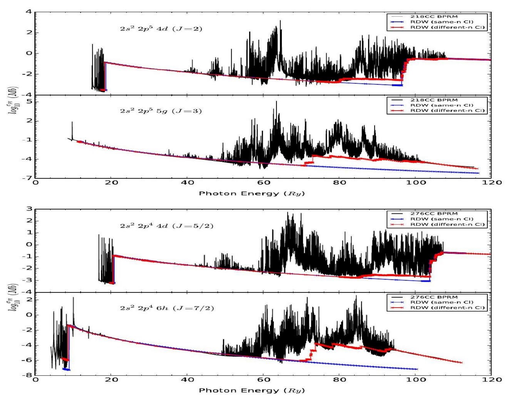

Figure 2. Most of the levels are matched on the first attempt with excellent consistency in photoionization cross section. The configuration is attached with each level. BPRM (black), RDW(blue and red). 'Same-n CI' means only same-n-complex CI is considered for core configurations, and 'different-n CI' refers to both same-n- and different-n-complex CI.

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Matching of RDA photoionization cross sections of Fe XVII and Fe XVIII from FAC with the background cross sections from BPRM method.

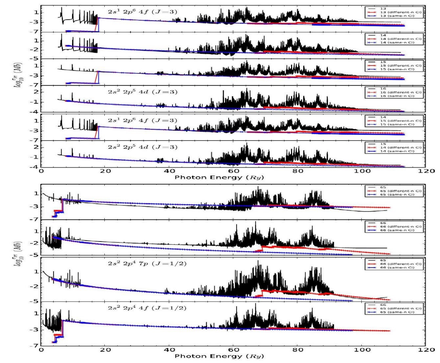

Figure 3. Multiple attempts are needed to ensure the correct matching when the levels are found with discrepancy in the photoionization cross section. The discrepancy is shown in the upper panel and the final matching in the lower one. Find the configuration attached for each level. BPRM (black), RDW(blue and red). 'Same-n CI' refers to only same-n-complex CI is considered for core configurations, and 'different-n CI' refers to both same-n- and different-n-complex CI are considered.

Matching of RDA photoionization cross sections of Fe XVII and Fe XVIII with the background cross sections from BPRM method.

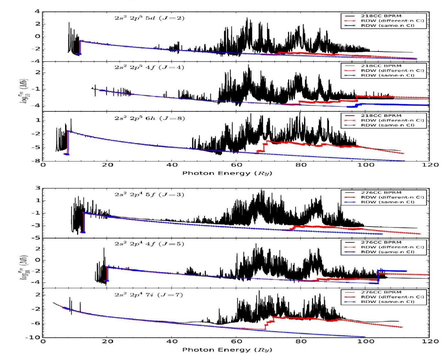

Figure 4. Different-n CI improves the background significantly, but there is still very large discrepancy in the right region of energy for some levels. BPRM (black), RDW(blue and red). 'Same-n CI' refers to only same-n-complex configuration interaction is considered for core configurations, and 'different-n CI' refers to both same-n- and different-n-complex configuration interaction are considered.

Matching the high energy tail from RDA photoionization cross sections for Fe XVII and Fe XVIII with the background cross sections from BPRM method.

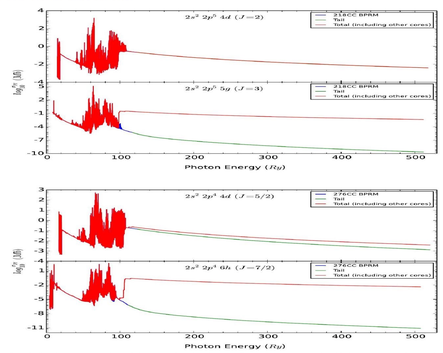

Figure 6. The photoionization cross section of the same four levels as in figure 2 are extended to higher energy region and the contribution from other core configurations with different-n-complex CI is added. Blue: BPRM calculation; green: RDW data multiplied by a ratio; red: total photoionization cross section.

CONCLUSION: Our investigation on the effect of configuration interaction which plays a significant role in correctly reproducing some background cross sections may not be important. Due to the fact that the additional RDW levels correspond to high-nl bound levels that are negligibly populated according to the Mihalas-Hummer-Däppen equation-of-state, the effect on opacities is expected to be small.

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