# Calculation of electron impact excitation cross-sections and collision strengths for non-LTE modelling

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LABORATÓRIO DE INSTRUMENTAÇÃO E FÍSICA EXPERIMENTAL DE PARTÍCULAS



# Non-LET atomic data needs



# Method

## Atomic energy levels

• Optimized potential (SMBO) and calibrated energies

## **Electron impact cross-sections**

• Distorted wave approximation

# Level populations

• Optically thin plasma assumed (no reabsorption)

# Col Rad Py

## **Emissivity and luminosities**

• Assuming elemental masses from Gillanders

**FAC** 

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### Kilonovae and r-process

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> When two neutron stars merge, we can detect gravitational waves from the explosion as well as an electromagnetic transient counterpart, known as kilonova. Reprocess reactions may take place, leading to the creation of heavy nuclei such as lanthanides and actinides [1]. The first kilonova observation in 2017 marked the first opportunity to observe and model the nucleosynthesis of elements in these circumstances.

- LTE modelling (approximation valid in the first few days after the merger):
- Level populations follow Maxwell Boltzmann distribution;
  Bolometric light curves can be reasonably approximated using grey opacities.
- NLTE modelling (necessary from 5 days after the merger) [2]: → Lower densities of the ejecta require a full solution for the rate equations;
- → A more extensive set of atomic data is required, for example, Electron-Impact Excitation (EIE) cross sections.
- Impact of correlation

Atomic structure, transition rates and EIE cross sections were calculated using FAC. As a Relativistic Configuration interaction (RCI) code, its accuracy is highly sensitive to the number of configurations included in the model.



 Added correlation (for improved wavefuncions) has a limited impact on the intensity of EIE cross sections and does not significantly affect the resulting luminosities

### DW, R-matrix and VRA



### Line luminosities

To investigate the impact of EIE cross-sections, we calculated spectral line luminosities following the same prescription as in McCann *et al* [3]. This was achieved by first determining the atomic level populations and photon emissivity coefficients (PECs) using COLRADPY [4] collisional-radiative solver.

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$$\operatorname{PEC}_{j \to i} = \frac{N_j A_{j \to i}}{n_e} \qquad \qquad L_{j \to i} = \frac{hc}{\lambda_{j \to i}} \frac{n_e \operatorname{PEC}_{j \to i}}{\sum_i N_i} \frac{M_{\text{ion}}}{m_{\text{ion}}}$$

All models presented are based on the following key parameters:

- Plasma Conditions: Te = 5000 K and ne = 10<sup>6</sup> cm<sup>-3</sup>
  Ion Abundances: Estimated from the Ye–0.29a model by Gillanders et al. [5]
  Atomic Data: Calculations were performed using the Flexible Atomic Code
- (FAC) [6], featuring an optimized local potential [7] and calibrated energy levels [8].





Level populations are concentrated in the

Luminosity predictions vary substantially between VRA and DW. The plasma is assumed to be optical thin > self-absorption meets are neglected > greater contribution from forbidden transitions is exacted within a more robust

### Conclusions

- Calibration and correlation are essential for peak identification, but not critical to gauge luminosities intensity
- Few levels significantly populated: incorporating a large atomic dataset in radiative transfer codes may not be necessary.
- Distorted wave calculations can provide better estimates to effective collisional strengths and level populations than VRA, and at a much lower computational cost when compared to R-Matrix calculations.

Impact of inclusion of resonances in the DW calculations to be studied in future works

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## T=5000 K, n=10<sup>6</sup> cm<sup>-3</sup>, M=0.05 M $_{\odot}$ , FWHM=0.1 c



- Optimization and calibration are essential for peak identification
- Few levels are populated: datasets in radiative transfer codes can be optimized;
- DW calculations provide better results but resonances need to be incorporated.