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Extending radiative transfer simulations in kilonovae towards non-equilibrium regimes

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The recent observations of several neutron-star merger events and associated electromagnetic transients, particularly AT2017gfo observation, provided robust indications that heavy r-process elements such as lanthanides and eventually actinides can be synthesised in these explosive environments [1]. Nonetheless, pinpointing particular features in the spectra, and linking them to the absorption and emission lines of distinct elements has presented a significant challenge [2,3,4].

One critical obstacle in the analysis is a severe lack of atomic data required to model the expansion's late epochs (> 4 days after the NSM). While it is reasonable to assume that the matter is in local thermodynamic equilibrium (LTE) and that atomic absorption processes dominate in the early hours (< 1 day after the NSM), LTE cannot be assumed for nebular epochs (non-LTE). During these late stages, significant processes include photoionization, ionisation and excitation by electronic impact, and electronic recombination, for which data is scarce.

In this work, we focus on performing large-scale atomic calculations on selected key elements, which are likely to have identifiable features in the spectra of the kilonova AT 2017gfo. Our approach, is therefore aimed at extending existing radiative transfer simulations to non-local thermodynamic equilibrium (NLTE) conditions. We try to overcome the limitations of current models, which often rely on approximations, leading to significant discrepancies in predicting spectral features. As highlighted by recent studies, conventional approaches, such as the Axelrod Van Regemorter treatments, can under- or overestimate effective collision strengths by orders of magnitude [5], impacting the accuracy of the simulated spectra and the intensity of line features.

The core of the calculations were done using the Flexible Atomic Code (FAC) [6] employing a configuration interaction approach, and a central potential that is optimised iteratively, making use of machine learning methods to better reproduce existing experimental data [7]. As to benchmark our calculations, we also use the general non-relativistic AUTOSTRUCTURE code, which has been extensively used and tested for opacity calculations in supernovae.[8]

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