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Convergence of Atomic Data for Kilonova Modelling

Gerrit Leck,[1,2,*] **Andreas Flörs,**[1] **Luke Shingles,**[1] **Ricardo da Silva**[3,4] **and Gabriel Martínez-Pinedo**[1,2]

[1] *GSI Helmholzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany*

[2] *Institut für Kernphysik (Theoriezentrum), Technische Universität Darmstadt, Schlossgartenstraße 2, 64289 Darmstadt, Germany*

[3] *Laboratório de Instrumentação e Física Experimental de Partículas, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal*

[4] *Universidade de Lisboa, Faculdade de Ciências, Rua Ernesto de Vasconcelos, Edifíco C8, 1749-016 Lisboa, Portugal*

E-mail: g.leck@gsi.de

The identification of signatures of heavy elements synthesized in the ejecta of two merging neutron stars requires the modelling of the electromagnetic signal following the merger, called kilonova. In order to reproduce these spectral features, corresponding radiative transfer models require input on the atomic transitions between bound states for ions of the first few ionization stages. Due to the complex electronic structures of the lanthanides and actinides in particular, experimental data is limited for heavy elements and the theoretical computation of atomic datasets involves a tradeoff between completeness and computation time. For the radiative transfer models, the datasets have to include all relevant transitions. We perform atomic structure calculations with different sets of electronic configurations and investigate the convergence of state densities and expansion opacities.

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1. Introduction: Spectral Features in Kilonovae

The origin of elements heavier than iron is not yet fully understood. Two regimes of neutron-capture processes are important for synthesizing these elements, the slow- and the rapid-neturon capture processes (s-process and r-process). The s-process operates close to the line of stability in the nuclear chart and the properties of the nuclei involved are experimentally well understood.
On the other hand, the r-process is characterized by its high neutron capture rate in an environment with a high density of free neutrons (number density of $\sim 10^{24}\,\mathrm{cm}^{-3}$). As a result, several neutron captures can occur before the resulting neutron-rich nuclei decay. Thus, the r-process operates close to the neutron dripline where nuclei are experimentally difficult to access [1].
In order to observe the operation of the r-process and investigate its properties, one has to find astrophysical sites in which it takes place and identify the presence of specific elements by their unique contributions to spectral features. In 1974, it had been suggested that a promising candidate for such an astrophysical r-process site is the merger of a black hole and a neutron star or a merger of two neutron stars (NSM) [2]. However, only in 2017 it was possible to observe the electromagnetic signal, nowadays called AT2017gfo, for the first time, arising from a NSM following the gravitational wave event GW170817 [3]. The electromagnetic signal is about 1000 times brighter than a classical nova and was thus named "kilonova" [4]. The kilonova is powered by the radioactive decay of heavy neutron-rich nuclei produced in the r-process.
The resulting spectra contain features of the heavy elements synthesized in the r-process. In the expanding merger ejecta, the decreasing temperature leads to a decreasing ionisation state. On a timescale of a few days, over which the temperature has dropped to a few thousand Kelvin, the Saha equation predicts that matter is mostly singly or doubly ionized. Under the right conditions, bound-bound atomic transitions can result in identifiable emission or absorption features in the spectra, although the high ejecta velocities mean that there will be significant Doppler broadening of these features. Further, some of the heavy elements, in particular lanthanides (atomic numbers $Z = 57 - 71$) and actinides ($Z = 89 - 103$) have a complex atomic structure and a large number of possible bound-bound transitions, making their spectral identification challenging. So far, only strontium has been identified in the spectra of AT2017gfo [5].
Proper kilonova spectral modelling requires data on the bound-bound transitions for all heavy elements in the relevant ionization stages. The calculation of such a dataset involves a compromise between completeness and feasible computation time. The completeness of atomic structure calculations depends on the number of included electronic configurations which give rise to energy levels and transitions. In this work we will examine sample atomic data for singly ionized neodymium and explore the effect of different numbers of used electronic configurations on two deduced quantities, the state density and expansion opacity.

2. Atomic Data for Spectral Modelling

Kilonova spectra are expected to contain a large variety of features of bound-bound atomic transitions. Spectral modelling requires information about all transitions that contribute meaningfully to the opacity, e.g. their oscillator strengths.
A dimensionless measure for the interaction probability of a transition from an initial state i to a

final state f is given by the optical depth. In the framework of an expanding medium (in our case the NSM ejecta), it is given by the Sobolev optical depth [6, 7]

$$\tau_{\mathrm{if}}^{\mathrm{Sob}} = \frac{\pi e^2}{m_e c} t_{\mathrm{exp}} n_{\mathrm{i}} \lambda_{\mathrm{if}} f_{\mathrm{if}} \tag{1}$$

where e is the elementary charge, m_e the electron mass, c the speed of light, t_{exp} the expansion time (after the merger), n_{i} the number density of the initial (lower) state and λ_{if} and f_{if} are the wavelength and oscillator strength of the transition.
In order to obtain a measure for the opacity of a large set of atomic transitions, the Sobolev optical depths for transitions contained in a wavelength bin of width $\Delta\lambda$ are combined in the expansion opacity [8]

$$\kappa_{\mathrm{exp}}(\lambda) = \frac{1}{\rho c t_{\mathrm{exp}}} \sum \frac{\lambda_{\mathrm{if}}}{\Delta\lambda} (1 - e^{-\tau_{\mathrm{if}}^{\mathrm{Sob}}}) \tag{2}$$

where ρ is the density of the ejecta. The sum is taken for all transitions falling into the bin of width $\Delta\lambda$ around a wavelength λ. Should the inclusion of transitions between additional electronic configurations yield no significant contribution to the expansion opacity, their role for spectral absorption may be neglected.

3. Atomic Structure Calculations

To compute the levels and transitions of heavy atoms, we use the Flexible Atomic Code (FAC, [9]). FAC uses a self-consistent scheme to calculate the full atomic wave functions ("configuration state function", CSF). It approximates a CSF as a linear combination of Slater determinants and then applies a variational principle to obtain the lowest energy state. An effective potential is used as an average representation of the many-body potentials.

4. Convergence of Neodymium Atomic Data

As a lanthanide, neodymium is of particular interest due to its complex atomic structure. We investigate singly ionized neodymium here (Nd II in spectroscopic notation) as it is expected to be the most abundant ion in the ejecta at around one day after the merger.
We compute atomic levels for Nd II in four different steps. In the first, the same atomic configurations as in [10] are used as a reference configuration set. In a second step, a few extra configurations are added which are expected to have low-lying energy levels. Then, we include all single excitations (see [11] for a description) and finally all single and double excitations ("SD") of electrons up to a fixed principal quantum number. The corresponding transitions between those levels are calculated for the first three datasets only as in the SD-case the computation time became too high.
Figure 1 shows the state density (number of states per energy interval) as a function of excitation energy. As can be seen, the calculated state density exceeds the experimental state density already beyond 2 eV. This underlines the fundamental problem that for heavy elements the data is very incomplete with many levels not yet identified, thus making atomic structure calculations necessary. The four calculations start to diverge from each other at excitation energies at around 6 eV. The SD

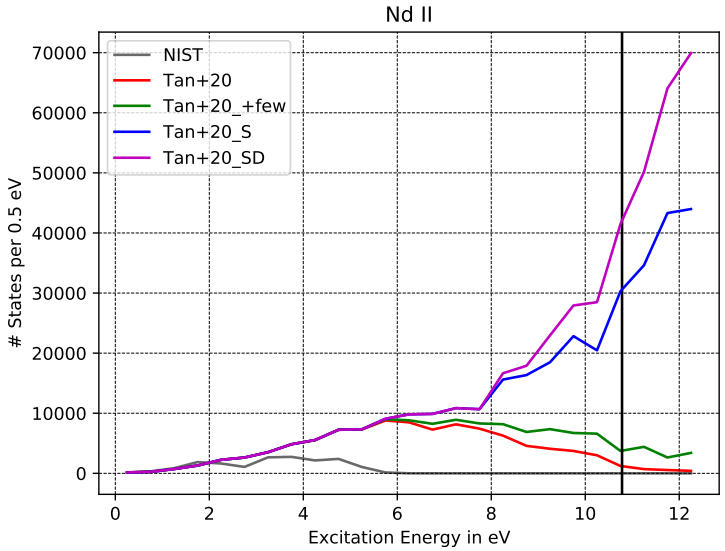

Figure 1: State density for singly ionized neodymium. The coloured lines correspond to a basis set of atomic configurations taken from [10] (red), a few additional configurations added on top by hand (green) as well as single (S, blue) and single+double (SD, purple) electronic excitations from the basis set. The state density using experimentally determined values from the NIST atomic spectra database (and therein taken from [12]) is shown for comparison (black). The vertical black line denotes the ionization edge of neodymium.

calculation shows a significantly higher number of states than the basis set used by [10].
Figure 2 shows the resulting expansion opacities calculated for typical NSM ejecta at at $t_{\mathrm{exp}} = 1\,\mathrm{d}$, i.e. density $\rho = 10^{-13}\,\mathrm{g\,cm^{-3}}$ and temperature $T = 5000\,\mathrm{K}$ (used by [10]). The lower-level number densities are calculated using the Saha and Boltzmann equations, i.e. we assume local thermodynamic equilibrium.
As can be seen, the increasing number of states does not have an impact on the opacity at high wavelengths (above the peak at around 4000 Å). However, below the peak, the high-energy shoulder of the opacity does not fully converge when more configurations are included. Consequently, in this regime, the high-energy transitions from low-lying levels to levels close to the ionization edge still give a contribution to the opacity. This behaviour and its actual consequences on modelled kilonova spectra have to be investigated further in future work.

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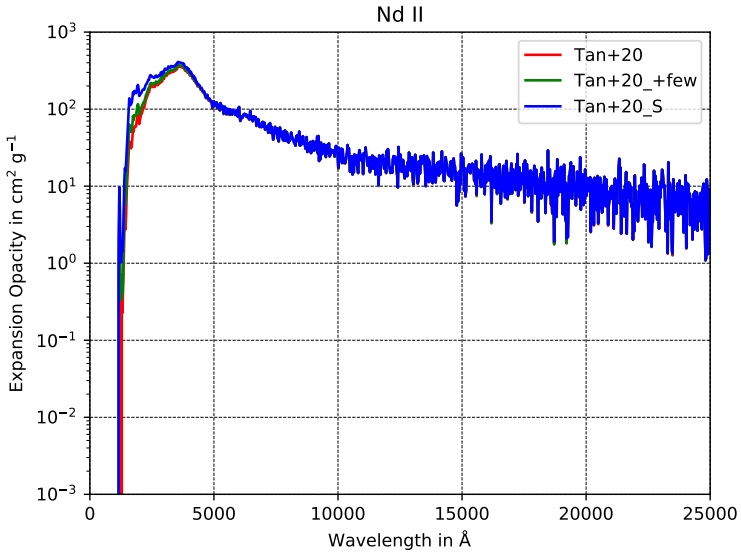

Figure 2: Expansion opacity of singly ionized neodymium for typical NSM ejecta conditions at $t_{\mathrm{exp}} = 1$ d, i.e. density $\rho = 10^{-13}$ g cm^{-3} and temperature $T = 5000$ K. The three curves correspond to the atomic data sets of the same colours as in fig. 1. Transitions for the single+double excitations case were not computed due to too high computation times.

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