Impact of using realistic partition functions to calculate kilonova opacities

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On August 17, 2017, the LIGO-VIRGO collaboration observed a neutron star merger thanks to the first detection of gravitational waves. They also detected an explosion of hot and radioactive matter called a kilonova [1]. In the latter, there are nuclear reactions that form heavy nuclei (heavier than iron) such as lanthanides (Z = 57 - 71) which play a particular role. In fact, given their rich spectra, they strongly contribute to the opacity affecting radiation emission [2]. In order to interpret the spectrum of a kilonova, it is therefore crucial to precisely know the radiative parameters characterizing these elements. Over the past few years, several studies have been carried out (see e.g. [3-4]), for the first degrees of ionisation (up to 3+) but almost all these investigations were limited to the analysis of kilonovae in a temperature range below 20000 K. To extend the study to early phases of kilonovae (i.e. $T > 20\,000$ K), it is essential to know the radiative parameters of lanthanide ions in higher charge stages (see e.g. [5-7]). Thanks to the calculation of lanthanides' atomic data for different degrees of ionization, we can calculate the expansion opacities using the expansion formalism [8-10]. In all of the works mentioned (except in [7]) the partition function, U(T), was approximated to the statistical weight of the ground level, g_0 , for the computation of the Sobolev optical depth. This approximation has a significant impact on the computed opacities. The main goal of this present work is to show how it can affect the expansion opacity for a couple of lanthanide examples, namely for samarium (Sm) in the case of early-phase kilonova conditions (t = 0.1 day after the merger), which is associated with moderately-charged species (Sm V - XI) and for neodymium (Nd) in the case of plausible conditions in the kilonova ejecta that should take place about 1 day after the neutron star merger (NSM), corresponding to the presence of lowly-ionized elements in the ejecta (Nd II - IV) [11].

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