Convergence of Atomic Data for Kilonova Modeling

Gerrit Leck

FAIR next generation scientists - 7th Edition Workshop
23rd May 2022

with Andreas Flörs, Gabriel Martínez-Pinedo, Luke Shingles,
and Ricardo da Silva (LIP Lisbon)

TECHNISCHE
UNIVERSITÄT
DARMSTADT

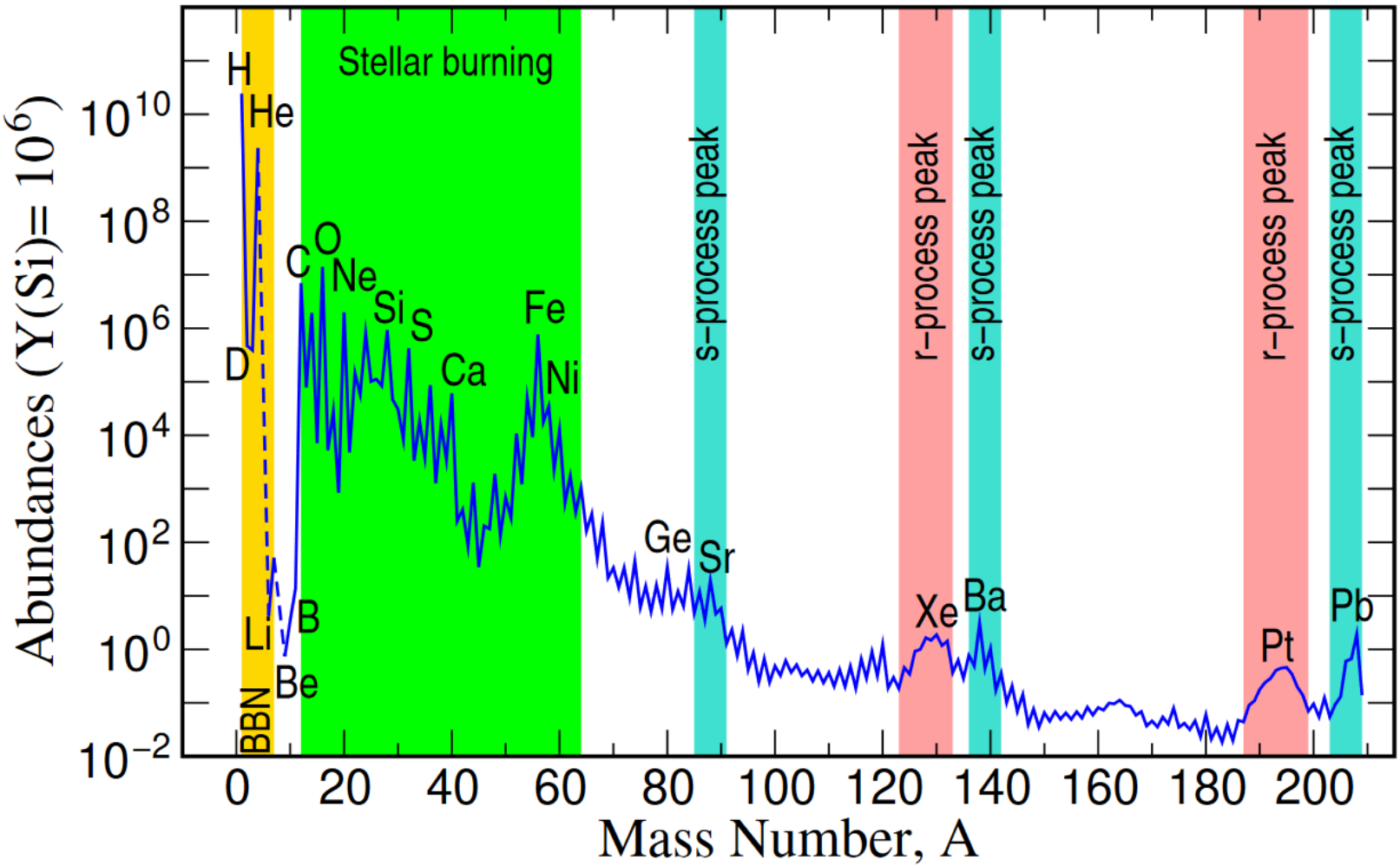
GSI Helmholtzzentrum für Schwerionenforschung GmbH

European Research Council
Established by the European Commission

LIP

Motivation: Where are Heavy Elements produced?

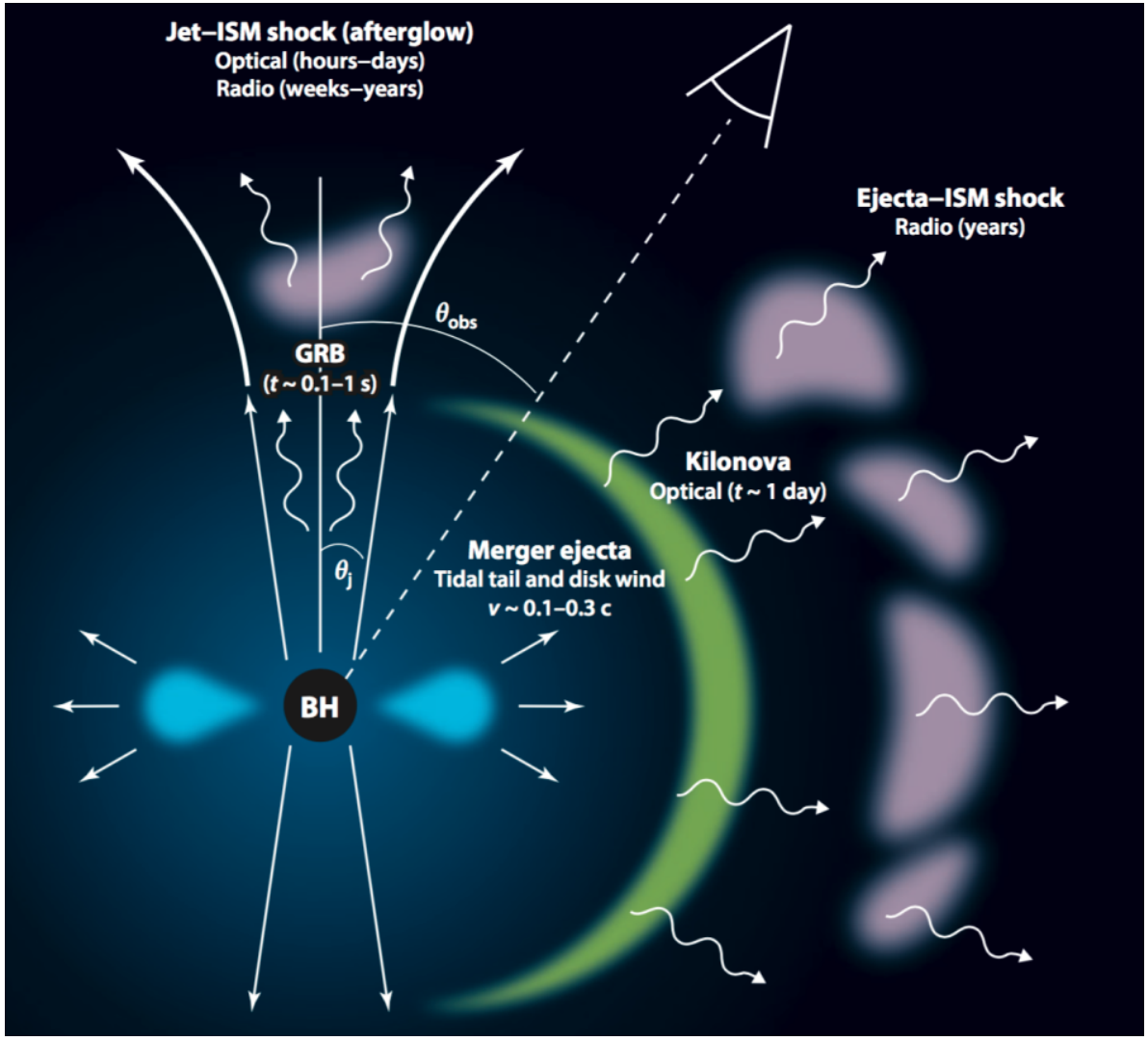
- astrophysical cite of r-process not fully understood yet



Cowan et al., 2021

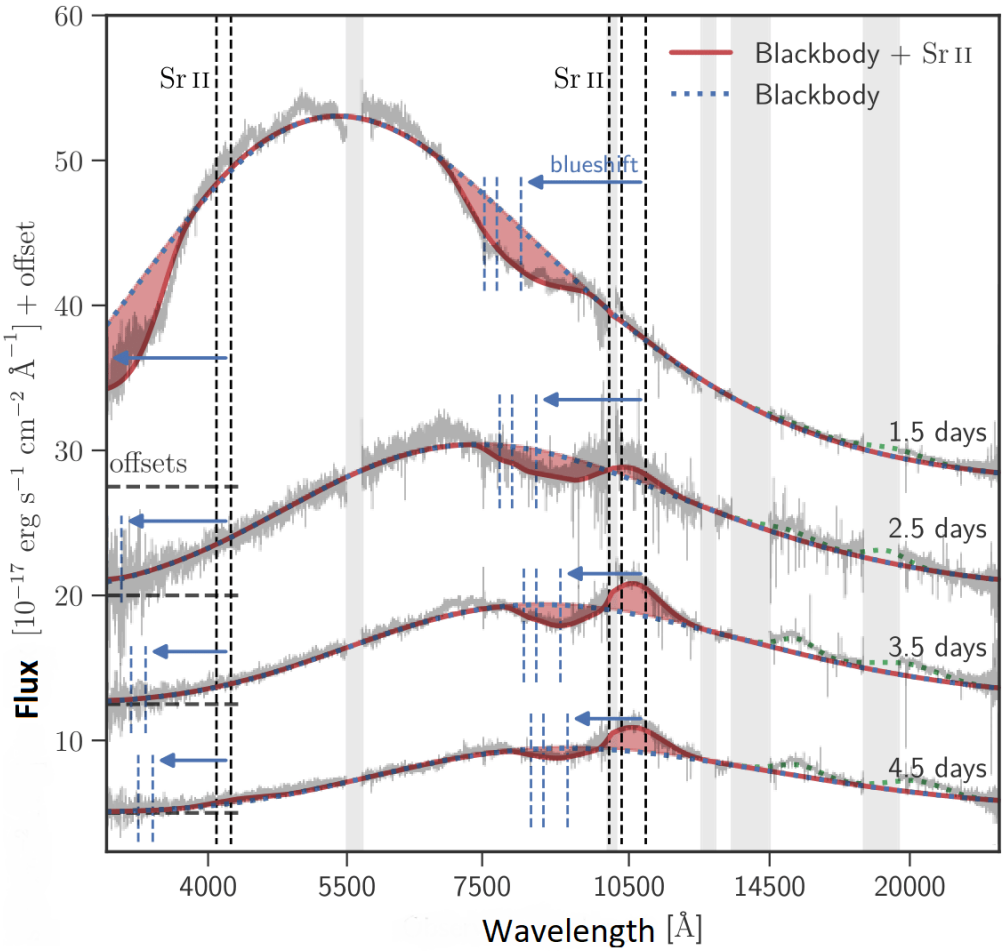
Neutron Star Mergers and Kilonovae

- kilonova: electromagnetic merger transient



Metzger & Berger, 2012

The Kilonova AT2017gfo



Adapted from Watson et al., 2019

- Watson et al., 2019: identification of Sr II
- identification via kilonova spectral modeling
- *fundamental issue*: limited experimental data for r-process atoms

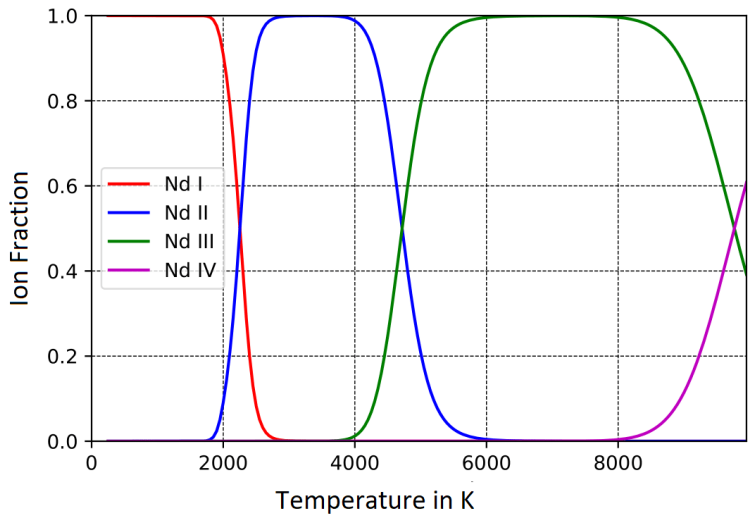
Atomic Data for Spectral Modeling

- bound-bound optical depth for a single line l:

$$\tau_l \propto \underbrace{t_{\text{exp}}}_{\text{expansion time}} \cdot \underbrace{n_{\text{lower}}}_{\text{lower-level density}} \cdot \underbrace{\lambda_l}_{\text{wavelength}} \cdot \underbrace{f_l}_{\text{oscillator strength}}$$

- n_{lower} via local thermodynamic equilibrium
- effective "expansion" opacity:

$$\kappa_{\text{exp}} := \frac{1}{\rho c t_{\text{exp}}} \sum_l \frac{\lambda_l}{\Delta\lambda} \left(1 - e^{-\tau_l}\right)$$



Atomic Calculations and Convergence

- two criteria for "convergence":
  1. accurate lowest-lying energy levels
  2. accurate level density at relevant energies
- we use the Flexible Atomic Code (FAC, Gu 2008)
- self-consistent scheme: number of input configurations impacts precision of results

$$\Psi = \sum_{k=1}^{N_{\mathrm{SD}}} c_k \Psi_k^{\mathrm{SD}}$$

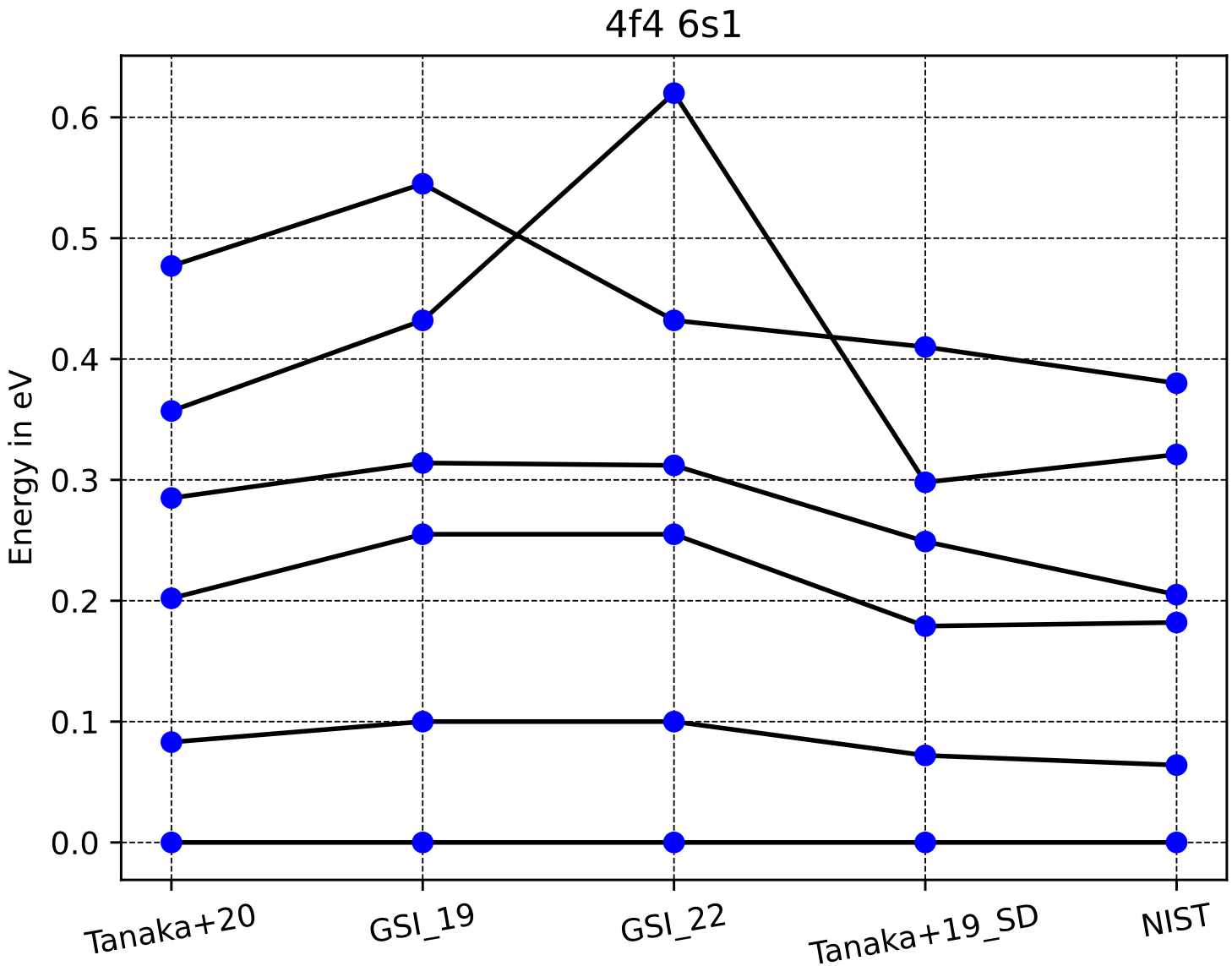
$\rightarrow$ but number of levels grows as

$$\#\ \text{levels} \sim \prod_k \binom{g_k}{N_{e,k}} = \prod_k \frac{g_k!}{N_{e,k}!(g_k - N_{e,k})!}$$

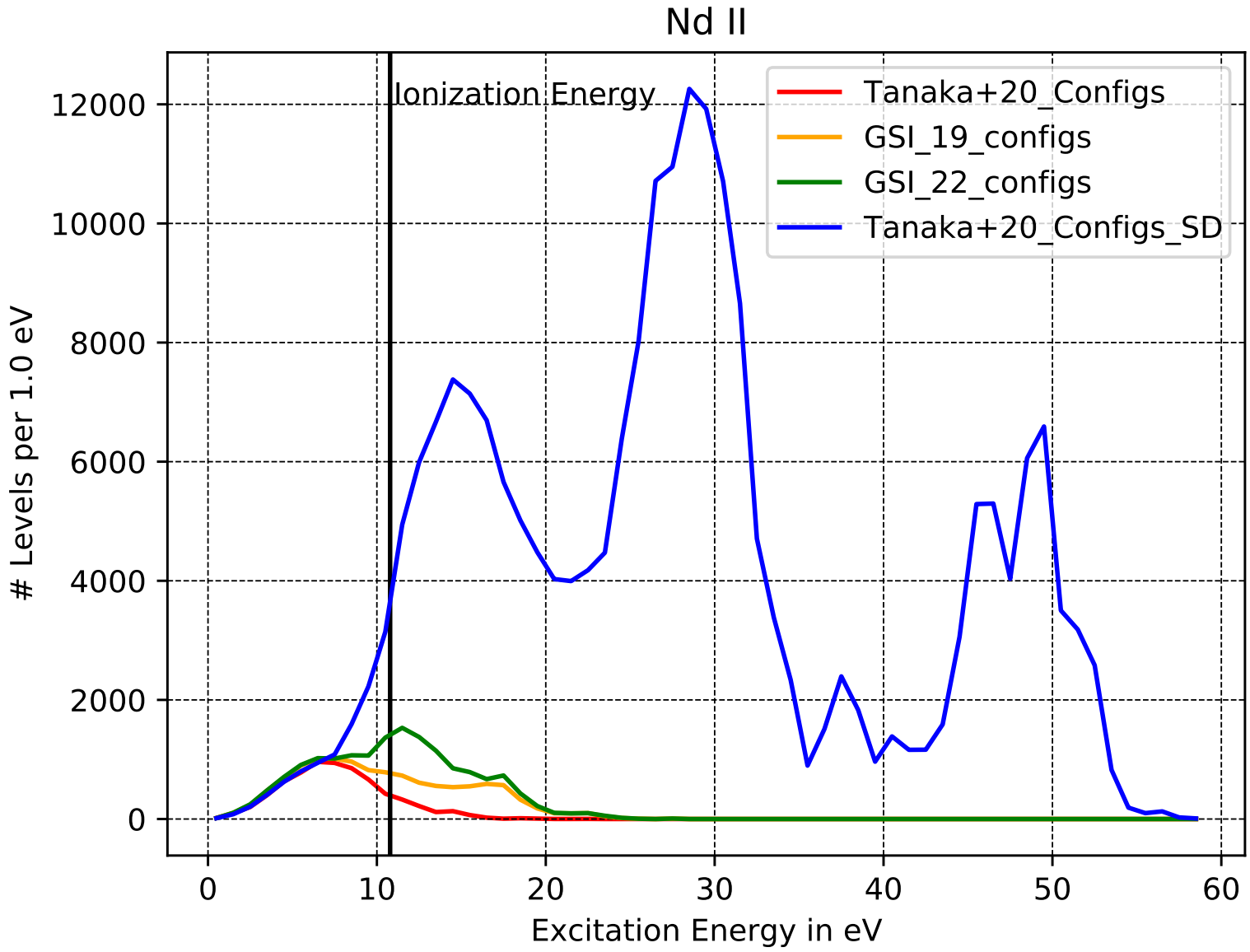
- *key challenge*: at which point may we truncate the calculations?

Example Results: Nd II Lowest Levels

- comparison of calculations to experimental NIST values



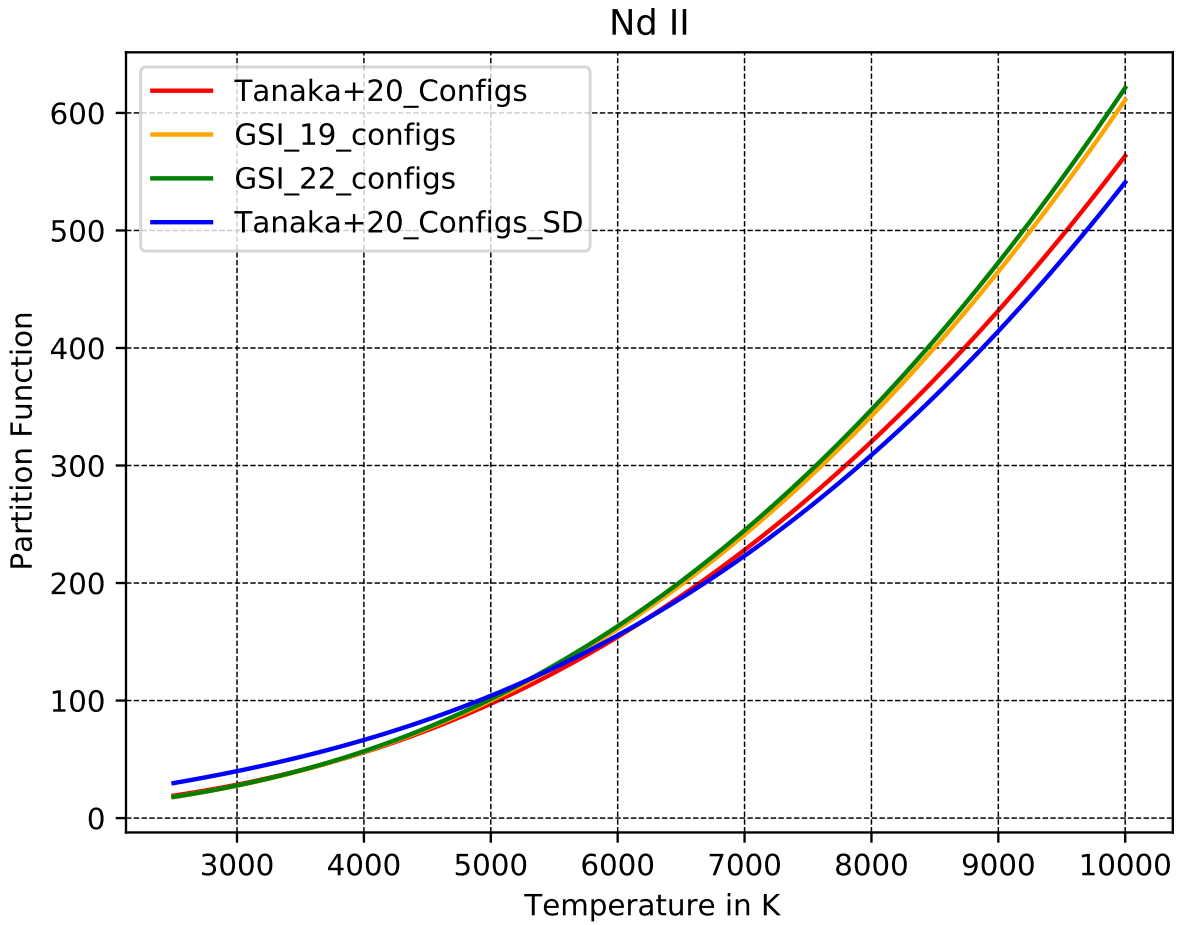
Level Density and Statistical Theory



Nd II Partition Functions

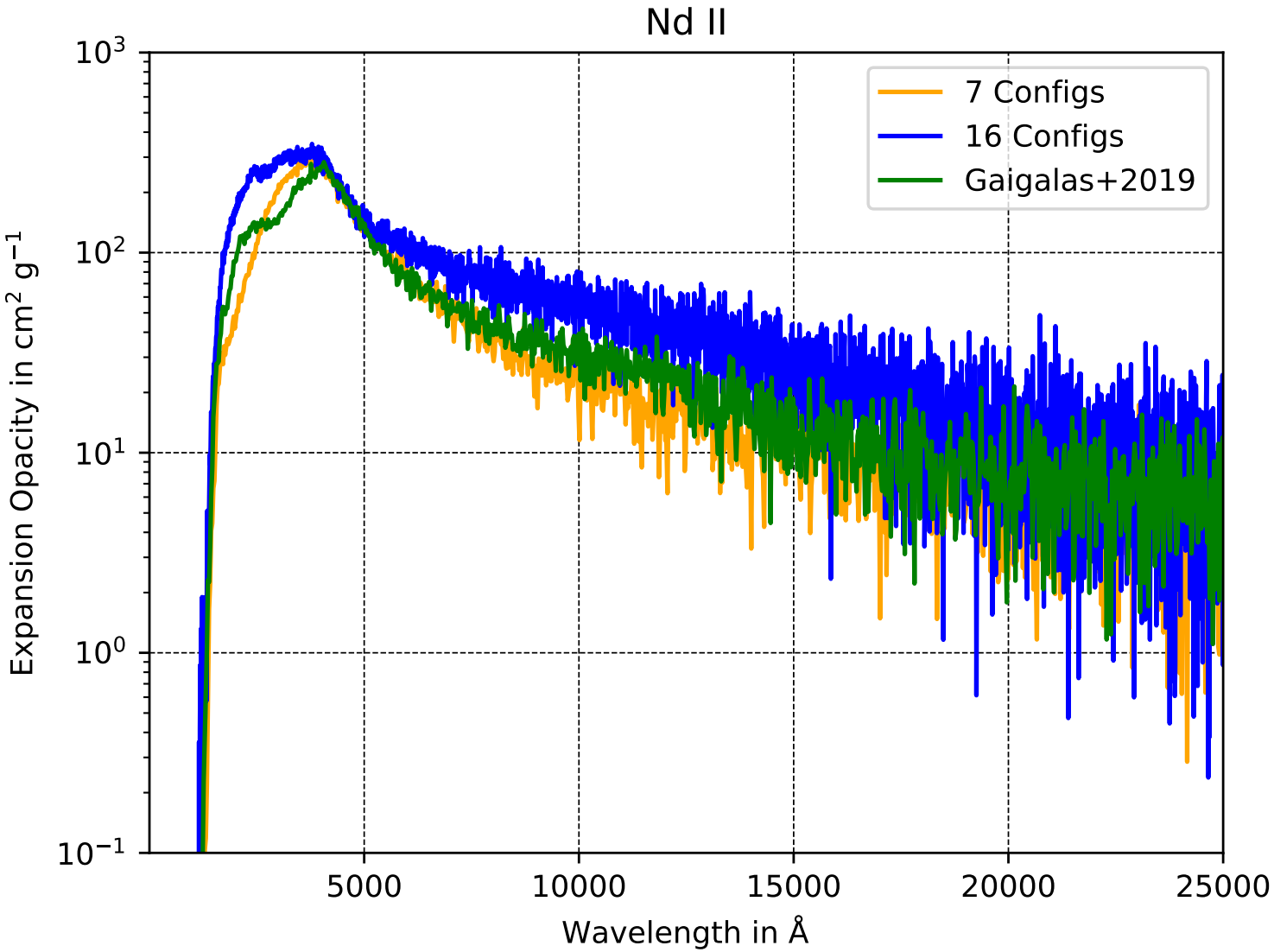
- canonical partition function:

$$Z := \sum_k g_k e^{-E_k/k_B T}$$



Nd II Expansion Opacity

- $t_{\mathrm{exp}} = 1\,\mathrm{d}$, $T = 5000\,\mathrm{K}$, $\rho = 10^{-13}\,\mathrm{g\ cm^{-3}}$



Summary

- aim: find spectral features of r-process elements in kilonovae
- we need detailed atomic data for:
  - accurate description of low-lying levels
  - appropriate description at high level densities
- example calculations: singly-ionized neodymium
- aim: extend this procedure to the other required ions