Lanthanide and Actinide Opacity Computations for Kilonova Modeling

Jérôme Deprince

Université Libre de Bruxelles
Astronomy and Astrophysics Institute

ASOS-14, Paris, France

July 10, 2023
Team

- ULB (Université Libre de Bruxelles):
  - Stéphane Goriely
  - Michel Godefroid

- UMONS (Université de Mons):
  - Pascal Quinet
  - Patrick Palmeri
  - Helena Carvajal Gallego
  - Sirine Ben Nasr
1. Neutron star mergers and kilonovae

2. Theoretical method
   Atomic structure computation: HFR
   Expansion opacity

3. Existing works

4. Results
   Opacity sensitivity to atomic properties
   Lanthanide and actinide expansion opacities
   Actinide VS lanthanide opacities

5. Conclusion
Kilonovae


NSMs also produce an electromagnetic signal powered by the ejection of hot and radioactive matter: kilonova (KN)

GW170817 EM counterpart also detected: KN AT2017gfo

KNe thought to be responsible for heavy element production

1. Neutron star mergers and kilonovae
Kilonova opacity

- KN light curve modeling strongly depends on atomic opacities
- KN opacity dominated by millions of lines from f-shell elements ($\rightarrow$ lanthanides + actinides) newly created by r-process
Kilonova opacity

⇒ Lanthanide and actinide contributions to the opacity are of paramount importance due to their large spectral density and abundances

1. Neutron star mergers and kilonovae
Many studies are based on a simple but powerful one-zone approximation (e.g. Metzger 2019, Hotokezaka & Nakar 2020) → Ejecta = expanding homogeneous sphere with gray opacity

Monte-Carlo approaches solve the radiative-transfer eqs very accurately using atomic-physics based opacities, but are computationally expensive and often assume analytic ejecta distributions (e.g. Kasen et al. 2017, Kawaguchi et al. 2019)

Intermediary approach: truncated two-moment approximation (so-called M1 scheme), which assumes a local closure relation ("equation of state") for the radiation field (Just et al. 2022) → fills the gap between the two approaches above in terms of both accuracy and complexity

1. Neutron star mergers and kilonovae
Kilonova opacity

So far, the KN total opacity in Just et al. 2022’s code is estimated using crude approx to atomic-physics based model, motivated by fits to bolometric KN light curves

$$\kappa(X_{LA}, T) = \kappa_{LA} \times \kappa_{T}$$

where the $X_{LA}$-dependent part is

$$\kappa_{LA} = \begin{cases} 
30 \text{ cm}^2 \text{ g}^{-1} (X_{LA} / 10^{-1})^{0.1} & , \quad X_{LA} > 10^{-1}, \\
3 \text{ cm}^2 \text{ g}^{-1} (X_{LA} / 10^{-3})^{0.5} & , \quad 10^{-3} < X_{LA} < 10^{-1}, \\
3 \text{ cm}^2 \text{ g}^{-1} (X_{LA} / 10^{-3})^{0.3} & , \quad 10^{-7} < X_{LA} < 10^{-3}, \\
0.2 \text{ cm}^2 \text{ g}^{-1} & , \quad X_{LA} < 10^{-7}, 
\end{cases}$$

and the temperature-dependent part is

$$\kappa_{T} = \begin{cases} 
1 & , \quad T > 2000 \text{ K} \\
\left( \frac{T}{2000 \text{ K}} \right)^5 & , \quad T < 2000 \text{ K}.
\end{cases}$$

$X_{LA}$: average lanthanide + actinide mass fraction

→ Realistic KN opacity would require big amounts of reliable atomic data (structure + radiative data for all transitions) for both lanthanides and actinides

1. Neutron star mergers and kilonovae
Kilonova: physical conditions

\[ 10^{-17} \text{ g/cm}^3 < \rho < 10^{-13} \text{ g/cm}^3 \]

and

\[ 1000 \text{ K} < T < 10000 \text{ K} \]

⇒ Only the first ionization stages (I – IV) of the elements are present in the KN ejecta

1. Neutron star mergers and kilonovae
Pseudo-relativistic Hartree-Fock Method

- Based on Schrödinger equation
- Orbitals obtained for each config. by solving the HF eqs (→ variational principle to the config. average energy)
- Relativistic corrections added perturbatively

Advantages of HFR method:

- Calculation is relatively quick, even for a large number of configurations considered (→ large number of transitions)
- States from all the configurations are optimized

⇒ Suitable to compute physical properties as opacity which requires to consider large numbers of transitions (→ lanthanides and actinides) all fairly well described
Expansion opacity:

\[ \kappa_{\text{exp}}^{bb}(\lambda) = \frac{1}{\rho c t} \sum_l \frac{\lambda_l}{\Delta \lambda} (1 - e^{-\tau_l}) \]

with the Sobolev optical depth:

\[ \tau_l = \frac{\pi e^2}{m_e c} t n_l \lambda_l f_l \]

⇒ Radiative wavelength \( \lambda_l \) and oscillator strength \( f_l \) are needed to compute the expansion opacity (+ level population \( n_l \))

\( n_l \) is determined using Boltzmann and Saha equations

2. Theoretical method
   b) Expansion opacity
Recent studies for weakly-charged lanthanide opacities, e.g.:

- Kasen et al. (2013) → Nd I – IV, Ce II – III using AUTOS
- Gaigalas et al. (2019) → Nd II – Nd IV using GRASP
- Gaigalas et al. (2020) → Er III using GRASP
- Radžiūtė et al. (2020) → Pr II – Gd II using GRASP
- Tanaka et al. (2020) → All lanthanides using HULLAC
- Fontes et al. (2020) → All lanthanides using Los Alamos codes
- Carvajal Gallego et al. (2021) → Ce II – IV using GRASP
- Rynkun et al. (2022) → Ce IV using GRASP and HULLAC
- Gaigalas et al. (2022) → Pr IV using GRASP
- Silva et al. (2022) → Nd III using FAC
- Flörs, Silva, Deprince et al. (2023, accepted)
  → Nd II – III using FAC and HFR (this work)

Several works on moderately-charged lanthanides (early-phase kilonovae) from Carvajal Gallego et al. and Banerjee et al.

3. Existing works
Only very few works focused on actinide opacities, e.g.:

- Silva et al. (2022) → (Nd III and) U III using FAC
- Fontes et al. (2023) → All actinides using Los Alamos codes
- Deprince, Carvajal Gallego, Godefroid et al. (2023)
  ↔ U II – IV using HFR (sensitivity studies, this work)
- Flörs, Silva, Deprince et al. (2023, accepted)
  ↔ (Nd II – III) and U II – III using FAC and HFR (this work)
Effect of the multiconfiguration model

Models for U \textsc{lll}

- Silva \textit{et al.} 2022 (FAC):
  \[ 5f^4 + 5f^3\{6d+6f\} + 5f^3\{7s+7p+7d\} + 5f^3\{8s+8p\} + 5f^2\{6d^2+6d7s\} \]
  (10 configurations)

- Our work (HFR):
  \[ 5f^4 + 5f^3\{6d+6f+6g\} + 5f^3\{7s+7p+7d+7f+7g\} + 5f^3\{8s+8p+8d+8f+8g\} + 5f^3\{9s+9p+9d+9f+9g\} + 5f^2\{6d^2+6d7s+6d7p+6d7d+7s^2+7s7p+7s7d\} \]
  (26 configurations)

How are the computed opacities affected by the multiconfiguration model (by the number of config.)? Convergence of the models?

4. Results

a) Opacity sensitivity to atomic properties
Model convergence for U III

Convergence of the opacity while considering growing models (more configurations added shell by shell)

HFR opacity computations ($T = 5000$ K, $\rho = 10^{-13}$ g/cm$^3$, $t = 1$ day)

4. Results

a) Opacity sensitivity to atomic properties
Calibration procedure

Calibration procedure used in HFR: adjustment of the configuration average energies to the ones deduces from available energy levels

In both UII and UIII, level inversion occurs in our computations between (namely) the ground state and one of the first excited states

→ Our calibration procedure solves this level inversion problem
  ▶ Is such an adjustment procedure worth it in order to compute opacities (at least in a first step)?

(Deprince, Carvajal Gallego, Godefroid et al. 2023)

4. Results
   a) Opacity sensitivity to atomic properties
4. Results

a) Opacity sensitivity to atomic properties

HFR opacity computations ($T = 5000$ K, $\rho = 10^{-13}$ g/cm$^3$, $t = 1$ day)
4. Results

a) Opacity sensitivity to atomic properties
Core-polarization effect

- HFR: not all the correlations are explicitly taken into account
  → Model = ionic core + config. involving valence electrons

- UMONS team (Atomic Physics and Astrophysics Unit) has modified Cowan’s codes to include a core-polarization correction to the potential (Quinet et al., MNRAS 307, 934, 1999)

- Can be tricky to include for elements for which nf subshell is partially filled (ionic core not clearly defined)

- Is this effect worth being included in our opacity computations (in a first step)?

  (Deprince, Carvajal Gallego, Godefroid et al. 2023)

4. Results
a) Opacity sensitivity to atomic properties
4. Results

a) Opacity sensitivity to atomic properties
Importance of considering realistic partition functions (Nd opacity case)

Significant difference between our HFR opacity and the one computed by Tanaka et al. 2020 using HULLAC

- Atomic data → Importance of the multiconfiguration model!
  (7 and 8 configs included for Nd II and Nd III in Tanaka et al.)

4. Results

a) Opacity sensitivity to atomic properties
Importance of considering realistic partition functions (Nd opacity case)

▶ Expansion opacity computation itself

→ In Tanaka et al. (2020) (as well as in Gaigalas et al. 2019), the partition function \( U(T) \) is approximated to \( g_0 \) in the evaluation of level populations \( n_l \) (→ \( \tau_l \)):

\[
n_l = \frac{g_l n}{U(T)} \exp \left( -\frac{E_l}{kT} \right)
\]

\[
\tau_l = \frac{\pi e^2}{m_e c} t \frac{n_l \lambda_l f_l}{m_e c}
\]

\[
U(T) = \sum_{i=0}^{\infty} g_i \exp \left( -\frac{E_i - E_0}{kT} \right), \quad g_i = 2J_i + 1
\]

4. Results

a) Opacity sensitivity to atomic properties
For Nd III, for $T = 5000$ K, $U$ is about 6 times greater than $g_0$!

Carvajal Gallego, Deprince, Godefroid et al. 2023

+ cf. Carvajal Gallego et al.'s poster (moderately-charged lanthanides)

4. Results
a) Opacity sensitivity to atomic properties
Comparison with other works

GRASP: Gaigalas, Kato, Rynkun et al. (2019)
HULLAC: Tanaka, Kato, Gaigalas et al. (2020)

(Opacities recomputed using their atomic data → $U(T)$ NOT approximated to $g_0$)

FAC + HFR (This work): Flörs, Silva, Deprince et al. (2023)

4. Results

b) Lanthanide and actinide expansion opacities
Comparison with other works

Fontes et al. (2020)
→ Line-binned opacities (instead of expansion)

Flörs, Silva, Deprince et al. (2023)

4. Results
b) Lanthanide and actinide expansion opacities
4. Results

b) Lanthanide and actinide expansion opacities
4. Results

b) Lanthanide and actinide expansion opacities
U VS Nd opacities

$\Rightarrow$ U opacity at least as large as Nd opacity

$\Rightarrow$ Importance of the actinide opacities as well

4. Results

c) Actinide VS lanthanide opacities
4. Results

c) Actinide VS lanthanide opacities
Conclusion

- **Opacity computations needed to model kilonova light curves**
  - Reliable atomic data for as many transitions as possible
    - Especially for lanthanides and actinides which are expected to dominate the KN opacity

- Lanthanides: several works exist but can be improved

- Actinides: very few works
  - Multiconfiguration model choice is of crucial importance
  - Partition functions fully-computed (not approximated to $g_0$)

- HFR expansion opacities computed for all weakly-charged lanthanides and actinides for a grid of $T$, $\rho$ and time

- Opacity for U as large as for Nd or even greater
  - Actinides can be as important as lanthanides concerning their contributions to the KN opacity

5. Conclusion
Prospects

▶ Average the computed opacities with the expected elemental abundances for several NSM cases (nucleosynthesis simulations from S. Goriely, ULB) to infer the KN total opacity

▶ Implement the new atomic opacity data in kilonova light curve model (O. Just’s code, Just et al. 2022)

▶ Try to improve atomic data (especially for the most contributing species)
  ⇒ Investigate impact on the computed opacities

▶ Exhaustive comparison with the opacities computed by other groups using other methods (GSI/Lisbon University, NIST-Los Alamos Lanthanide Opacity Database, Japan-Lithuania Opacity Database for Kilonova)

5. Conclusion