Open questions in neutron star mergers (Kilonova & r-process)

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- 1. What is the composition of merger ejecta?
- 2. What is the main energy source? α , β , γ , or fission?
- 3. Is it Sr II, He I or else, which forms 10⁴A signature in GW170817?
- 4. How much angular dependence will be?
- 5. What can we learn from the nebular phase?
- 6. How kilonova remnants look like?
- Technical questions
 - 8. How do we get good atomic data?
 - 9. Which elements can be seen as absorption lines in kilonova?
 - 10.Can we develop non-LTE transfer models?

What is the composition of merger ejecta?



Cumulative mass abundance in the sun







What we can surely say for GW170817



The 1st peak only cannot explain the observation.

What is the main energy source? a,β,γ,fission



 $Y(^{224}Ra) = 4.1 \times 10^{-5}$ ---- $Y(^{225}\text{Ra}) = 2.7 \times 10^{-5}$

10

time (days)

100

 $10^{3'}$

1

 β and γ dominate at early times (< a few days) Can α and fission dominate at the later times? This depends on the composition and nuclear model. (see, e.g., Barnes et al 2021)



Is it Sr II, He I or else?



Problems exist on the Sr interpretation:

- Sr mass changes with time (more Sr is needed at the first epoch).
- Total mass is too small to produce the luminosity (Gillandars +2022).
- It can be He I (Perego et al 2022).

He I & Sr II lines in non LTE

Spectrum structure of GW170817



He I & Sr II lines in non LTE

Sr II

- The level population is thermal because it is strongly coupled with thermal photons.
- But, Sr may be overionized by radioactivity in the line forming region.

He I

- No chance for thermal excitation.
- The level population is non thermal. 2³S is filled by recombination from He II.
- Radioactive ionization may enhance the population of He I 2³S.



He & Sr lines are comparable if their abundances are comparable

• Sobolev optical depth:

$$\tau_l = \frac{\pi e^2}{m_e c} t n_l \lambda_l f_l,$$
$$= 0.23 t_d \frac{\lambda_l}{1 \,\mu \mathrm{m}} n_l f_l$$

 $f_l({\rm He\,I}) \approx 0.54 \qquad f_l({\rm Sr\,II}) \approx 8.9 \cdot 10^{-2}$

*τ*_l>1 at 3.5 day:

n(He I, 2³S)>2cm⁻³ n(Sr II, ²D)>14cm⁻³

• Ejecta condition:

 $n_{atom} \sim 5 \times 10^{6} \text{ cm}^{-3} \text{ at } 0.2 \text{ c}$

 $n_{He} \sim n_{Sr} \sim 5 \times 10^4 (Y/0.01) \text{ cm}^{-3} \text{ at } 0.2 \text{ cm}^{-3}$

If the abundances of He and Sr are 1%.

He I & Sr II lines are comparable if their abundances are comparable

• Ionization in LTE:

He I ~ 1, He II ~ 0, He III ~ 0 Sr I ~ 0, Sr II ~ 1, Sr III ~ 0

• Level population in LTE:

He I, 2³S ~ 10⁻³⁰ Sr II, ²D ~ 4.6x10⁻³

 n_{LTE} (He I, 2³S)~0 cm⁻³ n_{LTE} (Sr II, ²D)~200 cm⁻³

cf. *τ*/>*1* at 3.5 day:

n(He I, 2³S)>2cm⁻³

n(Sr II, ²D)>14cm⁻³

In LTE, the Sr II line is very strong while the He I line is negligibly small.

Non-thermal electron spectrum

KH+ in prep.



He I & Sr II lines are comparable if their abundances are comparable

Ionization under β-radiation:



Recombination rate = $\alpha_i n_e n_{i+1}$

He I ~ 10⁻², He II ~ 0.5, He III ~ 0.5 Sr I ~ 0, Sr II ~ 0.05, Sr III ~ 0.9

• Level population:

Sr II, ²D ~ 5x10⁻³

He I, 2³S ~ 0.75x(recombination from He II)/(collision depopulation) ~ 10-4 n(He I, 2³S)~10 cm⁻³ n(Sr II, ²D)~10 cm⁻³

cf. $\tau_{l} > 1$ at 3.5 day:

n(He I, 2³S)>2cm⁻³ n(Sr II, ²D)>14cm⁻³

Is it Sr II, He I or else?



It seems that He I is more consistent with the observed data if non-LTE is include (Tarumi, KH+ in prep. but see Perego+2022). If Sr II, we need X(Sr) ~ 10⁻², if He I we need X(He) ~ a few 10⁻³. A bunch of lines from Lanthanides may also produce the structure.

How much angular dependence?

Kasen+2015, Tanaka, KH,+2014, Darbha & Kasen 2020, Korobkin+2021





What massive neutron star remnants do?



Ejecta is much faster and energetic than normal ejecta.

Kilonova should be redder.

Synchrotron radiation is much brighter than GW170817 (Udi raised why we haven't seen one?)

What can we learn from nebular phase?

Spitzer Telescope detection for GW170817



Kasliwal+21

λ and time
4.5µm 43day
4.5µm 74day
3.6µm 43day
3.6µm 74day

AB magnitude 21.88 (22.9) 23.86 (23.8) >23.21 >23.05

Detections

Upper limits

Kasliwal+21 (and Villar +18)

This implies strong line emitters around 4.5 µm.

Importance of Fine-structure lines in kilonova nebula



- Heavy elements: Wavelength ~ 1 10 μm and cooling rate ~ $\lambda^{\text{-4}}$
- M1 lines can carry away a significant fraction of radioactive heat.

Are M1 lines available in NIST? No

If you search forbidden lines of W III,

Error Message:

No lines are available in ASD with the parameters selected

Please inform the ASD Team about your data needs.

You may query the NIST Atomic Spectra Bibliography Database for references to published data:

Energy Levels:	Literature on W III Energy Levels
Lines:	Literature on W III Spectral Lines
Transition Probabilities:	Literature on W III Transition Probabilities

But energy levels of W III available, which are sufficiently accurate

NIST Atomic Spectra Database Levels Data

W III 236 Levels Found

Z = 74, Hf isoelectronic sequence

Example of how to reference these results:

Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2021). NIST Atomic Spectra Database (ver. 5.9), [Online]. Available: https://physics.nist.gov/asd [2022, March 17]. National Institute of Standards and Technology, Galthersburg, MD. DOI: https://doi.org/10.18434/T4W30F

BibTex Citation (new window)

Data on Landé factors are not available for this ion in ASD

Primary data source Query NIST Bibliographic Database for W III (new window) Kramida and Shirai 2009 Literature on W III Energy Levels

Configuration	Term	J	Level (cm ⁻¹)	Uncertainty (cm ⁻¹)	Leading percentages			Reference		
5d ⁴	°D	0	0.00	0.11	64		15	5d*	³ P1	L10405
		1	2 256.20	0.07	83		8	5d ⁴	³ P1	L10405
		2	4 461.19	0.05	93					L10405
		3	6 277.81	0.05	91					L10405
		4	7 686.68	0.05	78		12	5d ⁴	3F2	L10405
5 <i>d</i> ⁴	³ P2	0	9 984.38	0.07	35	°D	30	5d ⁴	³ P2	L10405
		1	12 881.03	0.04	38		18	5d ⁴	³ P1	L10405
		2	16 621.08	0.03	36		16	5d ⁴	³ P1	L10405
5d ⁸ (⁴ F)6s	δĘ	1	10 968.54	0.04	82		5	5d ⁸ (2D2)6s	3D	L10405
		2	12 427.09	0.03	79					L10405

M1 line list for kilonova nebula

- We have constructed a forbidden (M1) line list up to Eeinsteinium (Z=99).
- The experimentally calibrated levels and the LS selection rules are used.
- A values from an analytic formula (Pasternack 40, Shortley 40, Bahcall & Wolf 68)
- Some ions are missing because the energy levels are unknown.



A top-down approach for kilonova nebula

- All ions for which the experimental energy levels exist are included.
- Collision strengths are computed by HULLAC
- Ionization states, electron density, temperature are given.
- The wavelengths: \bigcirc , the intensities: \triangle .

KH+ 2022



We propose two interpretations for the Spitzer observation:

- 1) the first r-process peak elements are abundant and Se III dominates the flux.
- 2) W III, Os III, Rh III are the main sources.

Kilonova nebula: Heavy composition

Preliminary result (KH+ in prep)



- JWST will do an excellent job for this. But we have to improve the model.
- Once we see any spectral features, we can improve the relevant atomic data.

How kilonova remnants look like?



- 100 kyr remnants emit MeV γ -rays.
- How about emission at the other wavelengths on various time scales?

How good are atomic data?



How good on the second of the



Which elements can be seen ?



La III and Ce III may be in the observed spectrum.

Although spectra can be generated, the systematic errors cannot be put.

Can we develop non-LTE?

Local Thermodynamic Equilibrium (LTE)

A very powerful method but it is not always correct.

Input

- Atomic energy levels, *E_i*
- Electric dipole transition rates (E1), A_{ij} or f_{ji}
- Heating rate

Tremendous efforts on these for opacity.

Given a local *T* and *n*

- Free electron: Maxwell-Boltzmann distribution
- Level population: Boltzmann distribution
- Ionization: Saha equilibrium

Output - Photon spectrum

Non Local Thermodynamic Equilibrium (non LTE)

It can give in principle correct answers but demanding.

Input

- Atomic energy levels, E_i
- Transition rates including forbidden lines (E1, M2...), Aij or fij
- Photoionization cross sections $\sigma_{V,i}$
- Electron-impact excitation cross sections $\sigma_{ex,ij}$
- Electron-impact ionization cross sections $\sigma_{ion,i}$
- Recombination rate coefficients a_{y,i}
- Heating rate

Given a local *T* and *n*

- Free electron: Maxwell-Boltzmann distribution
- Level population: Boltzmann distribution
- Ionization: Saha equilibrium

Output

- Photon spectrum

Iteration



Tremendous efforts on these for opacity.

Can we develop non-LTE?

We can get radiative transition rates for M1 by an analytic formula (KH+ in prep).

Ion	$\lambda_{fs} \; (\mu \mathrm{m})$	$A ({\rm s}^{-1})$	$A_{\rm LS}~({\rm s}^{-1})$	Lower term	Upper term	
Sr II	0.6740252	2.559	—	${}^{2}\mathrm{S}_{1/2}$	${}^{2}\mathrm{D}_{5/2}$	E2
	0.6870066	2.299	—	${}^{2}\mathrm{S}_{1/2}$	${}^{2}\mathrm{D}_{3/2}$	M1+E2
Ac III	12.4846	$8.48 \cdot 10^{-7}$	_	$^{2}S_{1/2}$	$^{2}\mathrm{D}_{3/2}$	E2
	2.93863	$4.30 \cdot 10^{-1}$	$4.25 \cdot 10^{-1}$	${}^{2}\mathrm{D}_{3/2}$	${}^{2}\mathrm{D}_{5/2}$	M1
	2.37872	$3.745 \cdot 10^{-3}$	—	${}^{2}\mathrm{S}_{1/2}$	${}^{2}\mathrm{D}_{5/2}$	E2
Pt II	1.187671	8.75	9.66	$^{2}\mathrm{D}_{5/2}$	$^{2}\mathrm{D}_{3/2}$	M1
Sn II	2.352114	0.694	0.691	$^{2}P_{1/2}^{o}$	$^{2}\mathrm{P}_{3/2}^{o}$	M1
Bi III	0.4810426	86.3	80.75	${}^{2}\mathrm{P}^{o}_{1/2}$	${}^{2}\mathrm{P}^{o}_{3/2}$	M1+E2

Table 3Fine structure transitions of heavy elements. The atomic data are taken from NIST.

Can we develop non-LTE?

Collisional processes are always problematic. (preliminary values from Hullac)

Ion	Upper level	Lower level	Hullac	R-matrix	reference
C II	${}^{2}\mathrm{P}_{3/2}$	${}^{2}\mathrm{P}_{1/2}$	2.4	1.8	Tayal (2008)
Se III	$^{3}P_{1}$	$^{3}P_{0}$	0.96	1.80	Sterling et al. (2017)
	$^{3}\mathrm{P}_{2}$	$^{3}\mathrm{P}_{0}$	1.78	1.10	
	$^{3}\mathrm{P}_{2}$	$^{3}\mathrm{P}_{1}$	3.0	4.46	
	$^{1}\mathrm{D}_{2}$	$^{3}P_{0}$	0.34	0.65	
	$^{1}\mathrm{D}_{2}$	$^{3}\mathrm{P}_{1}$	1.07	2.08	
	$^{1}\mathrm{D}_{2}$	$^{3}\mathrm{P}_{2}$	0.68	0.14	
Te III	${}^{3}P_{1}$	$^{3}P_{0}$	0.87	5.81	Madonna et al. (2018)
	$^{3}\mathrm{P}_{2}$	$^{3}P_{0}$	2.1	2.57	
	$^{3}P_{2}$	$^{3}P_{1}$	3.63	8.74	
	$^{1}\mathrm{D}_{2}$	$^{3}P_{0}$	0.32	1.1	
	$^{1}\mathrm{D}_{2}$	$^{3}P_{1}$	1.09	4.32	
	$^{1}\mathrm{D}_{2}$	$^{3}P_{2}$	2.70	8.61	
W IV	${}^{4}\mathrm{F}_{5/2}$	${}^{5}\mathrm{F}_{3/2}$	3.17	4.54	Ballance et al. (2013)
	${}^{4}\mathrm{F}_{7/2}$	${}^{5}\mathrm{F}_{3/2}$	0.59	1.89	
	${}^{4}\mathrm{F}_{9/2}$	${}^{5}\mathrm{F}_{3/2}$	0.26	1.32	

 $\begin{array}{c} {\bf Table \ 4} \\ {\rm Collision \ strengths \ from \ HULLAC \ and \ the \ literature} \end{array}$