Atomic Structure and Opacities of r-process Elements

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INT Program on *Electromagnetic Signatures of r-process Nucleosynthesis in Neutron Star Binary Mergers*

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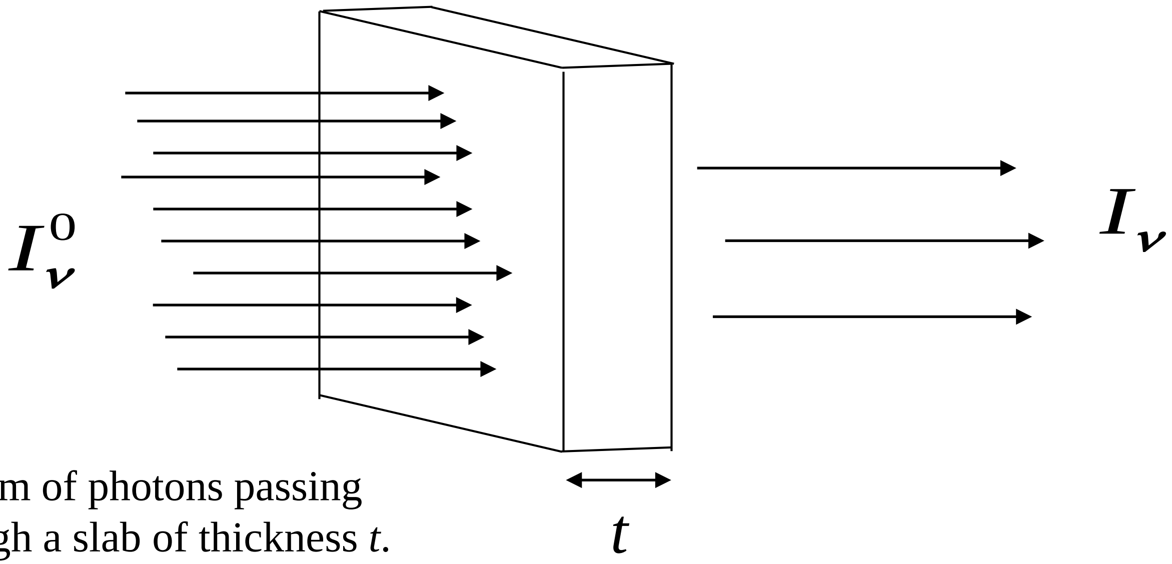
Overview

- The theory of opacities
- Specific application: r-process opacities and light curves for neutron star mergers

A useful illustration:
The classic opacity (transmission) experiment:

- Irradiate a thin slice of your favorite element and measure what gets transmitted to the other side:



A beam of photons passing through a slab of thickness *t*.

Why are opacities/emissivities important?

- These quantities are necessary to solve the radiation transport equation
- Assuming problem is time-independent and one-dimensional with isotropic radiation, the transport equation can be written:

emissivity

radiation intensity

$$\frac{1}{\rho}\frac{dI_\nu}{dx} = \frac{\varepsilon_\nu}{4\pi} - \kappa_\nu I_\nu$$

material density

opacity

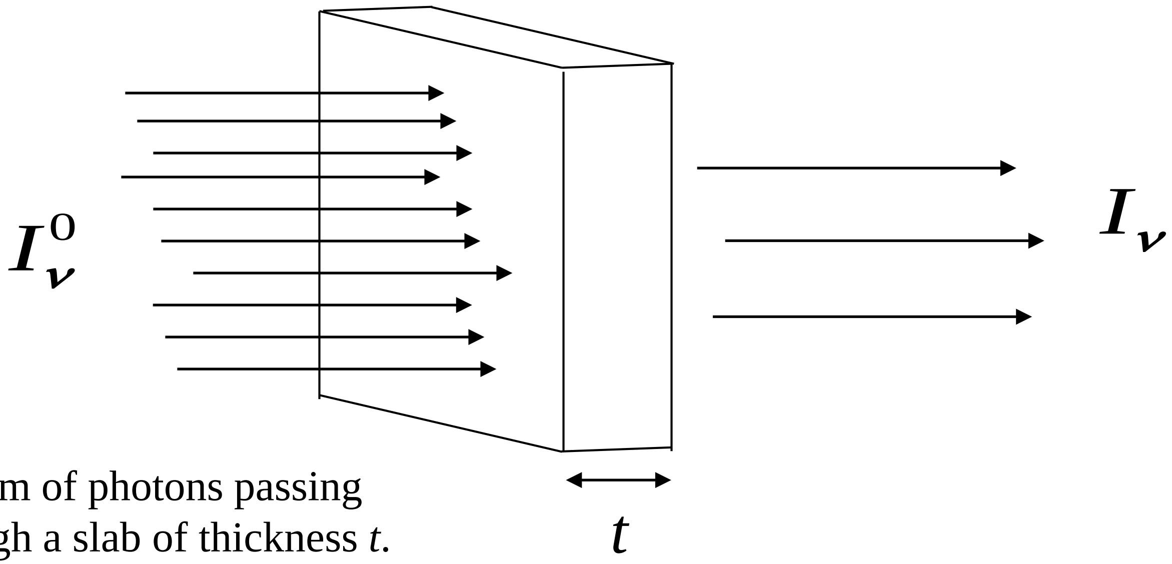
radiation frequency

The classic opacity (transmission) experiment: Optically thin plasma example

- If the plasma is “optically thin”, then the emitted radiation will escape and need not be considered in the radation transport equation:

$$\frac{1}{\rho}\frac{dI_\nu}{dx} = \xcancel{\frac{\varepsilon_\nu}{4\pi}} - \kappa_\nu I_\nu$$

- This situation can be illustrated by the following diagram:



A beam of photons passing through a slab of thickness *t*.

Optically thin plasma example (continued)

- The previous differential equation has a well-known solution:

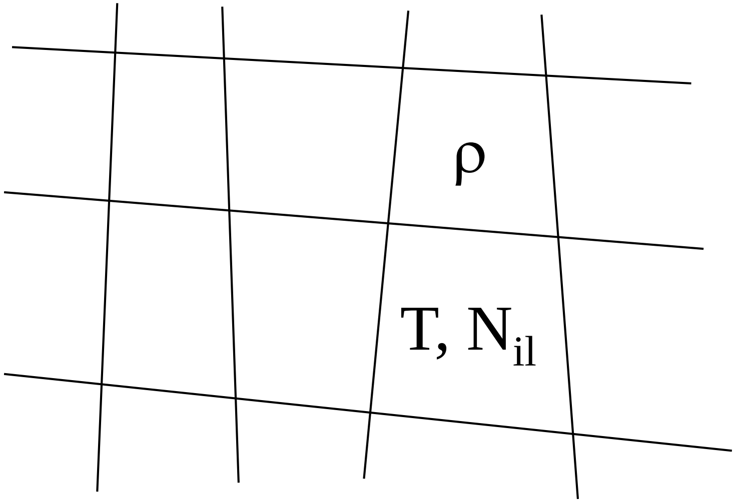
$$I_\nu = I_\nu^0 e^{-(\rho \kappa_\nu t)}$$

- This sort of “transmission experiment” is the typical way in which opacities are measured
- The quantity $\lambda_\nu^{\mathrm{mfp}} = (1/\rho\kappa_\nu)$ has the dimensions of length and is called the **optical mean free path**. The mean free path is a useful physical quantity and is defined as the average distance a photon can travel through a material without being absorbed or scattered. Optically thin plasmas have physical dimensions << $\lambda_\nu^{\mathrm{mfp}}$.

Connecting (macroscopic) opacity with (microscopic) atomic physics

Some helpful illustrations

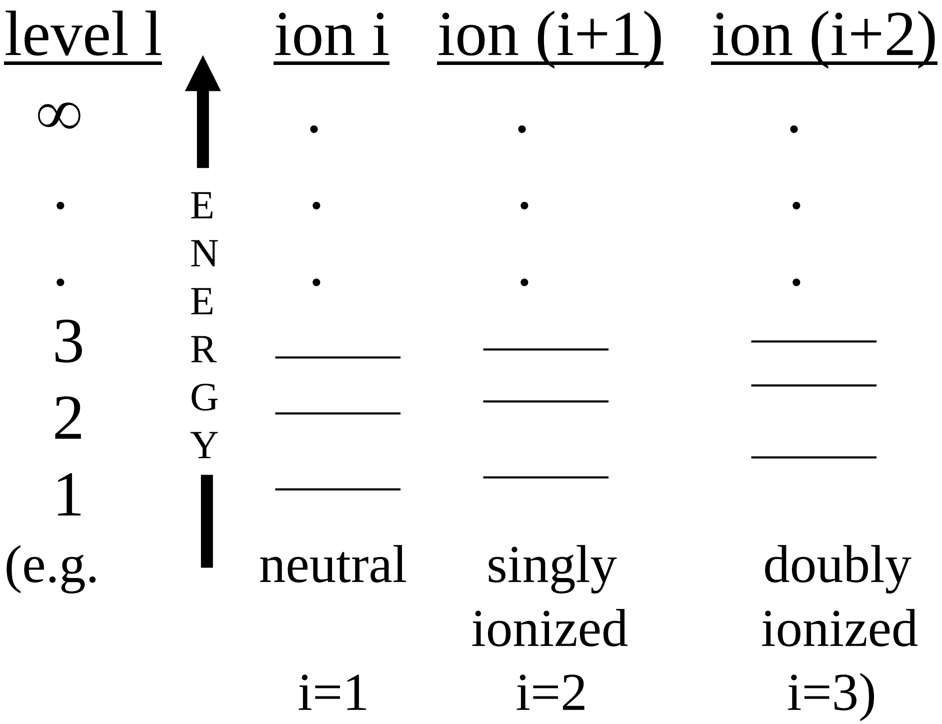
Our sample plasma made up of cells described by temperatures, densities, atomic populations, etc.



N_{il} = number density for level l, ion stage i

$[N_{il}] = 1/cm^3$

Our sample ions/atoms inhabiting each cell



Atomic kinetics modeling is an *ab-initio* effort

- There are far too many atomic processes to be measured experimentally
- Furthermore, there are not many experimental measurements of atomic physics data
- Nuclear data are obtained through evaluations which rely on both experimental data and theoretical calculations
- Atomic data (e.g. opacities) are obtained almost exclusively from first-principle calculations (quantum mechanics, wavefunctions, cross sections, etc.)

Road map to opacity

wavefunctions, level energies (Ψ_l, E_l)

↓

fundamental cross sections ($\sigma_{l\rightarrow l'}$)

↓

rate coefficients, rate equations

↓

atomic level populations (N_{il})

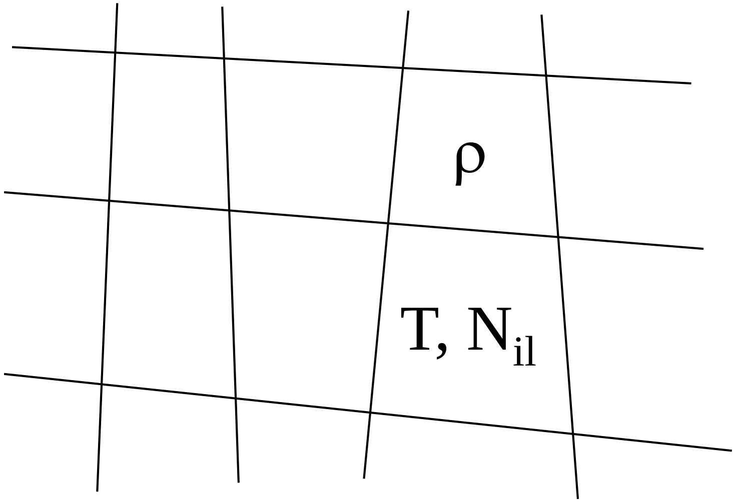
↓

opacity ($\kappa_\nu \sim N_{il} \times \sigma^{\mathrm{photo}}_{l\rightarrow l'}$)

Excitation and de-excitation processes

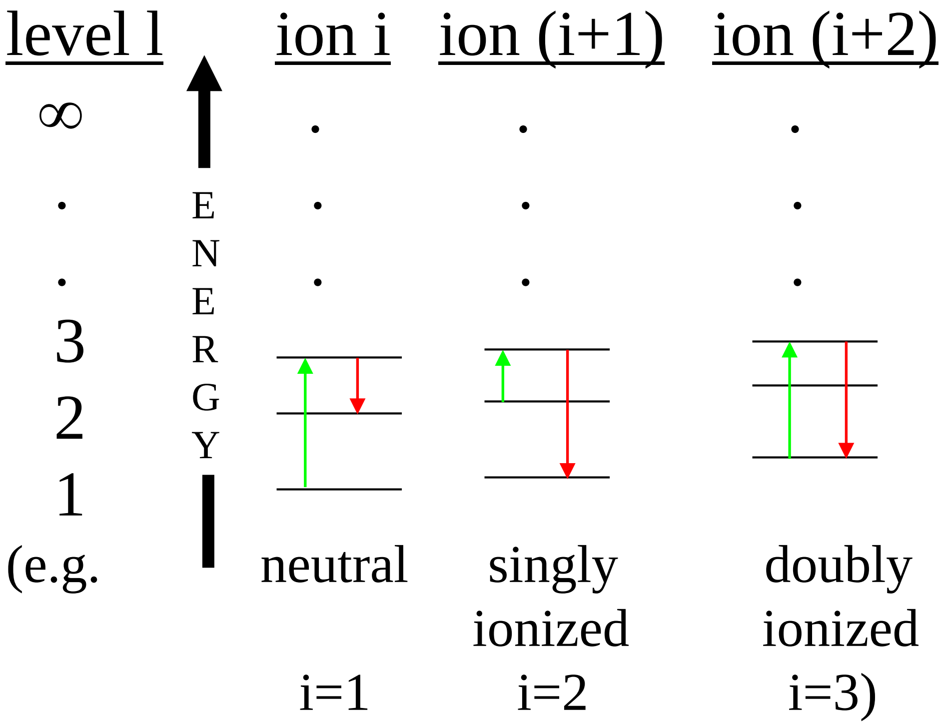
Our sample plasma made up of cells described by temperatures, densities, atomic populations, etc.

Our sample ions/atoms inhabiting each cell



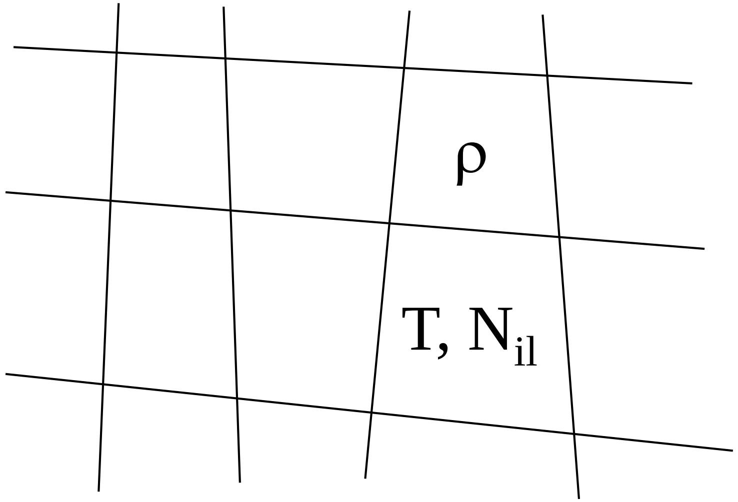
N_{il} = number density for level l, ion stage i

$[N_{il}] = 1/cm^3$



Ionization and recombination processes

Our sample plasma made up of cells described by temperatures, densities, atomic populations, etc.



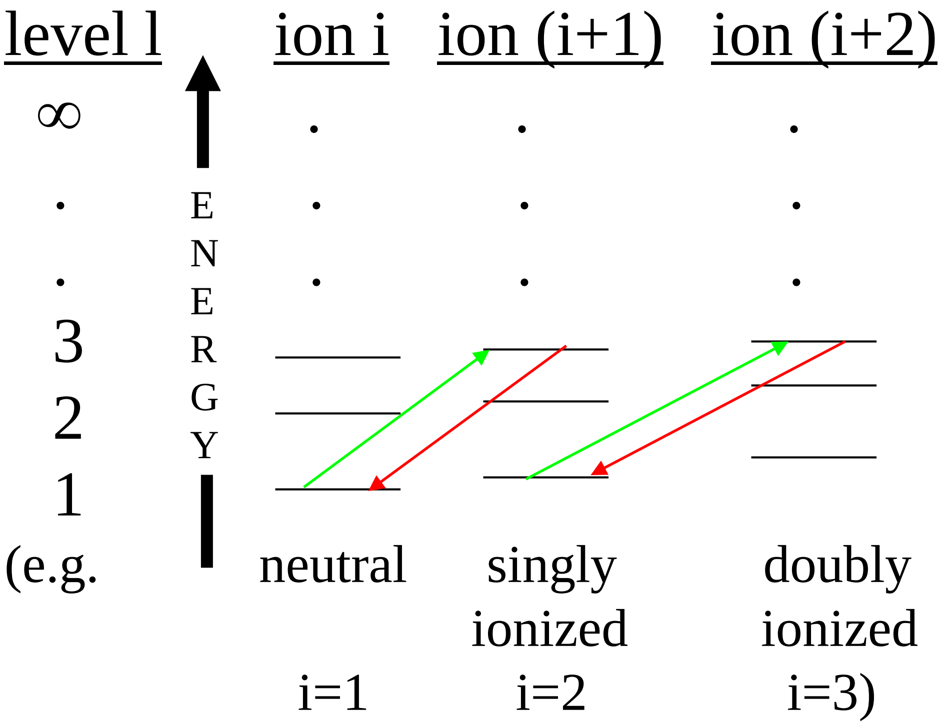
ρ

T, N_{il}

N_{il} = number density for level l, ion stage i

$[N_{il}] = 1/cm^3$

Our sample ions/atoms inhabiting each cell



level l

∞

.

.

3

2

1

ENERGY

ion i

ion (i+1)

ion (i+2)

(e.g.

neutral

i=1

singly ionized

i=2

doubly ionized

i=3)

Solving for the atomic level populations, N_{il}

- To obtain an opacity at each point in our sample plasma, we require the fundamental cross sections and the level populations, N_{il}
- The level populations are determined by the following basic atomic processes and their inverses:

process	inverse process
photoexcitation	photo de-excitation
photoionization	radiative recombination
electron collisional excitation	electron collisional de-excitation
electron collisional ionization	three-body recombination
autoionization	dielectronic recombination

- The cross sections for these processes are used in coupled, differential equations, known as “rate equations”, which determine the populations N_{il}

The rate equations

- In general, the level populations vary as a function of time
- One must consider all possible processes that can populate and depopulate each level
- The result is a set of non-linear, first-order differential equations
- $\frac{dN_{il}}{dt} =$ (Formation rates) - (Destruction rates)
- In matrix form

$$\begin{pmatrix} dN_{11}/dt \\ \ldots \\ dN_{il}/dt \\ \ldots \\ dN_{nn}/dt \end{pmatrix} = \begin{pmatrix} R_{11} & . & R_{1l} & . & R_{1n} \\ . & . & . & . & . \\ R_{i1} & . & R_{il} & . & R_{in} \\ . & . & . & . & . \\ R_{n1} & . & R_{nl} & . & R_{nn} \end{pmatrix} \begin{pmatrix} N_{11} \\ \ldots \\ N_{il} \\ \ldots \\ N_{nn} \end{pmatrix}$$

The rate equations (continued)

- The order of the rate matrix can vary greatly depending on the complexity of the atomic model
- Average-atom: order ~10, very crude, very fast to compute
- Configuration-average: order ~100-10^7, good compromise, some spectral detail, but maybe not enough to produce high-resolution spectra
- Fine-structure: order ~100-10^{10}, spectrally resolved features, very accurate if complete model can be considered, but can be impractical to solve numerically

Constructing the rate matrix

- Each element of the rate matrix is computed from fundamental cross sections associated with each process
- A “rate coefficient” is calculated from the cross section and the appropriate energy distribution (for electrons or photons)
- Rate coefficient $= \int$ [distribution(E,T)] x [cross section(E)] dE
- These concepts lead naturally to a discussion of LTE (local thermodynamic equilibrium) vs. non-LTE (NLTE) atomic physics

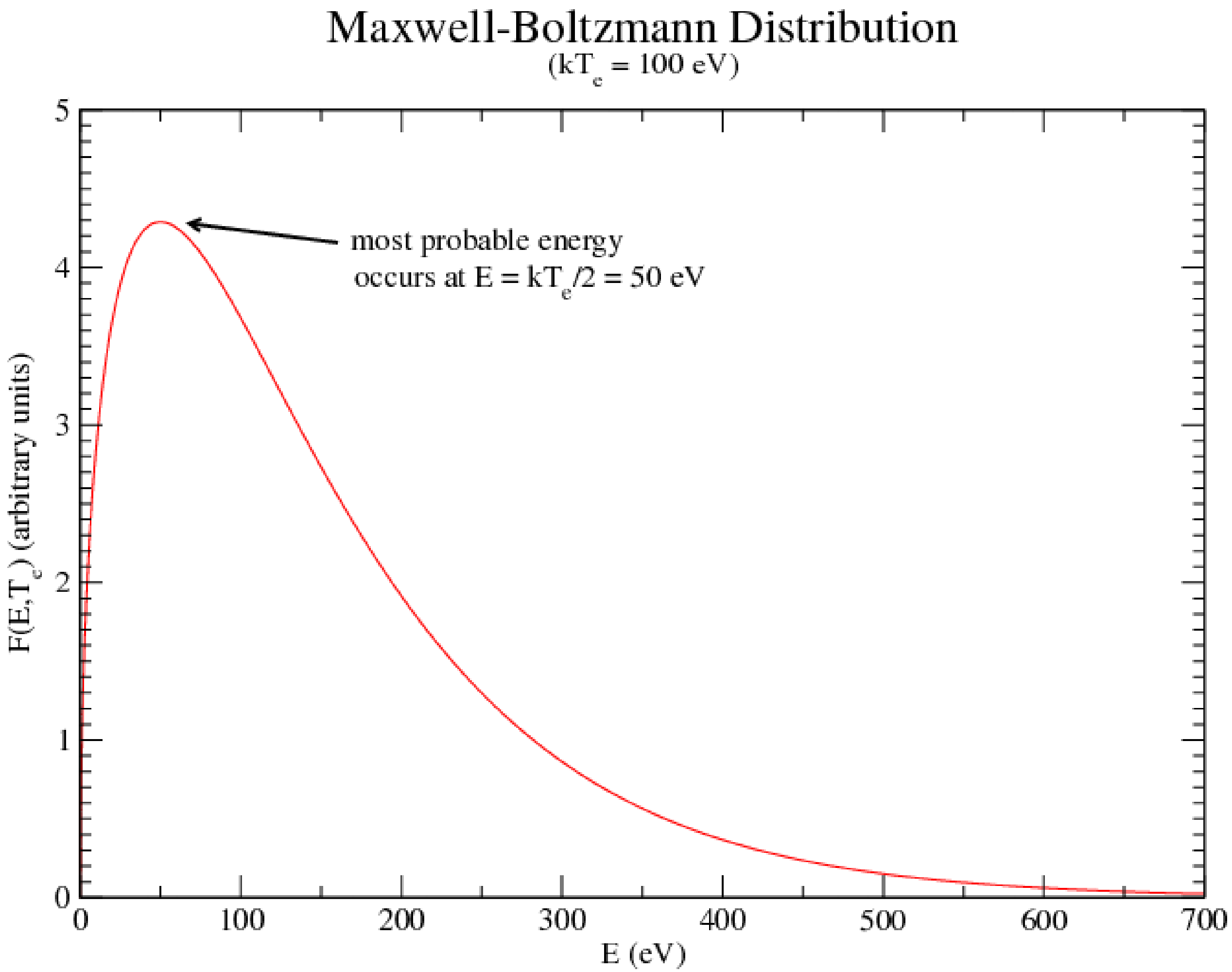
Free electrons in thermodynamic equilibrium

- If the free electrons are in thermodynamic equilibrium (TE) with themselves, then the energy distribution is given by the Maxwell-Boltzmann distribution at an electron temperature T_e

$$F(E,T_e)=\frac{2}{\sqrt{\pi}}\frac{\sqrt{E}}{(kT_e)^{3/2}}e^{-E/kT_e}$$

- This distribution represents the fraction of electrons per unit energy interval that have energies between E and E+dE

Maxwellian distribution at kT_e=100 eV



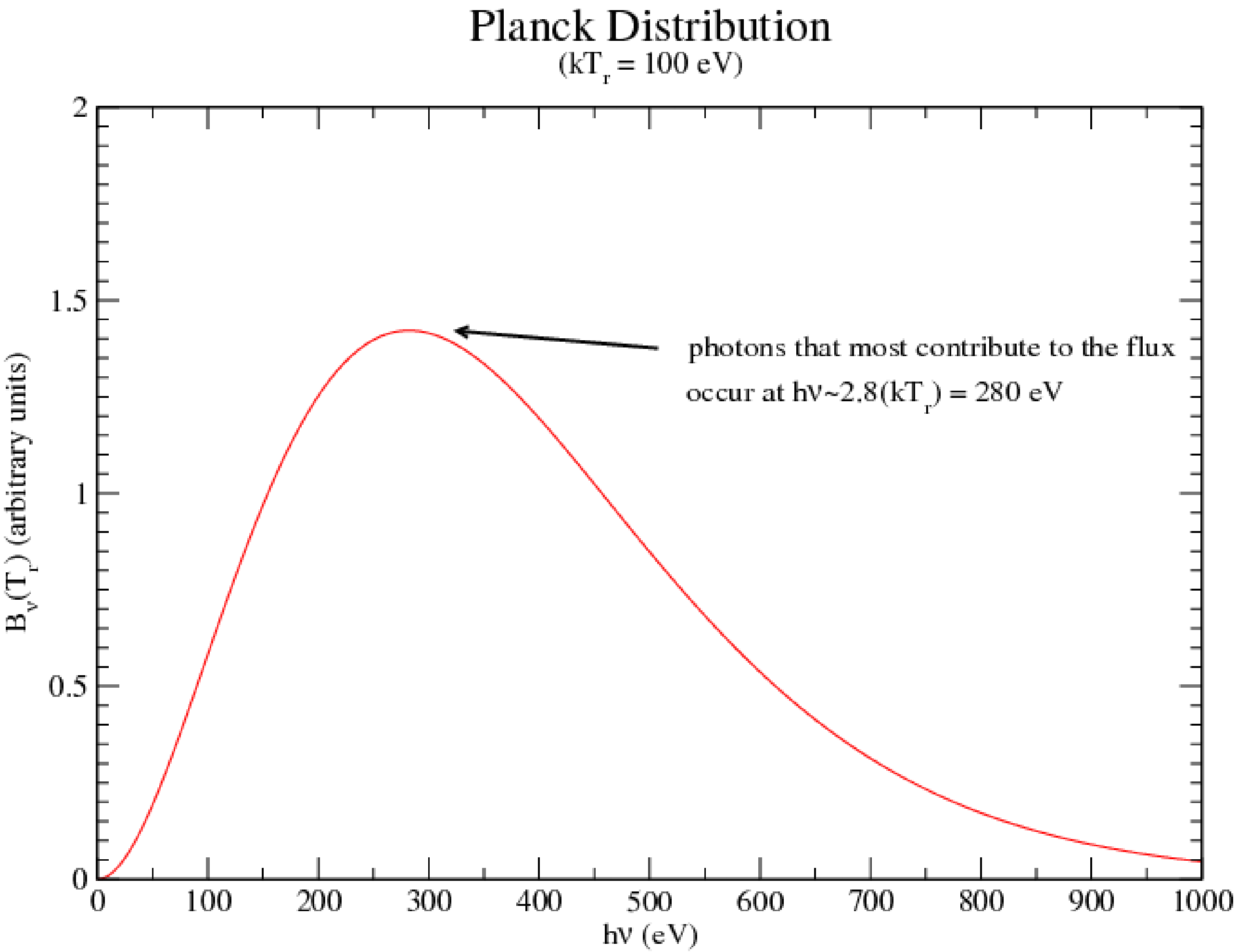
Photons in thermodynamic equilibrium

- Similarly, if the photons are in thermodynamic equilibrium (TE) with themselves, then the energy density distribution is given by the Planck distribution at a radiation temperature T_r

$$B_\nu(T_r) = \frac{2}{(hc)^2} \frac{(h\nu)^3}{e^{h\nu/kT_r} - 1}$$

- This is a flux distribution that represents the amount of radiation energy per unit frequency interval per unit area per unit time per unit solid angle

Planckian distribution at kT_r=100 eV



Local Thermodynamic Equilibrium (LTE) from a practical (computational) perspective

- From a computational perspective, LTE means that the atomic level populations, N_{il}, can be solved from the (relatively) simple Saha equation and the Boltzmann relationship

$$\boxed{N_{\mathrm{il}} \propto (N_{\mathrm{i}})e^{-E_{\mathrm{il}}/kT}}$$

- In this case, the N_{il} can be determined from a simple analytic formula that depends on the energy and temperature; there is ***no need to consider the fundamental cross sections***.

- Solving the detailed rate equations with a Maxwellian electron distribution and a Planckian radiation distribution results in a steady-state solution $(dN_{\mathrm{il}}/dt = 0)$ which could have been found by solving the much simpler Botzmann relationship above

Non-LTE
from a practical (computational) perspective

- For the NLTE case, the detailed rate equations must be solved to obtain the atomic level populations, N_{il}
- In practice, this solution requires the use of large-scale computing
- NLTE calculations can take as much as 3-4 ***orders of magnitude*** more computing time than LTE calculations

Computing an opacity from fundamental atomic cross sections

- Basically,

  opacity = (atomic population)(cross section)/(mass density)
  (NB: we are only interested in ***photo*** cross sections now)

- When interacting with electrons, a photon can be absorbed (most/all energy given to electrons) or scattered (some energy given to electrons, but photon survives with slightly decreased energy)

$$\kappa_\nu^{\text{TOT}}(\rho,T_e,T_r)=\kappa_\nu^{\text{ABS}}(\rho,T_e,T_r)+\kappa_\nu^{\text{SCAT}}(\rho,T_e,T_r)$$

Compton scattering

$$\kappa_\nu^{\text{ABS}}=\frac{1}{\rho}\sum_{\text{il}}N_{\text{il}}(\rho,T_e,T_r)[\sigma_{\text{il}}^{(\text{bound}-\text{bound})}(\nu)+\sigma_{\text{il}}^{(\text{bound}-\text{free})}(\nu)]+\kappa_\nu^{(\text{free}-\text{free})}$$

material density

atomic level populations

photoexcitation cross sections

photoionization cross sections

inverse Bremsstrahlung contribution

How to compute an opacity

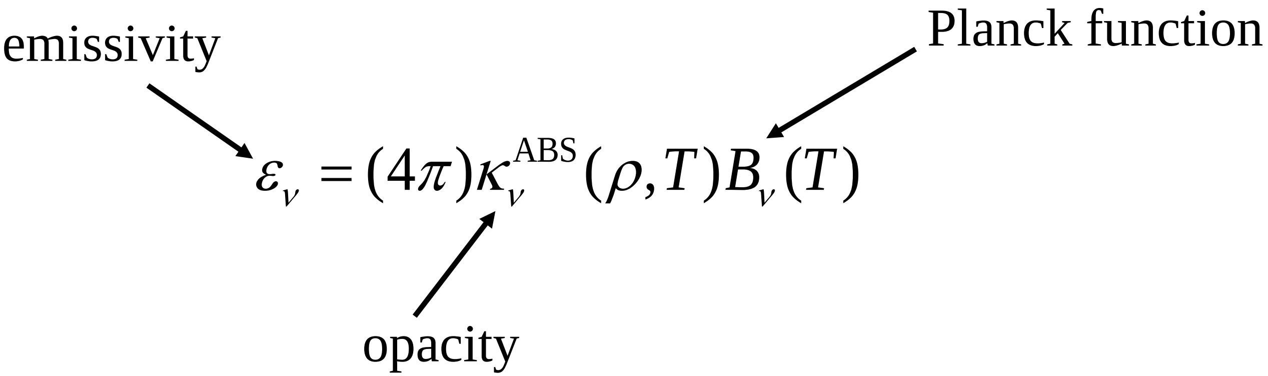
- Compton scattering uses a straightforward formula:

$$\kappa_\nu^{\mathrm{SCAT}} = N_e \sigma^{\mathrm{SCAT}}(\nu)/\rho \;\; [\approx 0.4\overline{Z}/A \; (\mathrm{cm}^2/\mathrm{g}) \text{ for Thomson scattering }]$$

- The free-free contribution is straightforward (Kramers' formula)
- The bound-bound and bound-free contributions are obtained by summing over ALL bound levels of ALL important ion stages
- This sum requires the populations, N_{il}, as well as the relevant photo cross sections, $\sigma_{il}^{\mathrm{photo}}$
- The previous opacity equations are valid for both LTE and NLTE conditions
- The LTE/NLTE difference ***is in how one calculates the atomic populations***, N_{il}

What about emissivities?

- Simple (Kirchoff) relation for LTE conditions:



emissivity

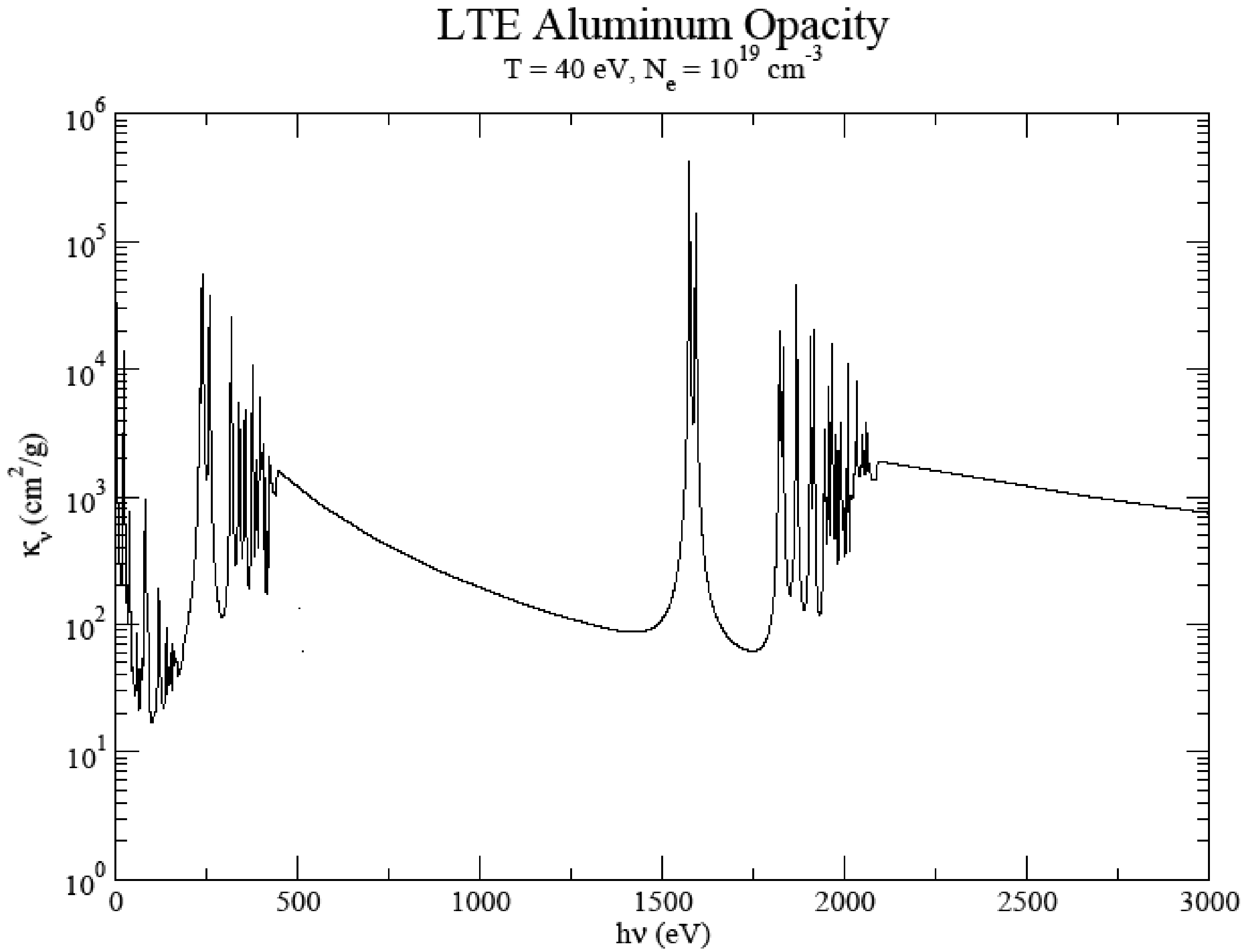
Planck function

$$\varepsilon_\nu = (4\pi)\kappa_\nu^{\mathrm{ABS}}(\rho, T)B_\nu(T)$$

opacity

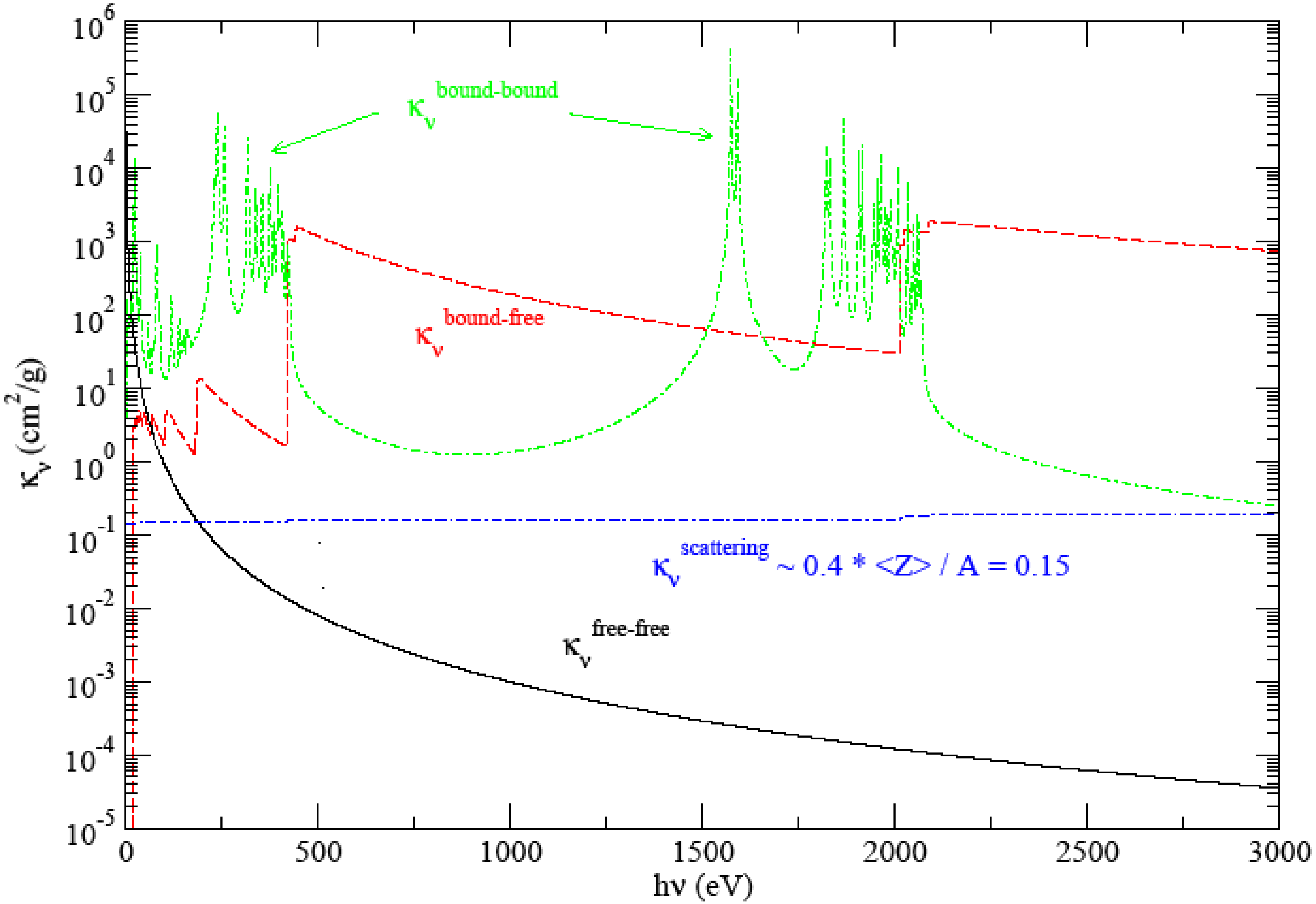
- One only needs the opacity to obtain the emissivity when doing LTE calculations
- Non-LTE emissivities require the level populations, N_{il}, along with the cross sections for the ***inverse*** of the photo-absorption processes that were considered for opacities

A specific example: the total LTE opacity of aluminum plasma (40 eV, 10^{19} electrons/cm^3)



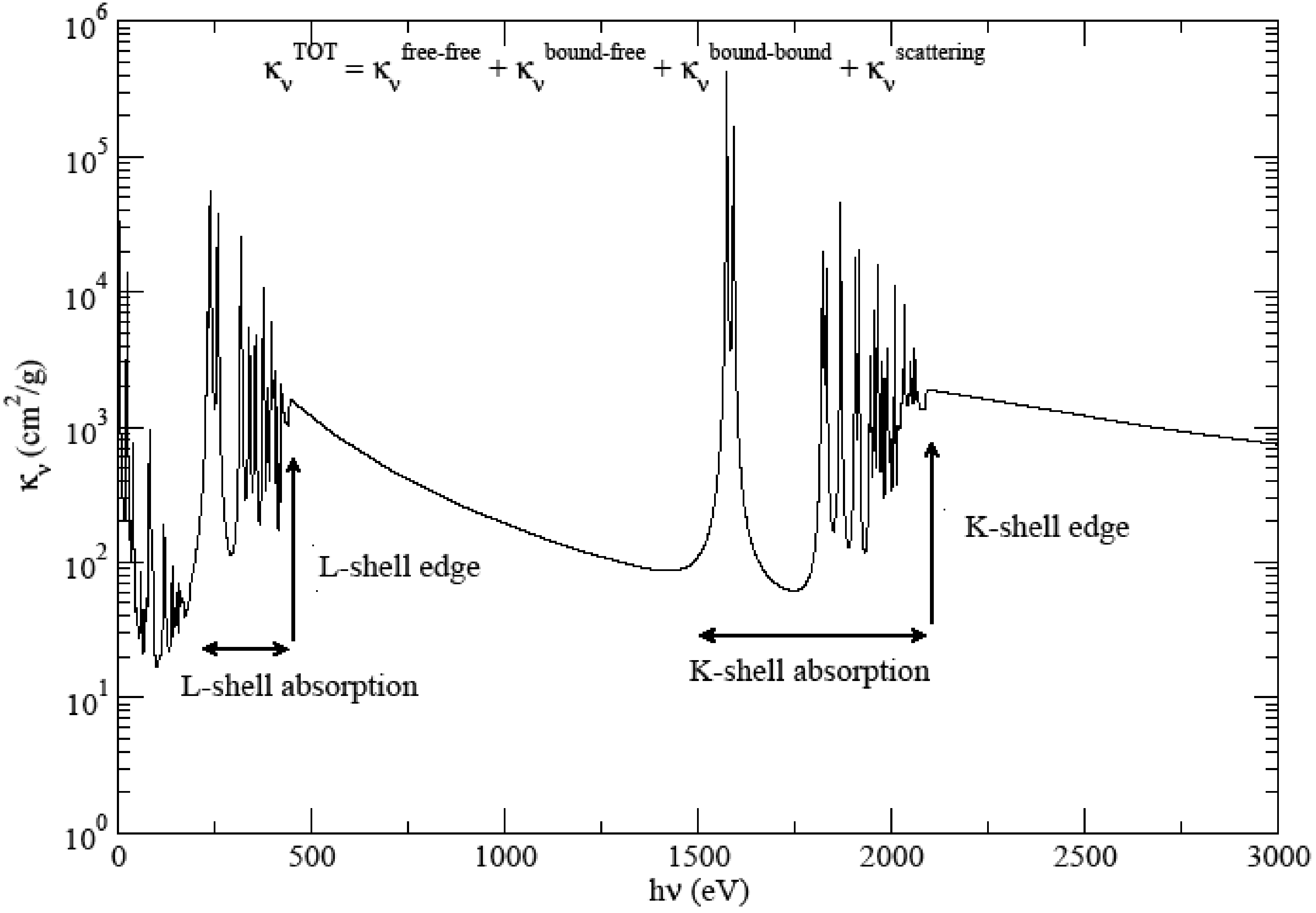
LTE Aluminum Opacity

T = 40 eV, $N_e = 10^{19}$ cm^{-3}



LTE Aluminum Opacity

T = 40 eV, $N_e = 10^{19}$ cm^{-3}



The LANL Suite of Atomic Modeling Codes (Fontes et al, JPB 48, 144014 (2015))

Atomic Physics Codes → Atomic Models → ATOMIC

CATS: Cowan Code

RATS: relativistic

ACE: e^- excitation

GIPPER: ionization

http://aphysics2.lanl.gov/tempweb

fine-structure
config-average
UTAs
MUTAs
energy levels
gf-values
e^- excitation
e^- ionization
photoionization
autoionization

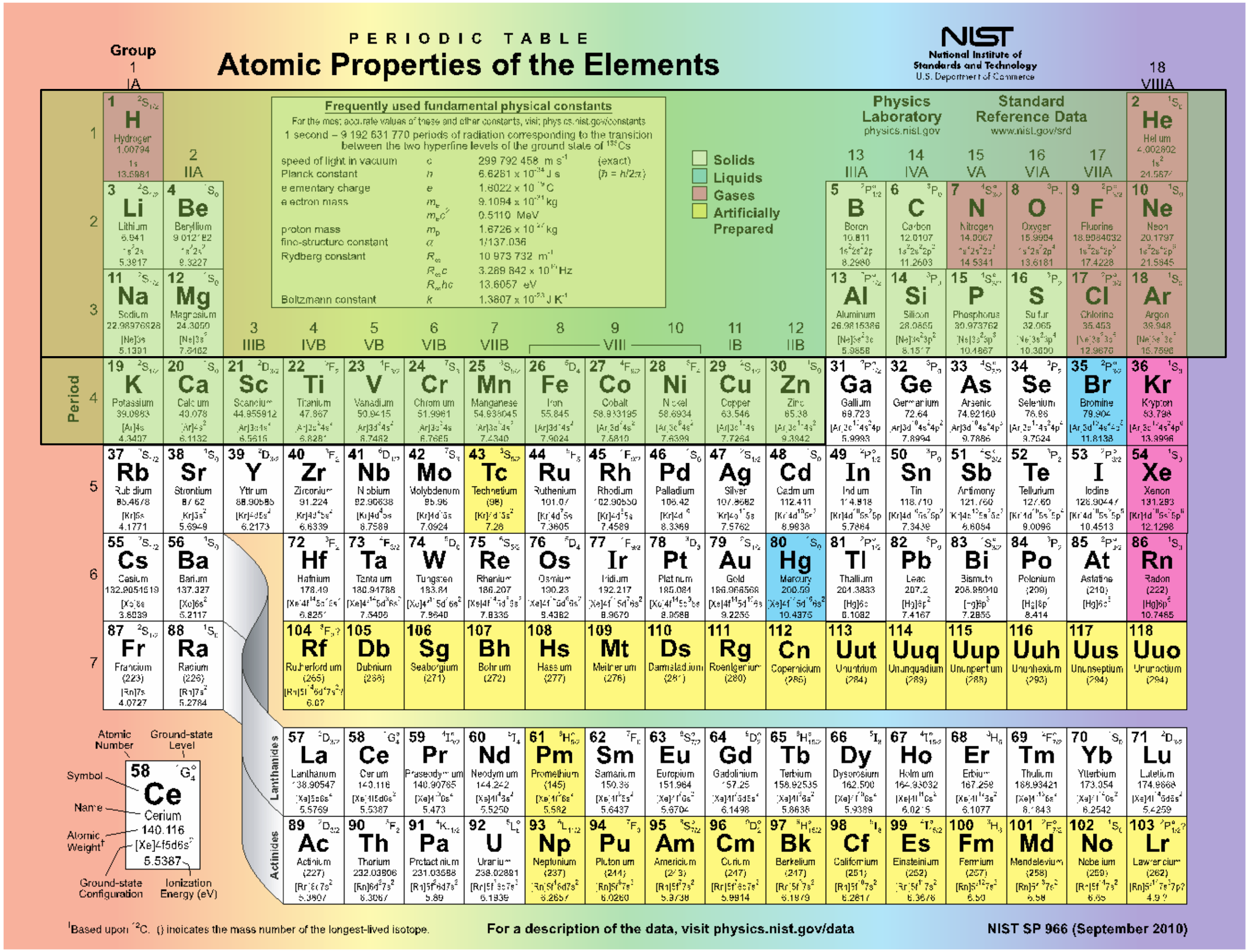
LTE or NLTE
low or high-Z
populations

spectral modeling
emission
absorption
transmission
power loss

LTE OPLIB tables
↓
TOPS

http://aphysics2.lanl.gov/opacity/lanl

The LANL Suite has been used to produce new LTE OPLIB tables for the first 30 elements


PERIODIC TABLE

Atomic Properties of the Elements

NIST National Institute of Standards and Technology U.S. Department of Commerce

Frequently used fundamental physical constants

For the most accurate values of these and other constants, visit physics.nist.gov/constants

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.6261×10^{-34} J s	($\hbar = h/2\pi$)
elementary charge	e	1.6022×10^{-19} C	
electron mass	m_e	9.1094×10^{-31} kg	
	m_ec^2	0.5110 MeV	
proton mass	m_p	1.6726×10^{-27} kg	
fine-structure constant	α	1/137.036	
Rydberg constant	R_∞	10 973 732 m^{-1}	
	$R_\infty c$	$3.289\,842 \times 10^{15}$ Hz	
	$R_\infty hc$	13.6057 eV	
Boltzmann constant	k	1.3807×10^{-23} J K^{-1}	

☐ Solids
☐ Liquids
☐ Gases
☐ Artificially Prepared

Physics Laboratory physics.nist.gov

Standard Reference Data www.nist.gov/srd

Atomic Number	Symbol	Name	Atomic Weight	Ionization Energy (eV)
1	H	Hydrogen	1.00794	13.5984
2	He	Helium	4.002602	24.5874
3	Li	Lithium	6.941	5.3917
4	Be	Beryllium	9.012182	9.3227
5	B	Boron	10.811	8.2980
6	C	Carbon	12.0107	11.2603
7	N	Nitrogen	14.0067	14.5341
8	O	Oxygen	15.9994	13.6181
9	F	Fluorine	18.9984032	17.4228
10	Ne	Neon	20.1797	21.5645
11	Na	Sodium	22.98976928	5.1391
12	Mg	Magnesium	24.3050	7.6462
13	Al	Aluminum	26.9815386	5.9858
14	Si	Silicon	28.0855	8.1517
15	P	Phosphorus	30.973762	10.4867
16	S	Sulfur	32.065	10.3600
17	Cl	Chlorine	35.453	12.9676
18	Ar	Argon	39.948	15.7596
19	K	Potassium	39.0983	4.3407
20	Ca	Calcium	40.078	6.1132
21	Sc	Scandium	44.955912	6.5615
22	Ti	Titanium	47.867	6.8281
23	V	Vanadium	50.9415	6.7462
24	Cr	Chromium	51.9961	6.7665
25	Mn	Manganese	54.938045	7.4340
26	Fe	Iron	55.845	7.9024
27	Co	Cobalt	58.933195	7.8810
28	Ni	Nickel	58.6934	7.6399
29	Cu	Copper	63.546	7.7264
30	Zn	Zinc	65.38	9.3942
31	Ga	Gallium	69.723	5.9993
32	Ge	Germanium	72.64	7.8994
33	As	Arsenic	74.92160	9.7886
34	Se	Selenium	78.96	9.7524
35	Br	Bromine	79.904	11.8138
36	Kr	Krypton	83.798	13.9996
37	Rb	Rubidium	85.4678	4.1771
38	Sr	Strontium	87.62	5.6949
39	Y	Yttrium	88.90585	6.2173
40	Zr	Zirconium	91.224	6.6339
41	Nb	Niobium	92.90638	6.7589
42	Mo	Molybdenum	95.96	7.0924
43	Tc	Technetium	(98)	7.28
44	Ru	Ruthenium	101.07	7.3605
45	Rh	Rhodium	102.90550	7.4589
46	Pd	Palladium	106.42	8.3369
47	Ag	Silver	107.8682	7.5762
48	Cd	Cadmium	112.411	8.9938
49	In	Indium	114.818	5.7864
50	Sn	Tin	118.710	7.3439
51	Sb	Antimony	121.760	8.6084
52	Te	Tellurium	127.60	9.0096
53	I	Iodine	126.90447	10.4513
54	Xe	Xenon	131.293	12.1298
55	Cs	Cesium	132.9054519	3.8939
56	Ba	Barium	137.327	5.2117
57	La	Lanthanum	138.90547	5.5769
58	Ce	Cerium	140.116	5.5387
59	Pr	Praseodymium	140.90765	5.473
60	Nd	Neodymium	144.242	5.5250
61	Pm	Promethium	(145)	5.582
62	Sm	Samarium	150.36	5.6437
63	Eu	Europium	151.964	5.6704
64	Gd	Gadolinium	157.25	6.1498
65	Tb	Terbium	158.92535	5.8638
66	Dy	Dysprosium	162.500	5.9389
67	Ho	Holmium	164.93032	6.0215
68	Er	Erbium	167.259	6.1077
69	Tm	Thulium	168.93421	6.1843
70	Yb	Ytterbium	173.054	6.2542
71	Lu	Lutetium	174.9668	5.4259
72	Hf	Hafnium	178.49	6.8251
73	Ta	Tantalum	180.94788	7.5496
74	W	Tungsten	183.84	7.8640
75	Re	Rhenium	186.207	7.8335
76	Os	Osmium	190.23	8.4382
77	Ir	Iridium	192.217	8.9670
78	Pt	Platinum	195.084	8.9588
79	Au	Gold	196.966569	9.2255
80	Hg	Mercury	200.59	10.4375
81	Tl	Thallium	204.3833	6.1082
82	Pb	Lead	207.2	7.4167
83	Bi	Bismuth	208.98040	7.2855
84	Po	Polonium	(209)	8.414
85	At	Astatine	(210)	
86	Rn	Radon	(222)	10.7485
87	Fr	Francium	(223)	4.0727
88	Ra	Radium	(226)	5.2784
89	Ac	Actinium	(227)	5.3807
90	Th	Thorium	232.03806	6.3067
91	Pa	Protactinium	231.03588	5.89
92	U	Uranium	238.02891	6.1939
93	Np	Neptunium	(237)	6.2657
94	Pu	Plutonium	(244)	6.0260
95	Am	Americium	(243)	5.9738
96	Cm	Curium	(247)	5.9914
97	Bk	Berkelium	(247)	6.1979
98	Cf	Californium	(251)	6.2817
99	Es	Einsteinium	(252)	6.3676
100	Fm	Fermium	(257)	6.50
101	Md	Mendelevium	(258)	6.58
102	No	Nobelium	(259)	6.65
103	Lr	Lawrencium	(262)	4.9 ?
104	Rf	Rutherfordium	(265)	6.0 ?
105	Db	Dubnium	(268)	
106	Sg	Seaborgium	(271)	
107	Bh	Bohrium	(272)	
108	Hs	Hassium	(277)	
109	Mt	Meitnerium	(276)	
110	Ds	Darmstadtium	(281)	
111	Rg	Roentgenium	(280)	
112	Cn	Copernicium	(285)	
113	Uut	Ununtrium	(284)	
114	Uuq	Ununquadium	(289)	
115	Uup	Ununpentium	(288)	
116	Uuh	Ununhexium	(293)	
117	Uus	Ununseptium	(294)	
118	Uuo	Ununoctium	(294)	

†Based upon ^{12}C. ( ) indicates the mass number of the longest-lived isotope.

For a description of the data, visit physics.nist.gov/data

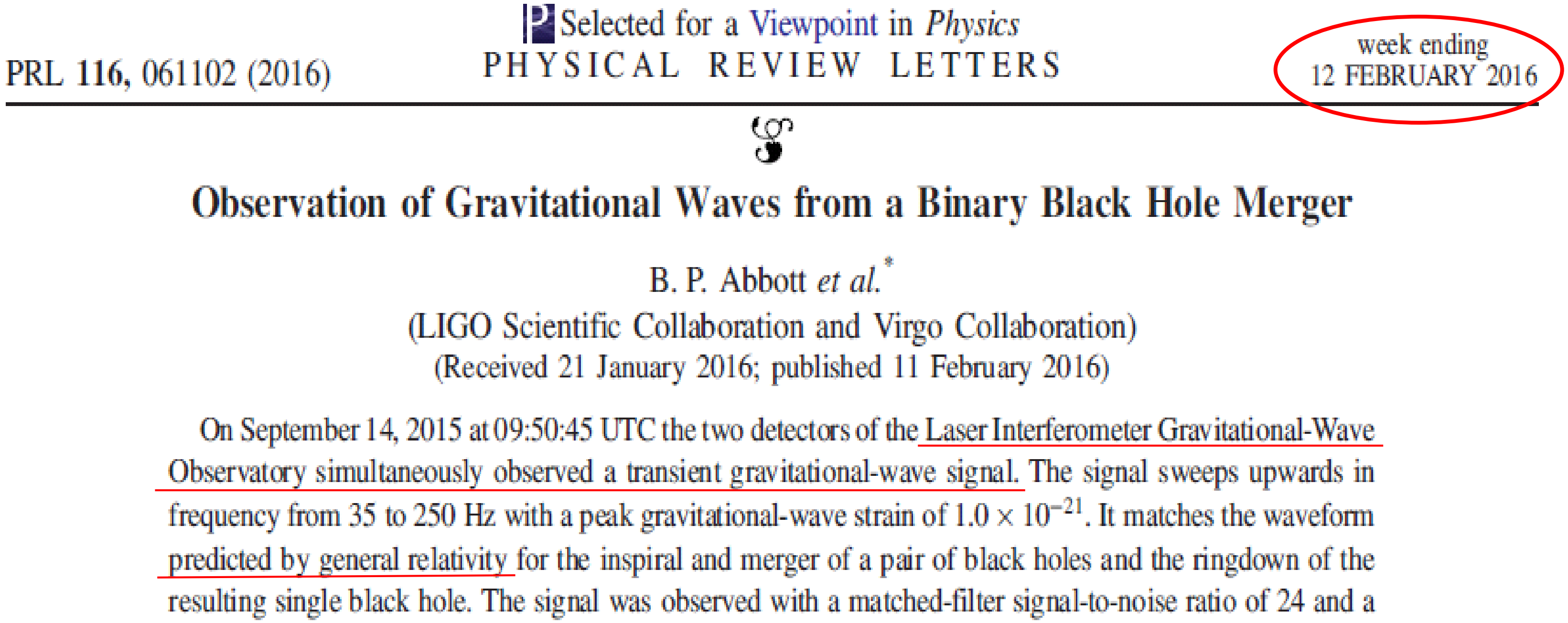
NIST SP 966 (September 2010)

Colgan et al, ApJ **817**, 116 (2016)

http://aphysics2.lanl.gov/opacity/lanl

LTE Opacity Application: light curves for neutron star mergers

We have entered the age of gravitational wave spectroscopy!



Selected for a Viewpoint in *Physics*

PRL **116,** 061102 (2016) PHYSICAL REVIEW LETTERS week ending 12 FEBRUARY 2016

Observation of Gravitational Waves from a Binary Black Hole Merger

B. P. Abbott *et al.**

(LIGO Scientific Collaboration and Virgo Collaboration)

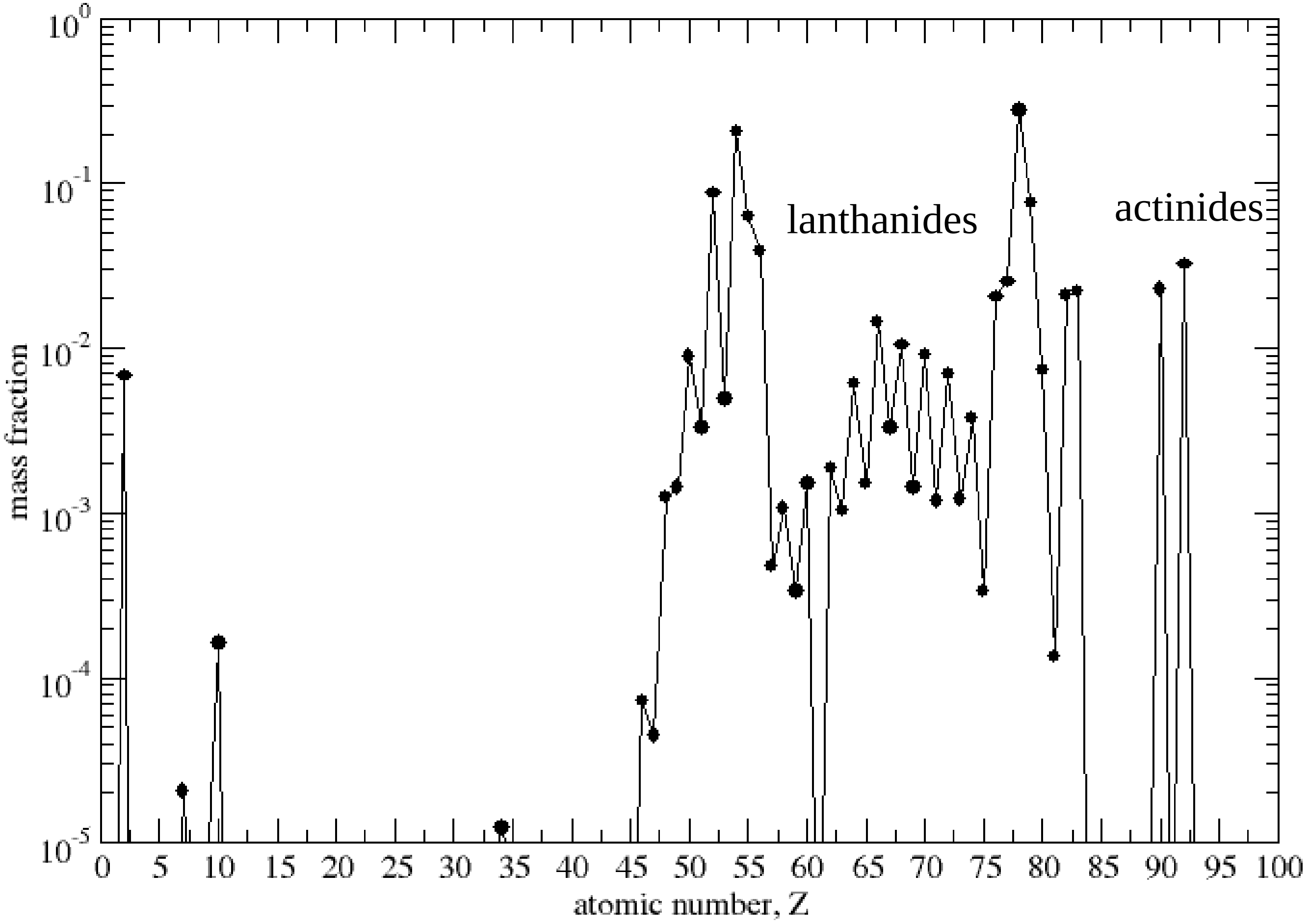
(Received 21 January 2016; published 11 February 2016)

On September 14, 2015 at 09:50:45 UTC the two detectors of the Laser Interferometer Gravitational-Wave Observatory simultaneously observed a transient gravitational-wave signal. The signal sweeps upwards in frequency from 35 to 250 Hz with a peak gravitational-wave strain of 1.0×10^{-21}. It matches the waveform predicted by general relativity for the inspiral and merger of a pair of black holes and the ringdown of the resulting single black hole. The signal was observed with a matched-filter signal-to-noise ratio of 24 and a

Can we observe gravitational waves with an electromagnetic counterpart?

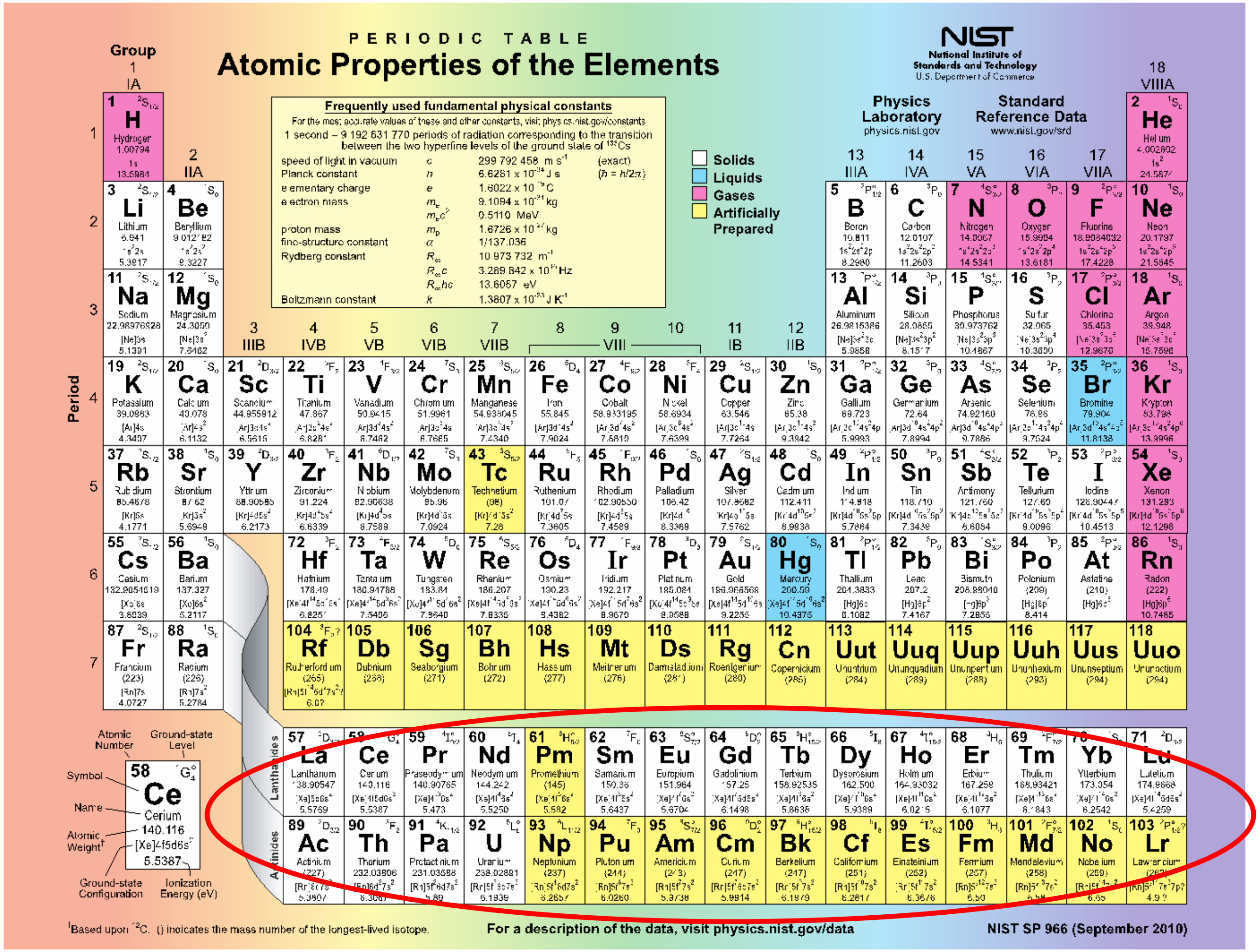
- Theory predicts that neutron star mergers will produce short gamma ray bursts (GRBs) and light curves
- The remainder of this talk deals with r-process opacities and their application to NSM light curves

Predicted elemental abundances in the ejecta of a neutron star merger (NSM)



courtesy of Stephan Rosswog

The lanthanides and actinides



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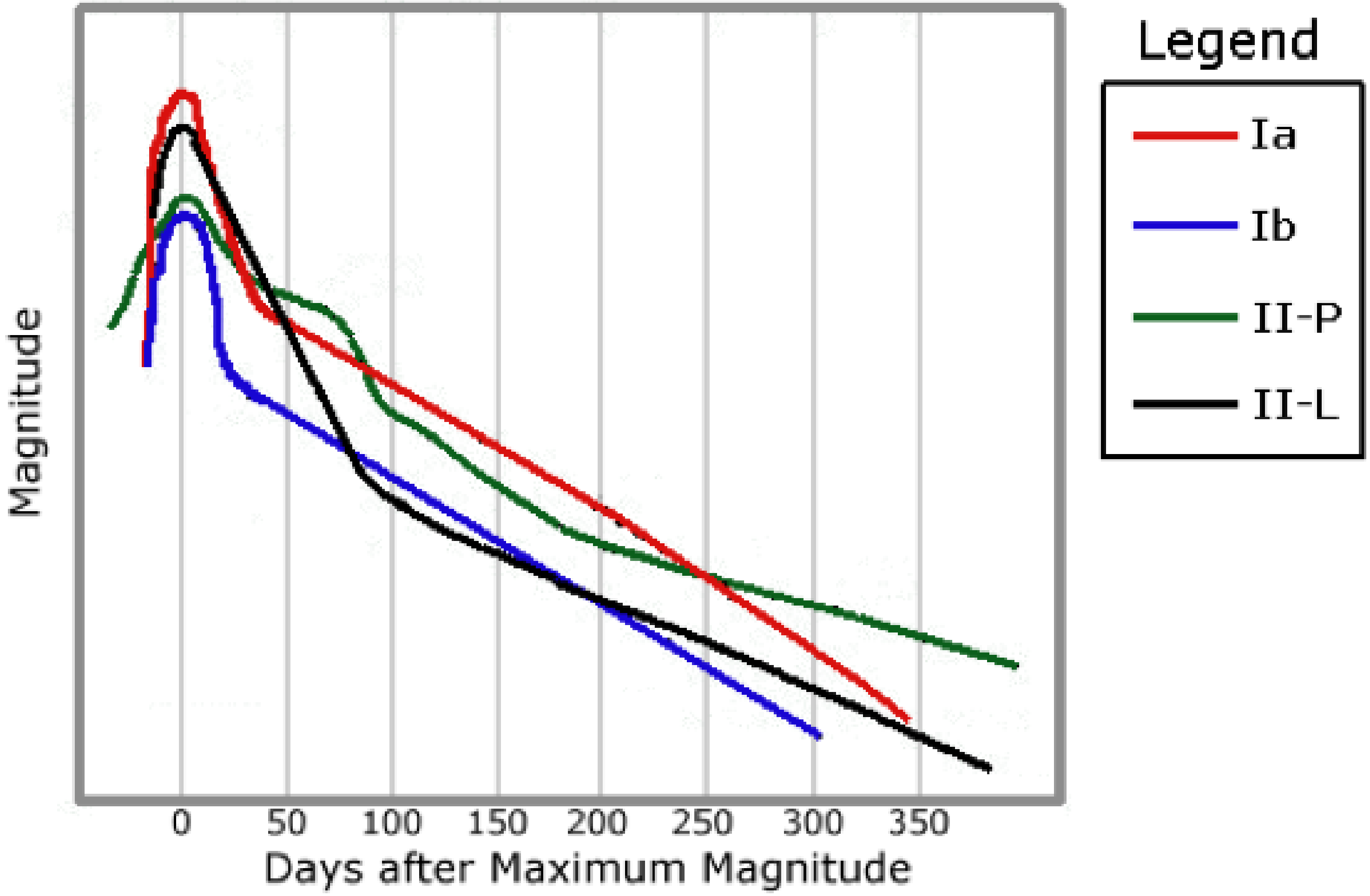
NIST SP 966 (September 2010)

Supernova light-curve examples



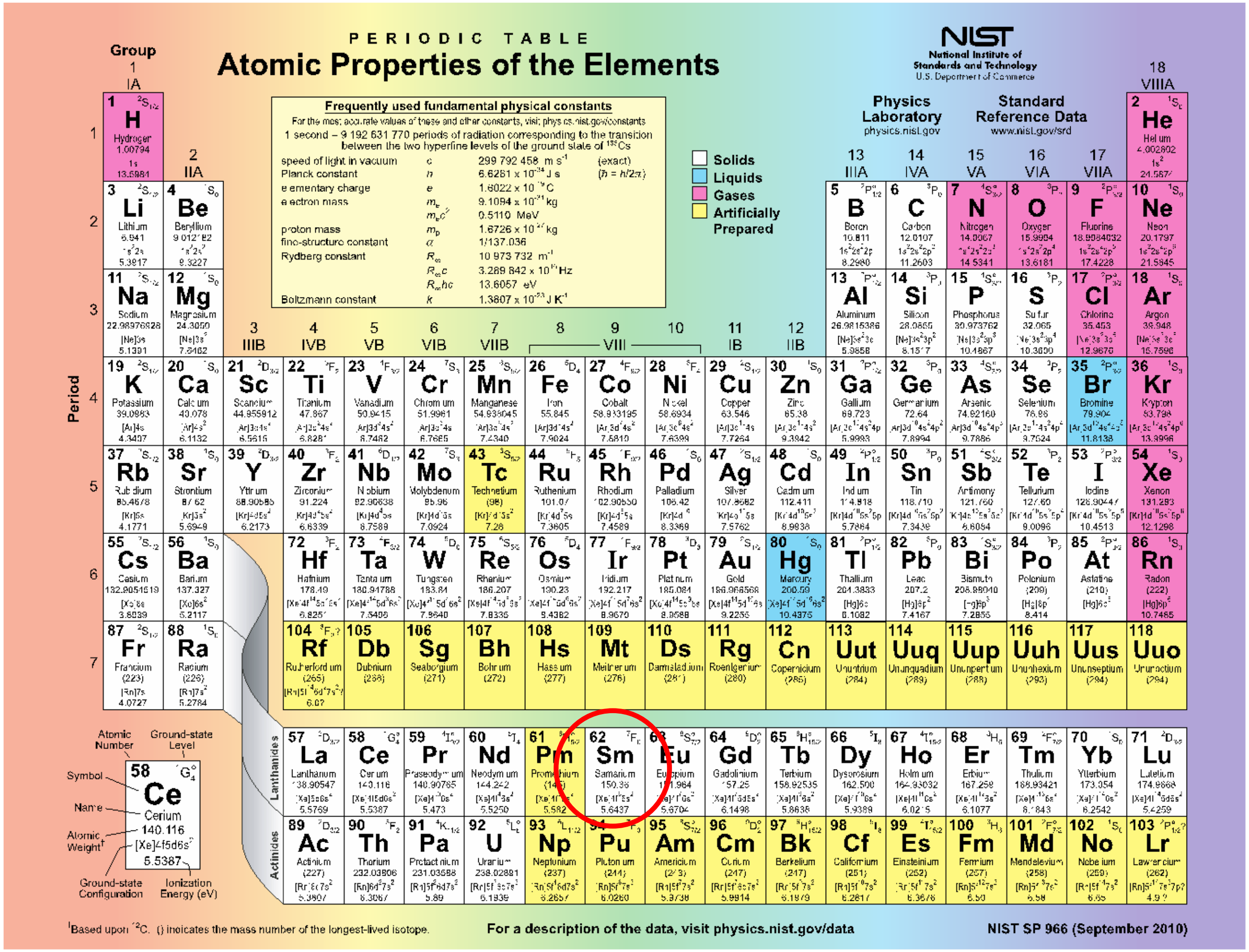
NSM light-curve ("macronova") examples

???

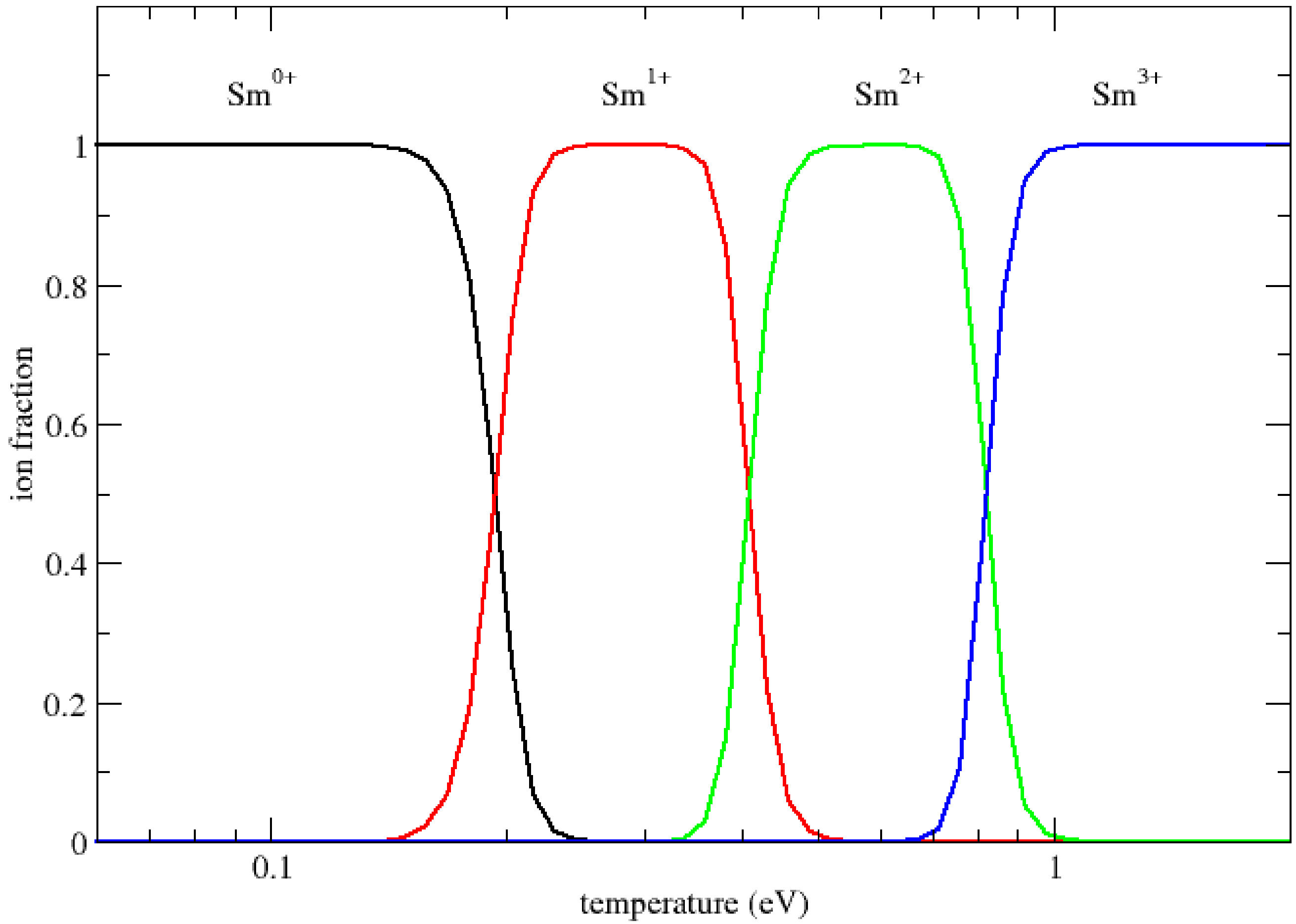
Conditions for neutron star mergers

- Initial conditions: $T \approx 1$ MeV, $\rho \approx 10^{14}$ g/cm^3
- Light curve approaching peak brightness: $T \approx 1$ eV, $\rho \approx 10^{-20} – 10^{-10}$ g/cm^3 ("low"); (if $\langle Z \rangle \approx 1$, then $N_e \approx 10 – 10^{11}$ el./cm^3)
- The presence of heavy elements at such cold temperatures requires the calculation of near-neutral ions with many (> 50) bound electrons. (Very complicated and difficult to calculate!!!)

Consider the opacity of cold samarium (Z=62) as an example (Sm^{0+} - Sm^{3+})

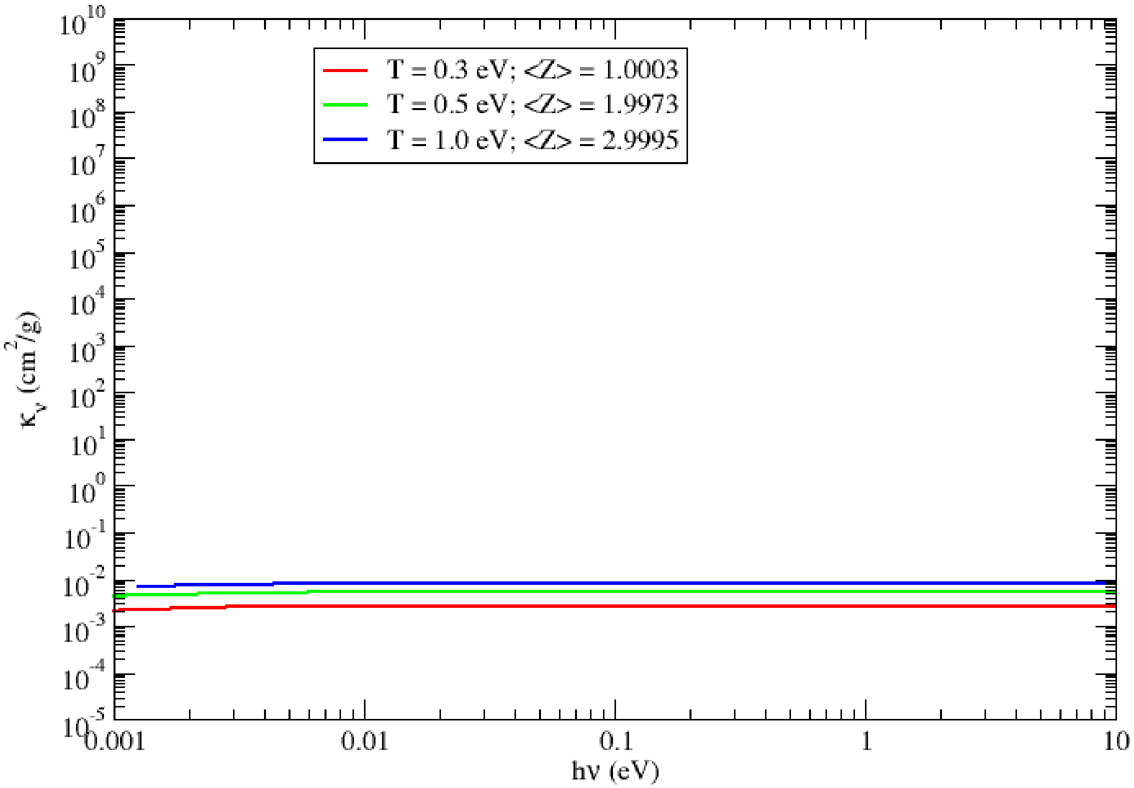


Sm (Z=62) LTE ionization balance
(ρ = 10^{-13} g/cm^3)



Consider opacity of Sm (Z=62) at T ~ 0.5 eV and $\rho = 10^{-13}$ g/cm^3

- A simple estimate of the opacity: assume Thomson/Compton scattering is the dominant mechanism
- Opacity ~ 0.4 <Z>/A (cm^2/g)
- Original light curve estimates were based on this simple approximation (e.g. Li & Paczyński 1998)

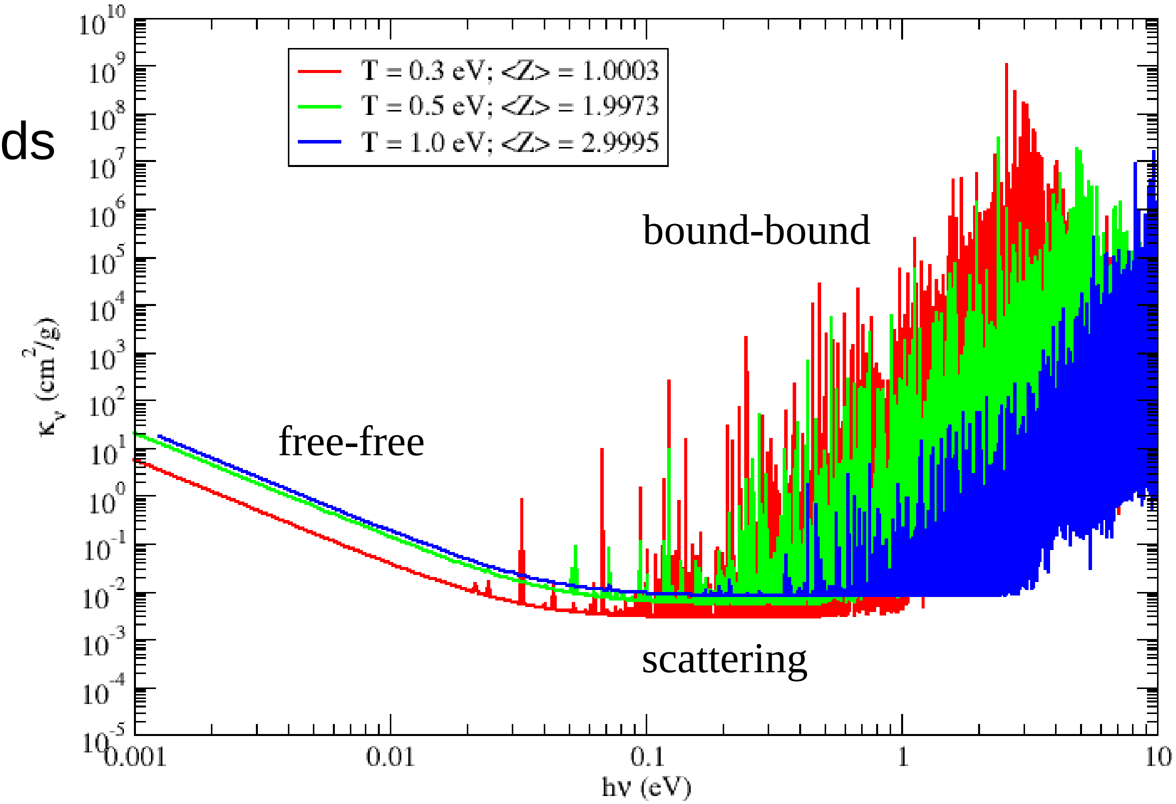


Consider opacity of Sm ($Z=62$) at $T \sim 0.5$ eV and $\rho = 10^{-13}$ g/cm^3 (configuration list, assume [Xe])

- 25 configurations
- Sm^{0+}: $4f^6\ 6s^2$, $4f^5\ 5d\ 6s^2$, $4f^6\ 5d\ 6s$, $4f^6\ 5d^2$, $4f^5\ 5d\ 6s\ 6p$, $4f^6\ 5d\ 6p$, $4f^6\ 6s\ 6p$
- Sm^{1+}: $4f^6\ 6s$, $4f^6\ 5d$, $4f^6\ 6p$, $4f^5\ 5d^2$, $4f^5\ 5d\ 6s$, $4f^5\ 5d\ 6p$, $4f^5\ 6s\ 6p$
- Sm^{2+}: $4f^6$, $4f^5\ 6s$, $4f^5\ 5d$, $4f^5\ 6p$, $4f^4\ 5d$, $4f^4\ 5d\ 6s$, $4f^3\ 5d^2\ 6s$
- Sm^{3+}: $4f^5$, $4f^4\ 6s$, $4f^4\ 5d$, $4f^4\ 6p$
- $\sim 10^5$ energy levels
- $\sim 3.3\times10^8$ radiative transitions

Consider opacity of Sm (Z=62) at T ~ 0.5 eV and $\rho = 10^{-13}$ g/cm^3

- Next, consider detailed bound-electron treatment
- Just 25 configurations leads to 100,000 levels and 330,000,000 lines!



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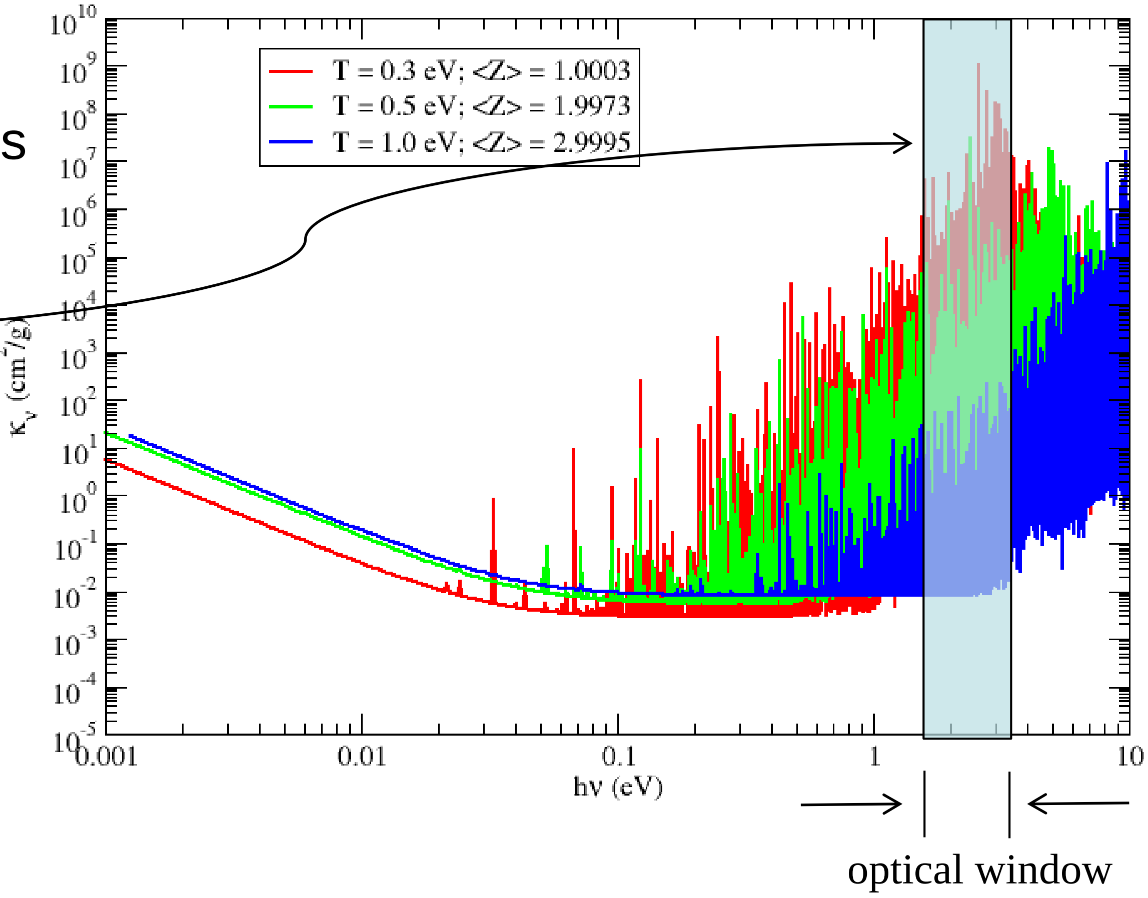
- Next, consider detailed bound-electron treatment
- Just 25 configurations leads to 100,000 levels and 330,000,000 lines!
- Visible photons have a low probability of escape ➔ infrared spectroscopy is required to see these objects



How to combine such detailed opacities with radiation transport?

- There are too many narrow lines to accurately resolve (w.r.t. photon energy) for a radiation transport calculation
- Recall the bound-bound opacity:

Line shape profile

$$\kappa_{\mathrm{bb}}(\nu) = \frac{\pi e^2}{4\pi\varepsilon_0 m_{\mathrm{e}} c} \sum_i N_i \left| f_i \right| L(\nu, \Delta\nu_i)$$

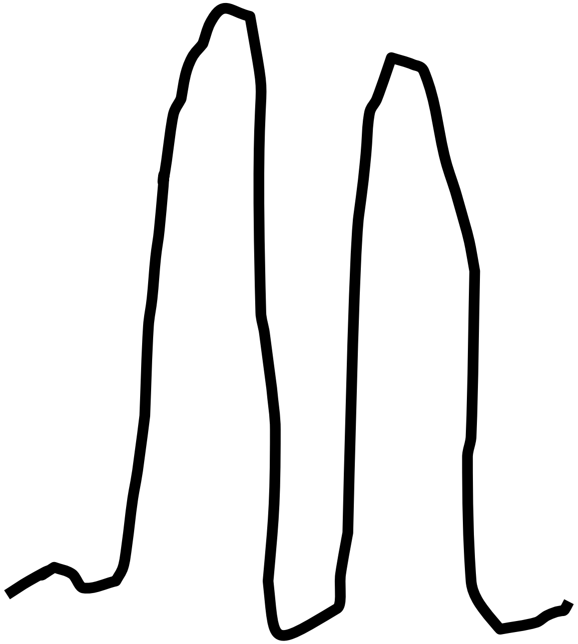
- Natural broadening is inherently narrow:

$$\Delta\nu_i = \frac{A_i}{2\pi}$$

- Doppler broadening becomes narrower as ν decreases:

$$\Delta\nu_i = \nu_i \left(\frac{2kT}{Mc^2} \right)^{1/2}$$

Effect of velocity gradients in expanding medium produces quasi-continuum opacity



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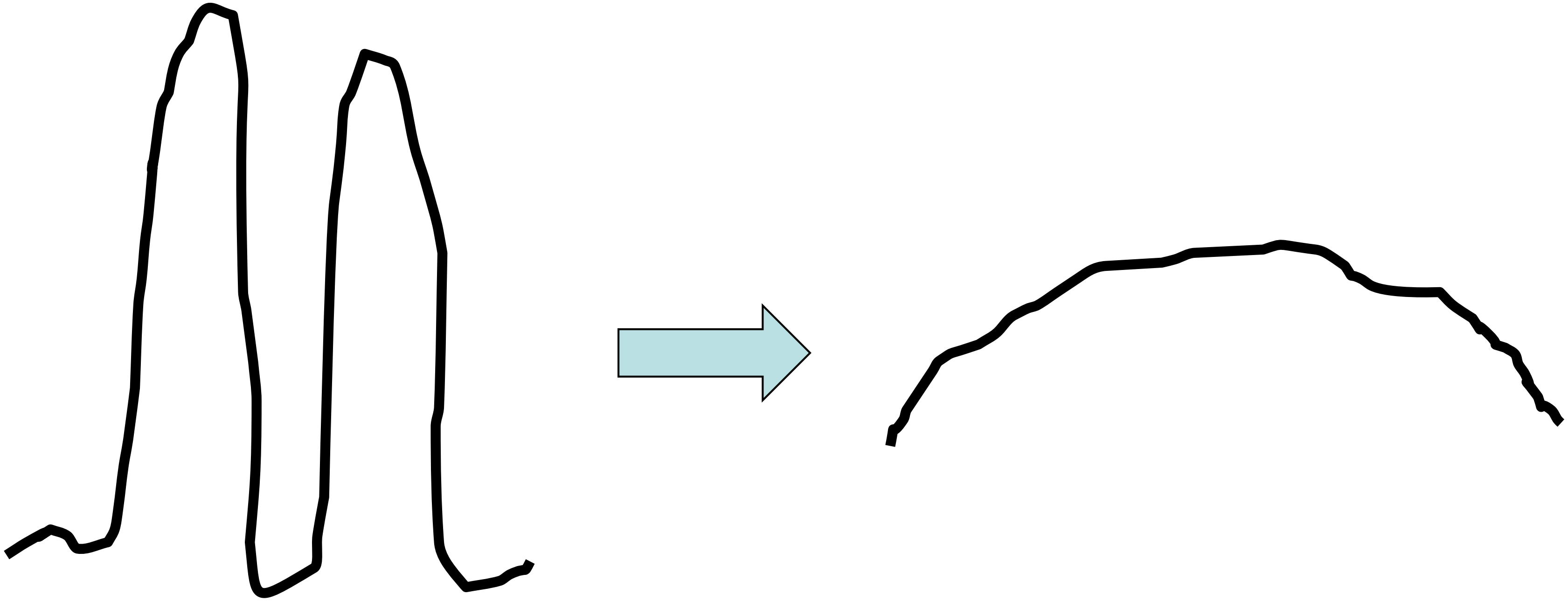


quasi-continuum opacity

Make an approximation based on the rapidly expanding ejecta

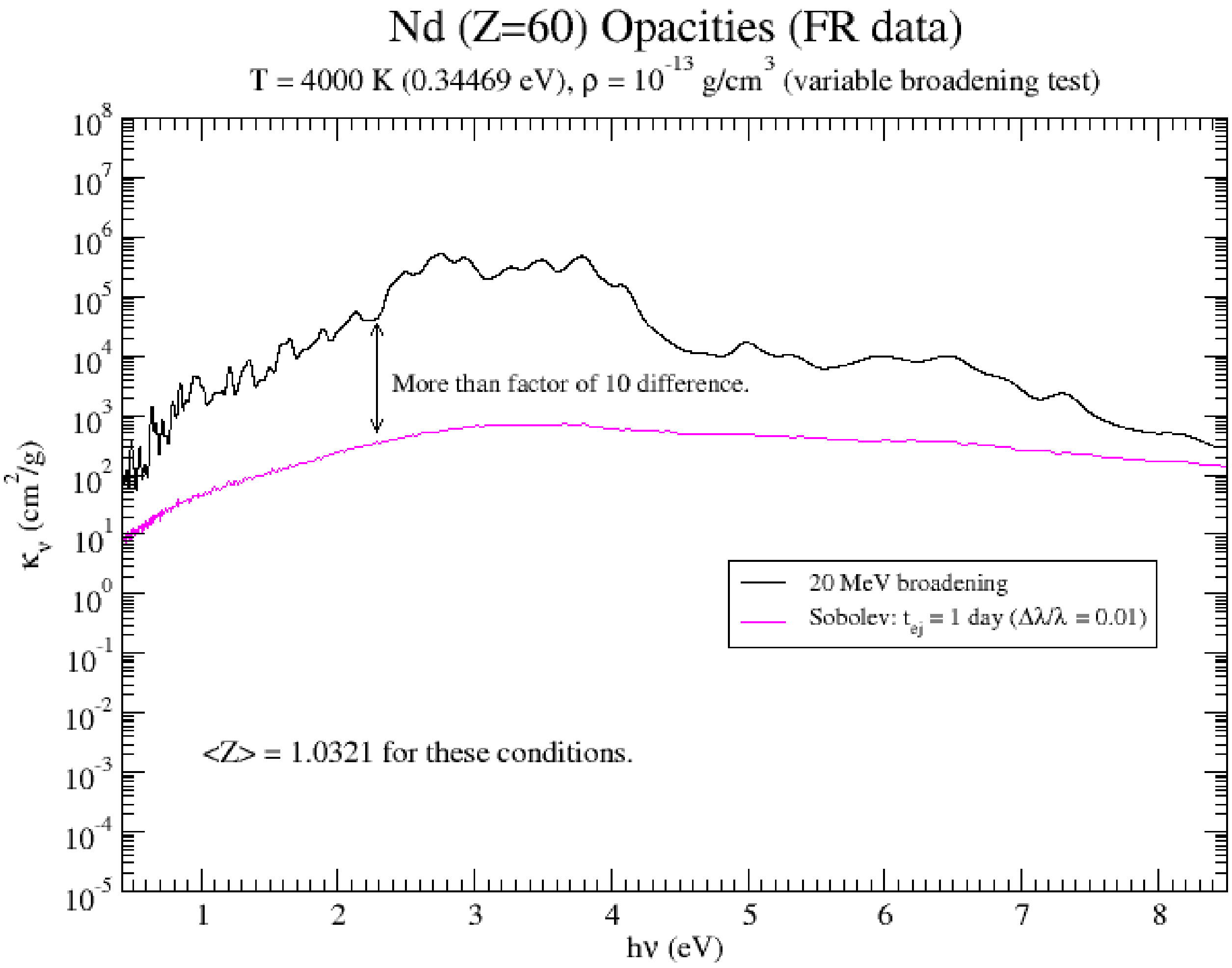
- Option 1: traditional **expansion opacity** (based on Sobolev)
  - Simply sum all lines in a given wavelength bin
  - Fast and easy; assumes reduction in line opacity
  - Recently applied to NSMs (Kasen, Badnell, Barnes, ApJ 2013)

$$\kappa_{\mathrm{bb}}^{\mathrm{exp}}(\Delta\nu_{\mathrm{bin}}) = \frac{1}{\rho c t_{\mathrm{eject}}} \sum_i \frac{\nu_i}{\Delta\nu_{\mathrm{bin}}}(1 - e^{-\tau_i})$$

- Option 2: Explore ***line smearing*** using effective temperature
  - Apply a profile to every line that preserves area under curve
  - Requires ~10^3 more time to calculate than Sobolev method
  - Assumes full strength of line opacity

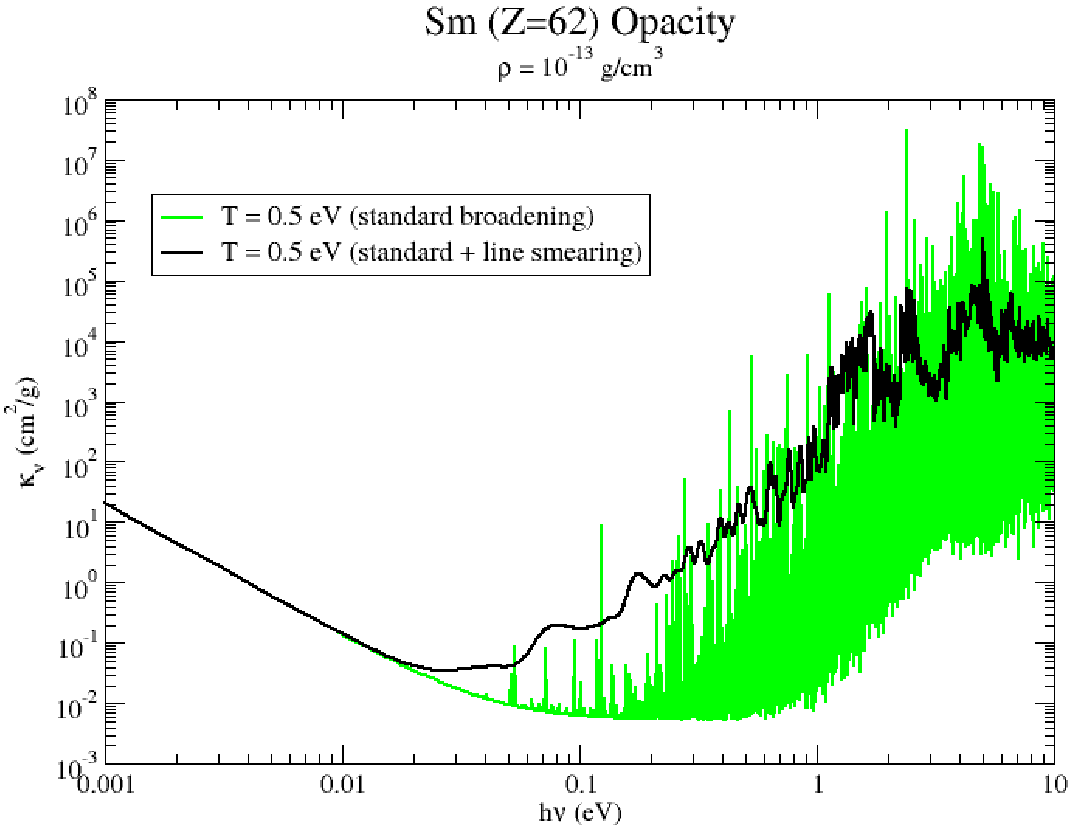
$$\kappa_{\mathrm{bb}}^{ls}(\nu) = \frac{\pi e^2}{4\pi\varepsilon_0 m_{\mathrm{e}} c} \sum_i N_i \left|f_i\right| L(\nu, \Delta\nu_i);\ \ \Delta\nu_i = \nu_i \left(\frac{2kT_{ls}}{Mc^2}\right)^{1/2}$$

Sobolev vs line-smeared opacity [Nd (Z=60) example]



Returning to Sm (Z=62) at T ~ 0.5 eV and ρ = 10^{-13} g/cm^3

- We investigate the limiting case of using the *full opacity* for determining which photons will escape the ejecta, using line-smeared opacities
- Assume a line smearing consistent with resolution allowed by spatial zone size
- Velocity change across a typical zone is ($\Delta v/c$) ~ 0.01, which can be used to obtain the effective line-smearing temperature



Fontes et al HEDP (2015); arXiv:1702.02990 (2016)

$$\frac{\Delta v}{c} = \frac{\Delta \nu}{\nu_i} = \left(\frac{2kT_{ls}}{Mc^2}\right)^{1/2} \Rightarrow T_{ls} \approx 20 \text{ MeV}$$

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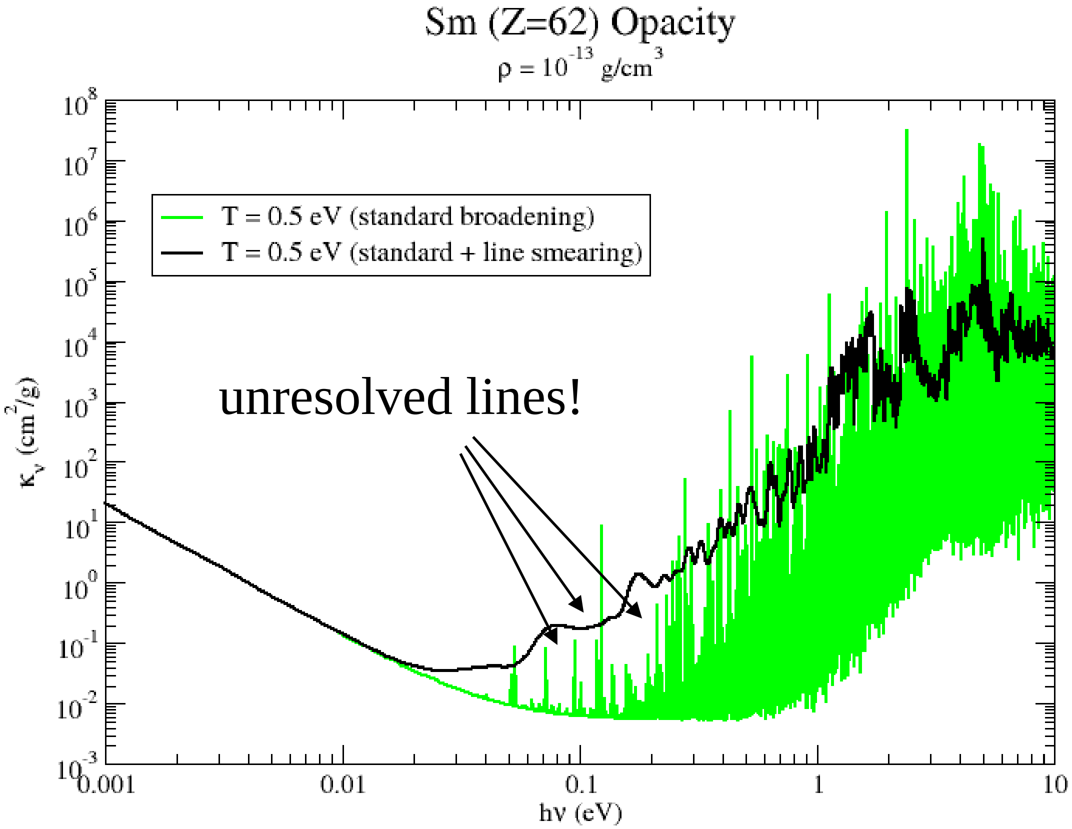

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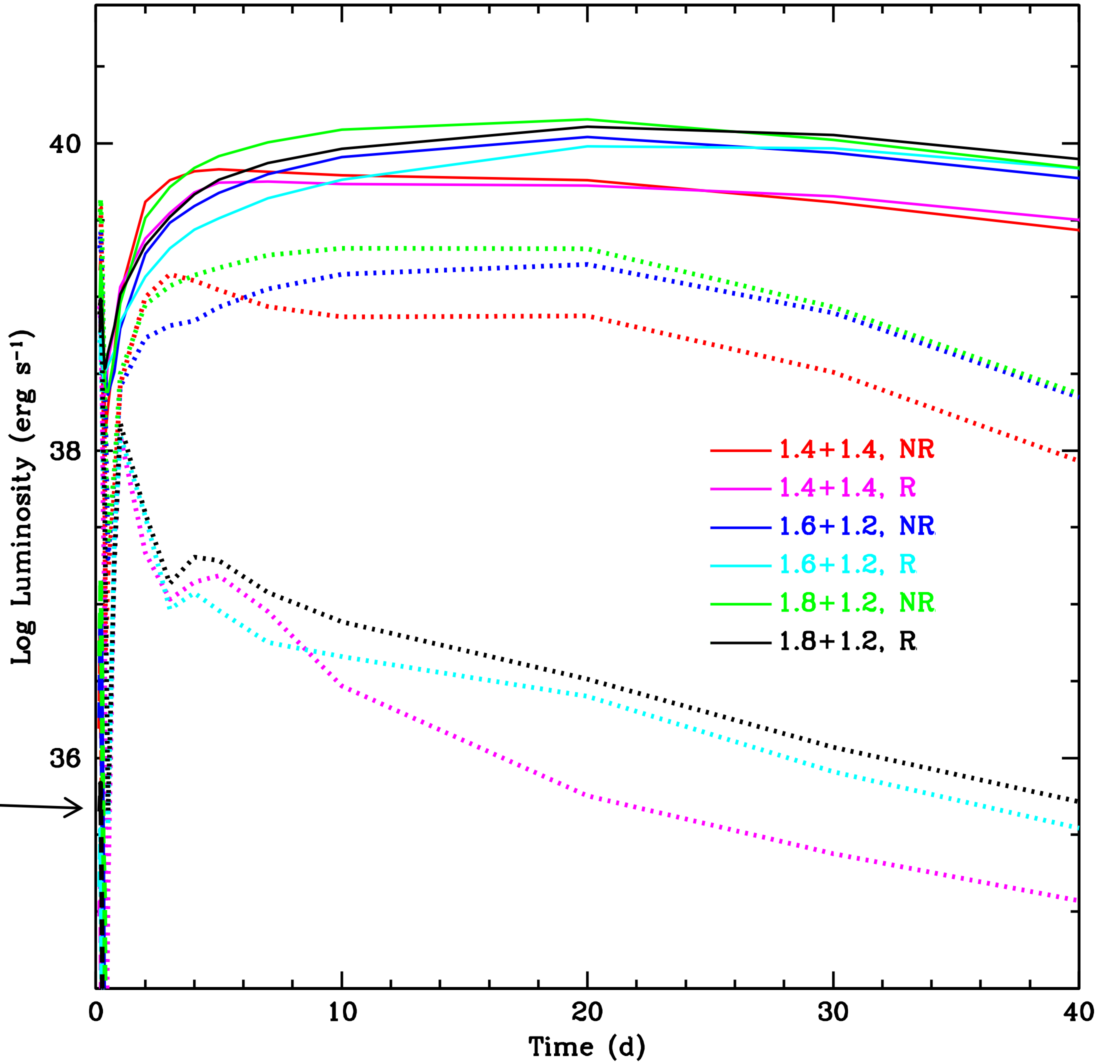
Light curves for 3 different neutron star systems (R=relativistic, NR=semi-relativistic)



Infrared band (most intense, longest duration, easiest to observe)

Near-infrared band

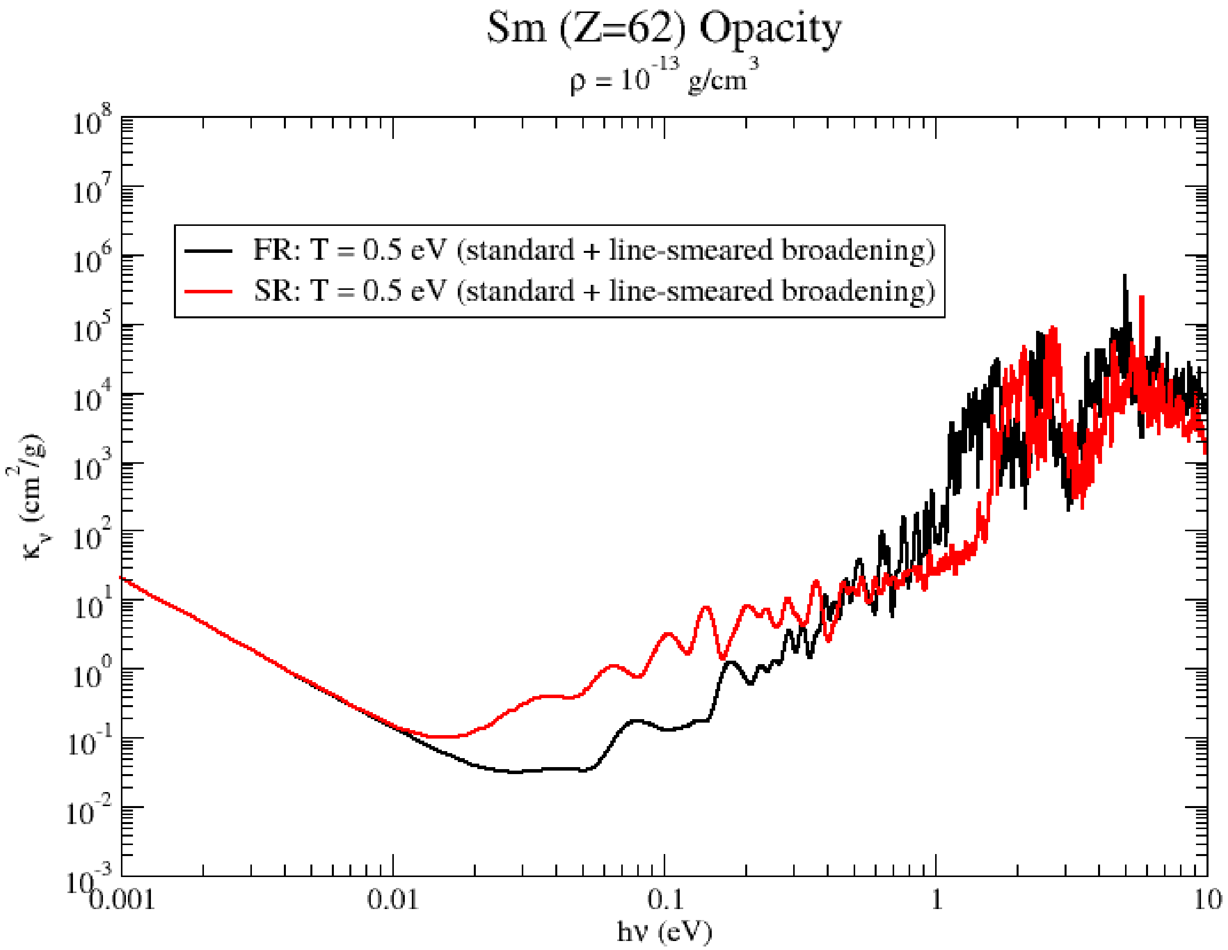
Optical band

Fontes et al, arXiv: 1702.02990 (2016)

Atomic structure considerations

- There are a variety of atomic structure codes that are available to calculate energies and radiative transition probabilities (Einstein A coefficients or oscillator strengths)
- The LANL Suite has both semi- and fully relativistic options, based on solutions of the Schrödinger and Dirac equations, respectively
- Other structure codes that are generally available include AUTOSTRUCTURE, HULLAC, FAC, MCHF and GRASP
- A more accurate path to calculating cold r-process atomic data could be the many-body perturbation theory (MBPT) approach, e.g. I. Savukov, JPB **50**, 165001 (2017)

Semi- and fully relativistic calculations can produce different opacity features…



Versatility of the LANL Suite

- The LANL Suite has been used to calculate opacity data for a broader range of elements for simulating electromagnetic signatures of NSMs
- Current list of elements: Cr, Pd, Se, Te, Br, Zr, Sm, Ce, Nd, U
- See Wollaeger, Korobkin, et al, arXiv:1705.07084 (2017) for more detailed study of ejecta morphology and composition on electromagnetic signatures of NSMs

Summary

- Opacity is typically calculated from first principles, based on fundamental (microscopic) atomic physics theory
- The calculation of accurate atomic data for cold lanthanide and actinide elements is very challenging; this is a possible topic of future exploration
- The use of these opacities in rad-hydro simulations to model macronovae is complicated by the detailed line structure of these elements and LTE vs non-LTE conditions
- The assumption of line-smeared opacities produces macronovae that peak in the mid-IR, with slightly lower luminosities compared to light curves produced with the traditional expansion-opacity approach