Atomic Cross Section Calculations: The Distorted-Wave Method

Christopher Fontes
Computational Physics Division (XCP-5)
Los Alamos National Laboratory

21st Meeting on Atomic Processes in Plasmas

Vienna, Austria

May 15-19, 2023

Atomic Cross Section Calculations: The Distorted-Wave Method (Where are the resonances?)

Christopher Fontes
Computational Physics Division (XCP-5)
Los Alamos National Laboratory

21st Meeting on Atomic Processes in Plasmas

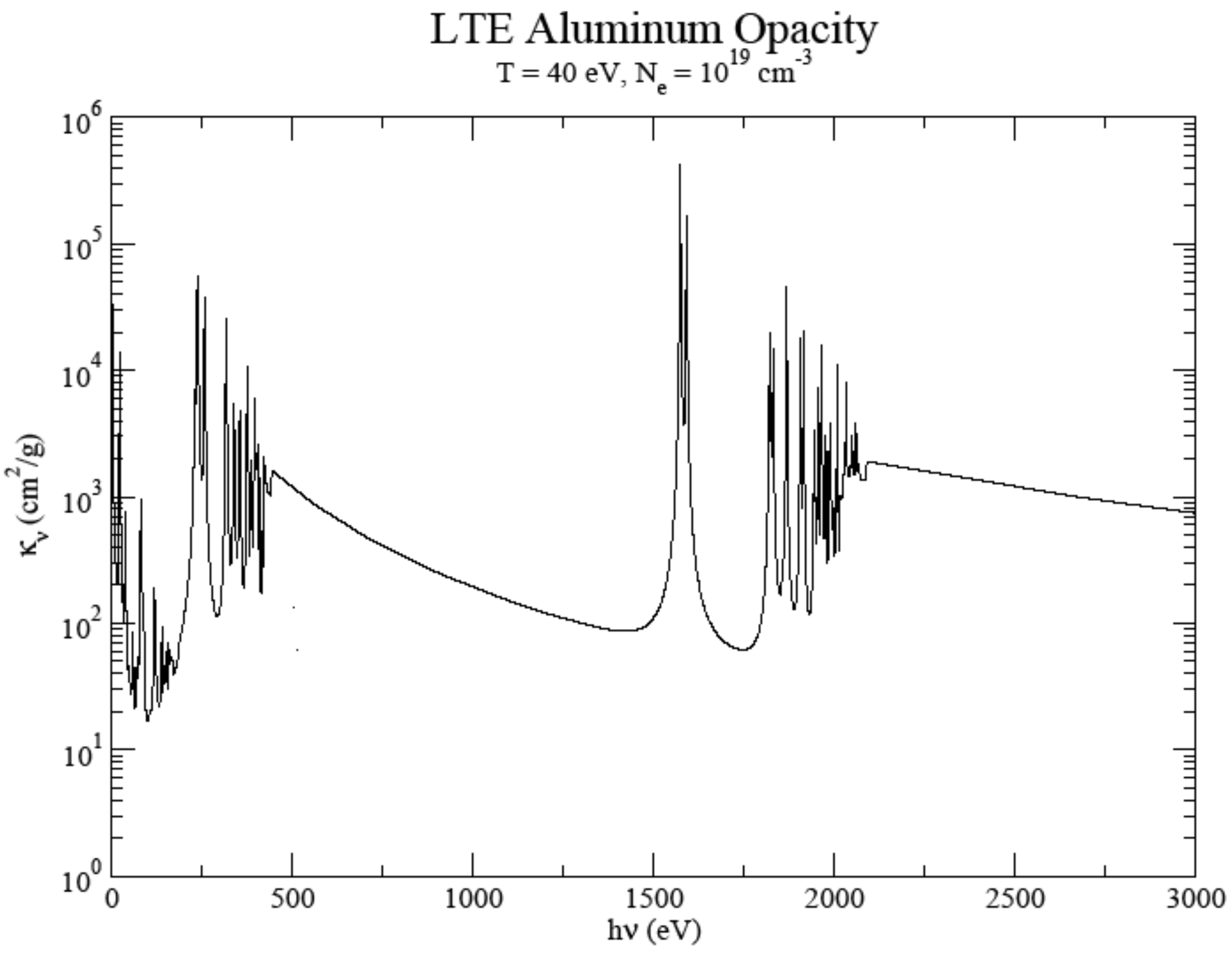
Vienna, Austria

May 15-19, 2023

Overview

- In this talk, I will discuss the connection between distorted-wave (DW) and R-matrix (RM) cross sections
- I will only consider the process of photoionization (PI), but the same basic concepts also apply to electron-impact excitation (EIE) and electron-impact ionization (EII)
- Shocking statement #1: Rather than start at “the beginning” (microscopic scale), I will start at the end (macroscopic scale) with opacities
- Shocking statement #2: I will not actually explain how to calculate DW cross sections (the basic concepts are the same as what you heard in the previous talk)!!!

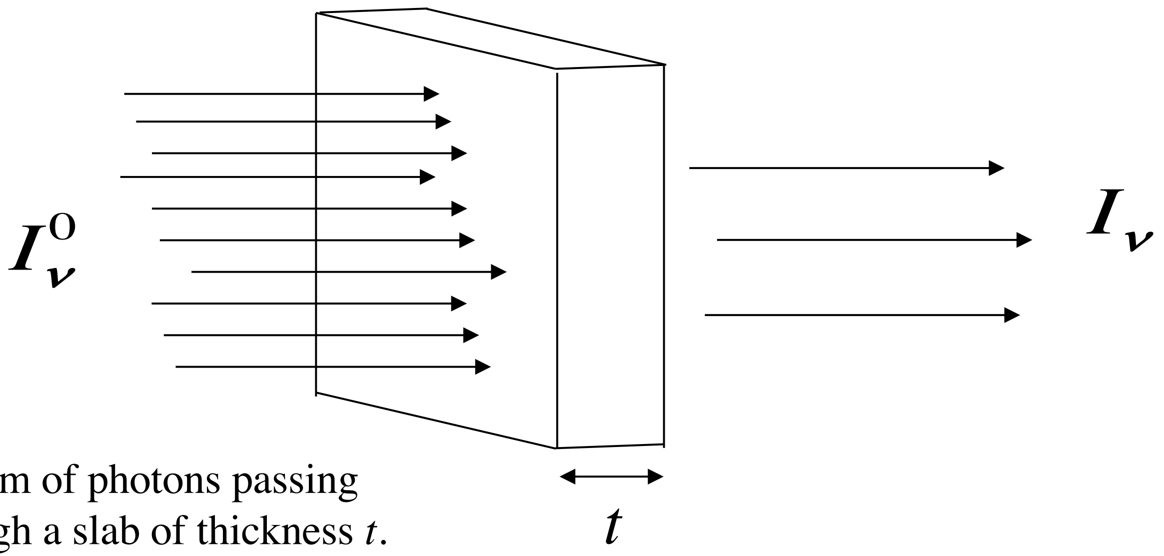
A random opacity: an (LTE) aluminum plasma at a particular temperature and density...



Los Alamos OPLIB database: https://aphysics2.lanl.gov/opacity

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.

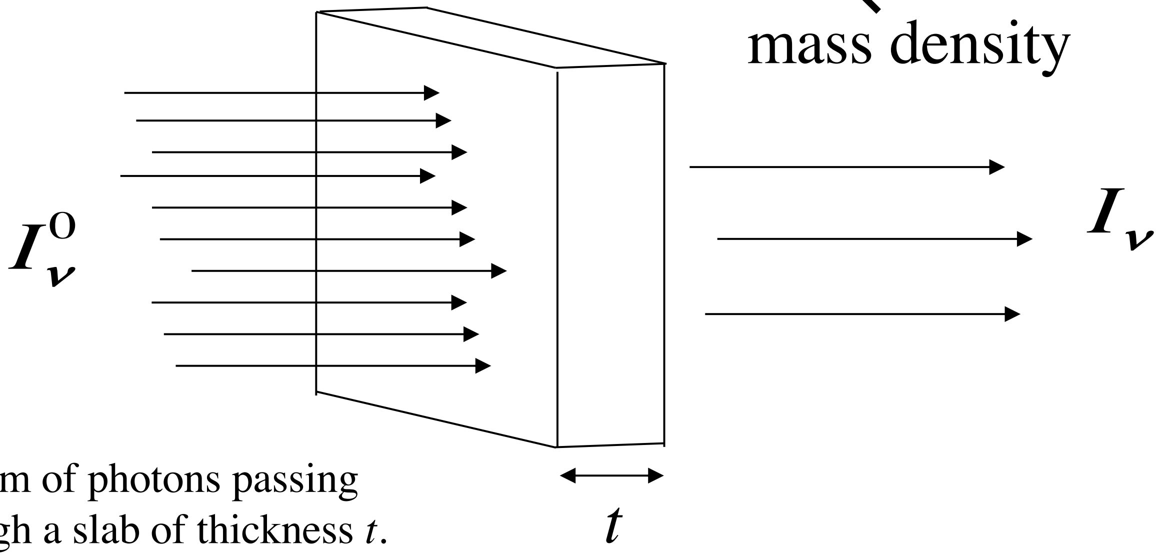
A useful illustration:
The classic opacity (transmission) experiment:

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

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

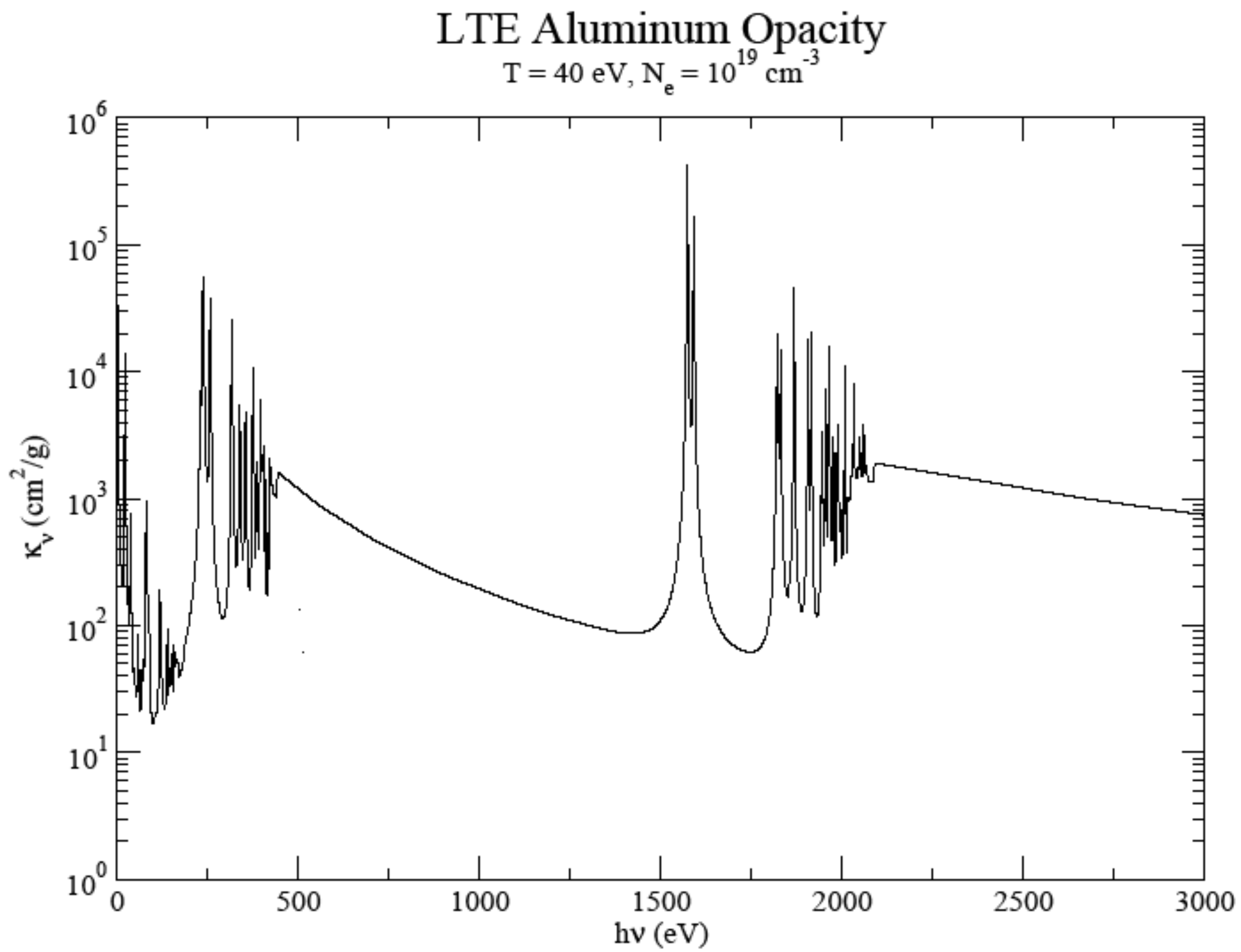
opacity

mass density



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

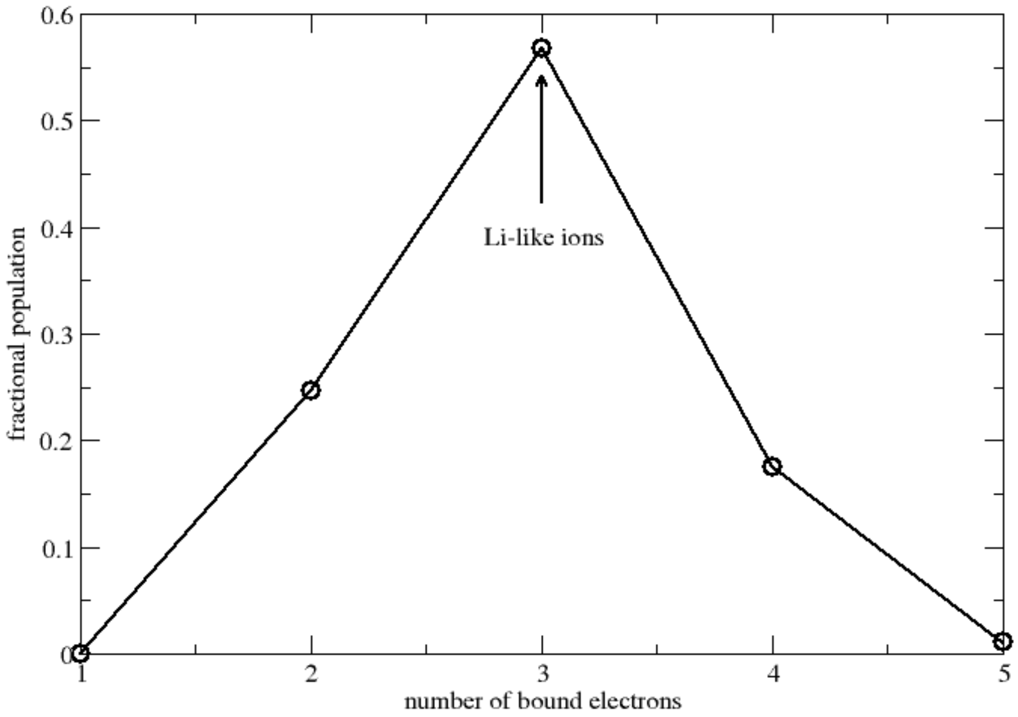
A random opacity: an (LTE) aluminum plasma at a particular temperature and density...

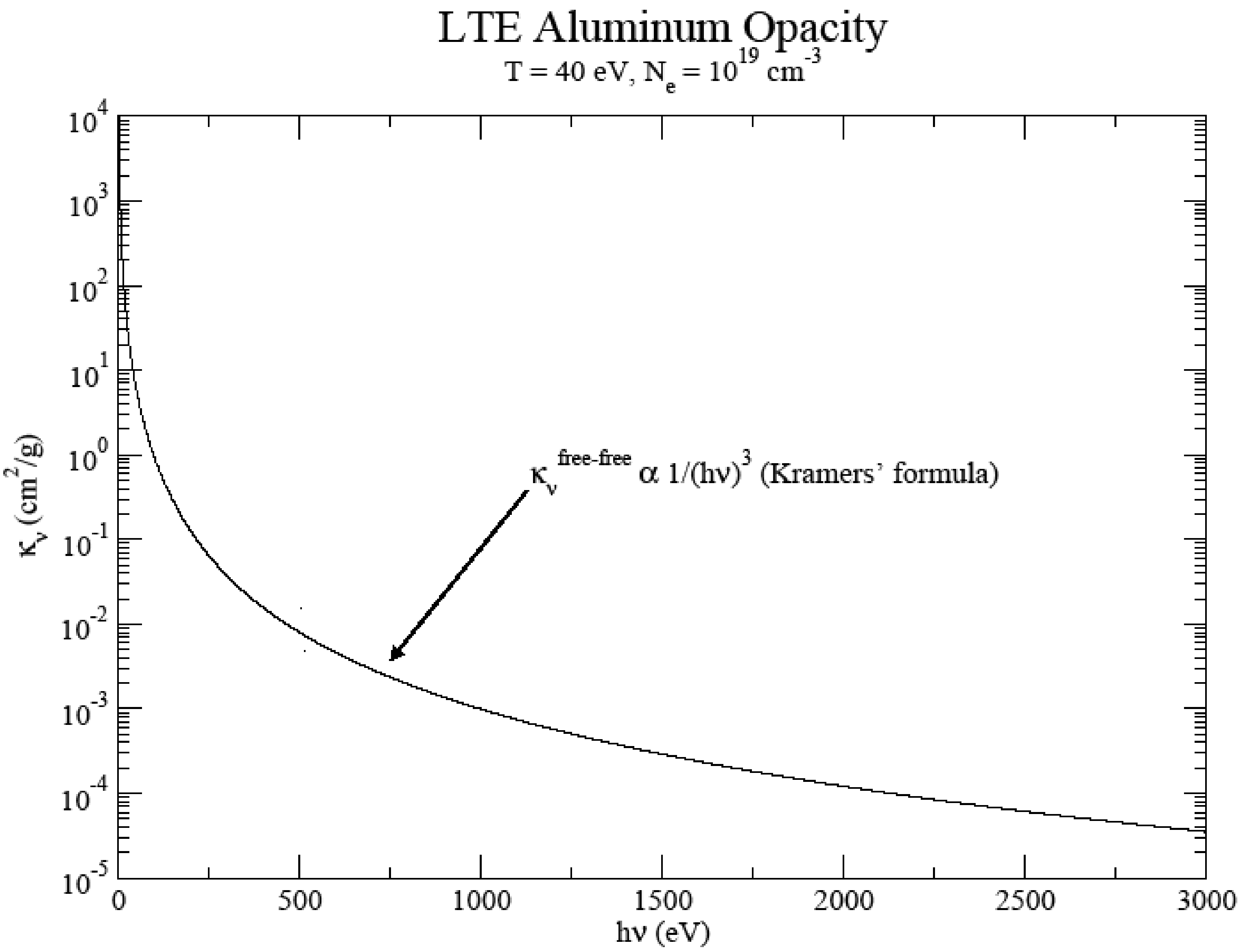


Los Alamos OPLIB database: https://aphysics2.lanl.gov/opacity

Numerical example of an LTE opacity: Aluminum plasma at kT = 40 eV, $N_e = 10^{19} cm^{-3}$

- For these conditions, <Z>=10.05 ⇒ there is an average of ~2.95 bound electrons/ion (Li-like ions are dominant)
- Here is the charge state distribution:





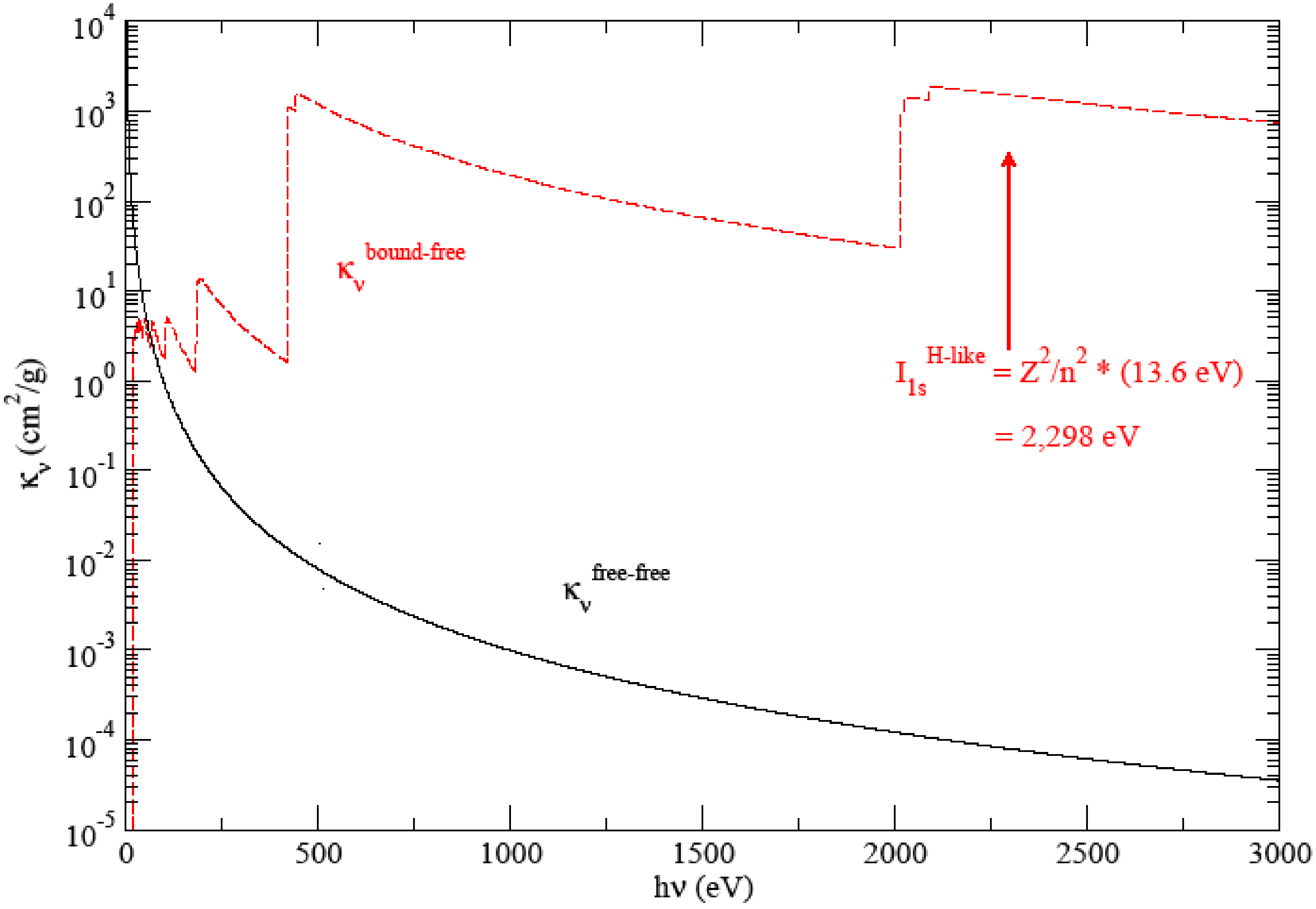
LTE Aluminum Opacity

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

$\kappa_\nu^{\text{free-free}}$ α $1/(h\nu)^3$ (Kramers' formula)

LTE Aluminum Opacity

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

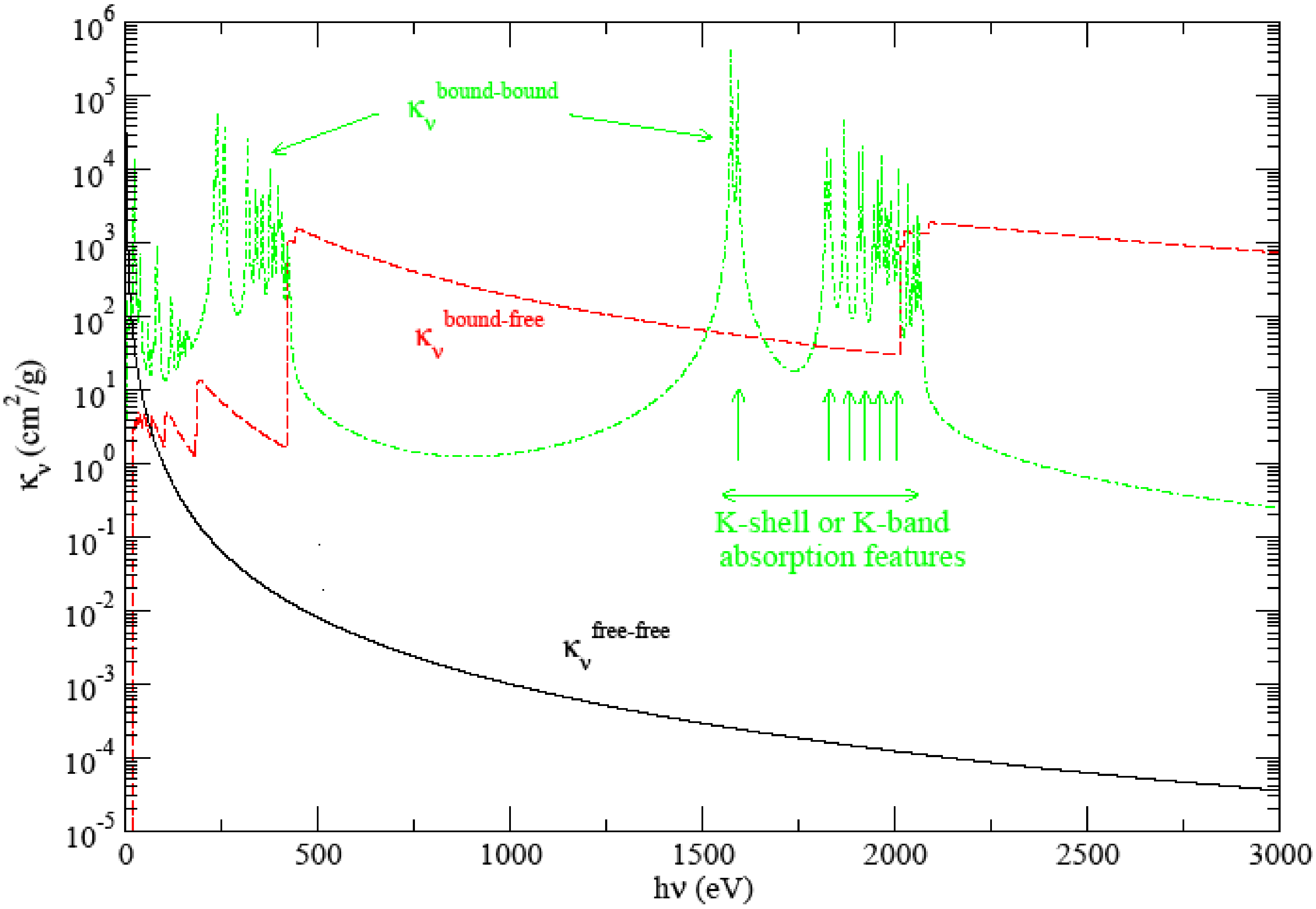


$I_{1s}^{\text{H-like}} = Z^2/n^2 * (13.6\text{ eV})$

$= 2{,}298$ eV

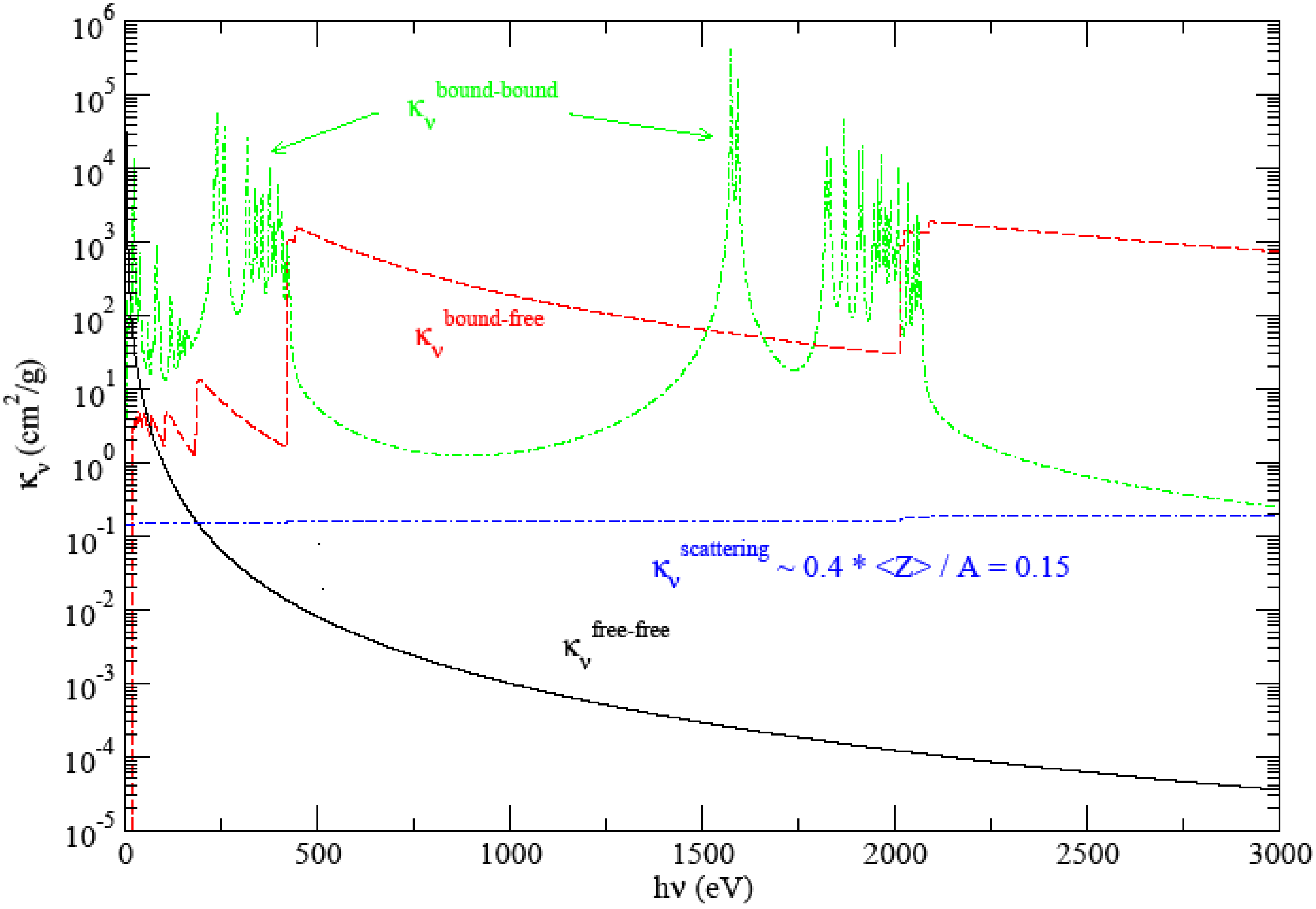
LTE Aluminum Opacity

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



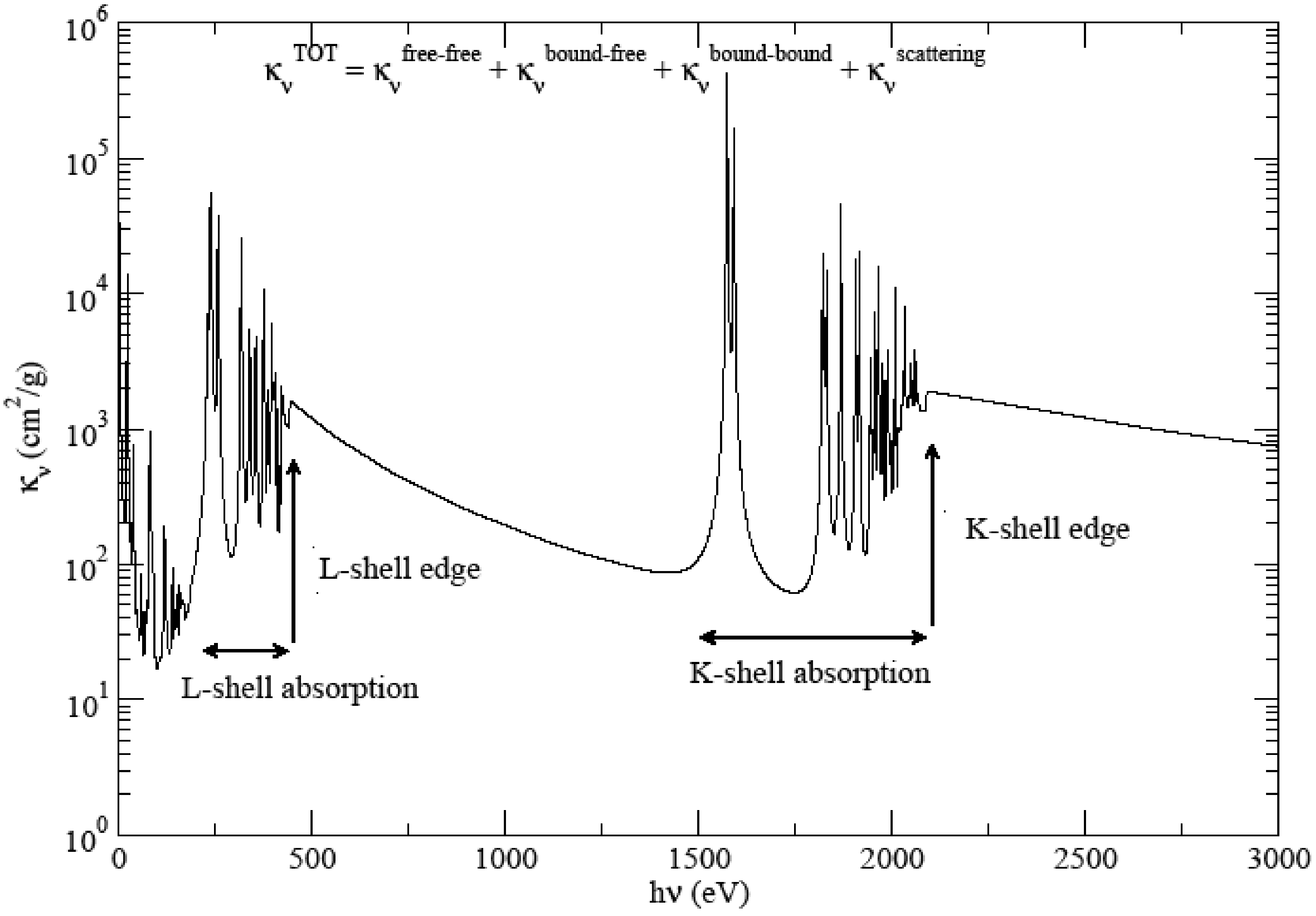
LTE Aluminum Opacity

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



LTE Aluminum Opacity

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



$$\kappa_\nu^{TOT} = \kappa_\nu^{free\text{-}free} + \kappa_\nu^{bound\text{-}free} + \kappa_\nu^{bound\text{-}bound} + \kappa_\nu^{scattering}$$

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 here)

- 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)

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

Compton scattering

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

material density

atomic level populations

photoexcitation cross sections

photoionization cross sections

inverse Bremsstrahlung contribution

How to compare a DW cross section with an RM cross section? Bookkeeping!

For a given initial level (l), you take all of the bound-free contribution and some parts of the bound-bound contribution, i.e. you take the parts that photo-excite to an AI level.

Take part of this.

Take all of this.

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

material density

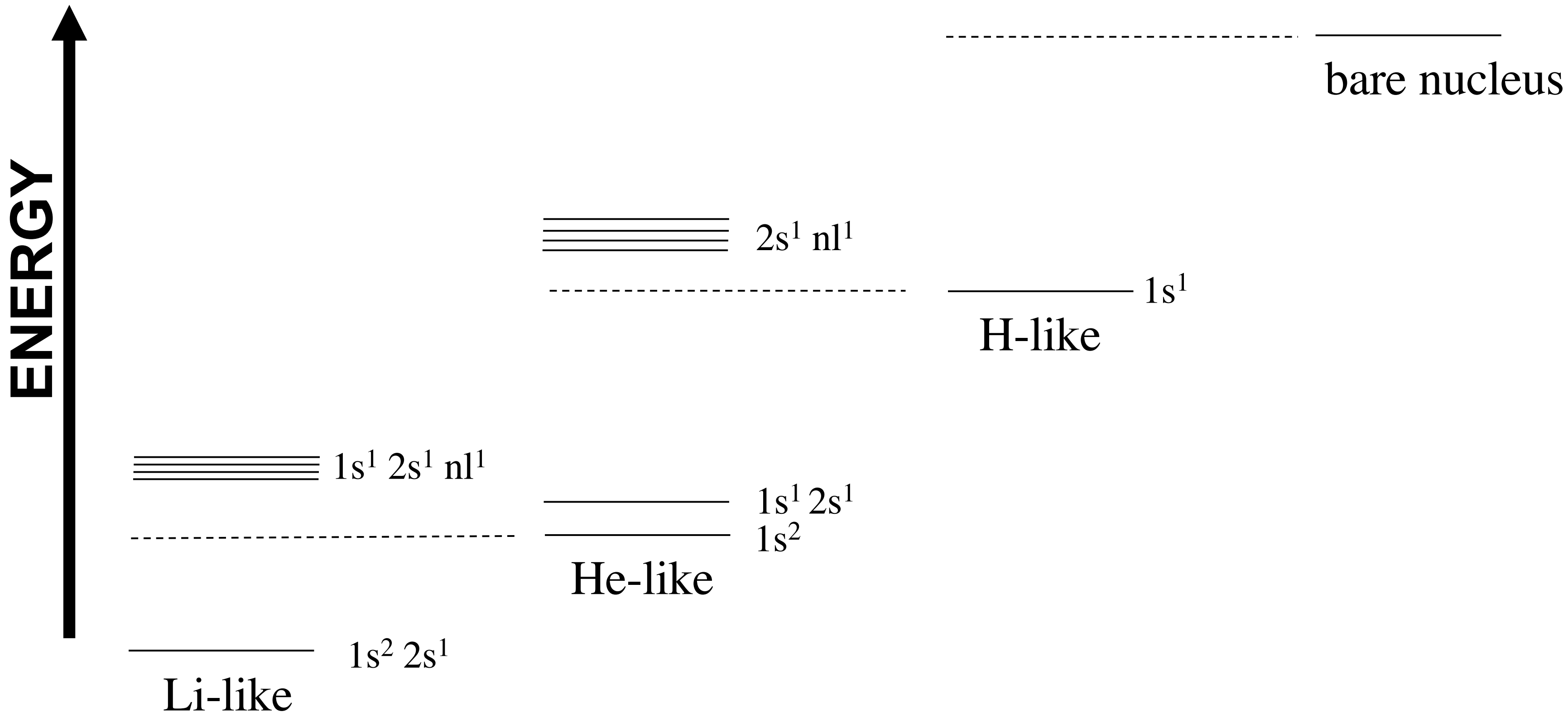
atomic level populations

photoexcitation cross sections

photoionization cross sections

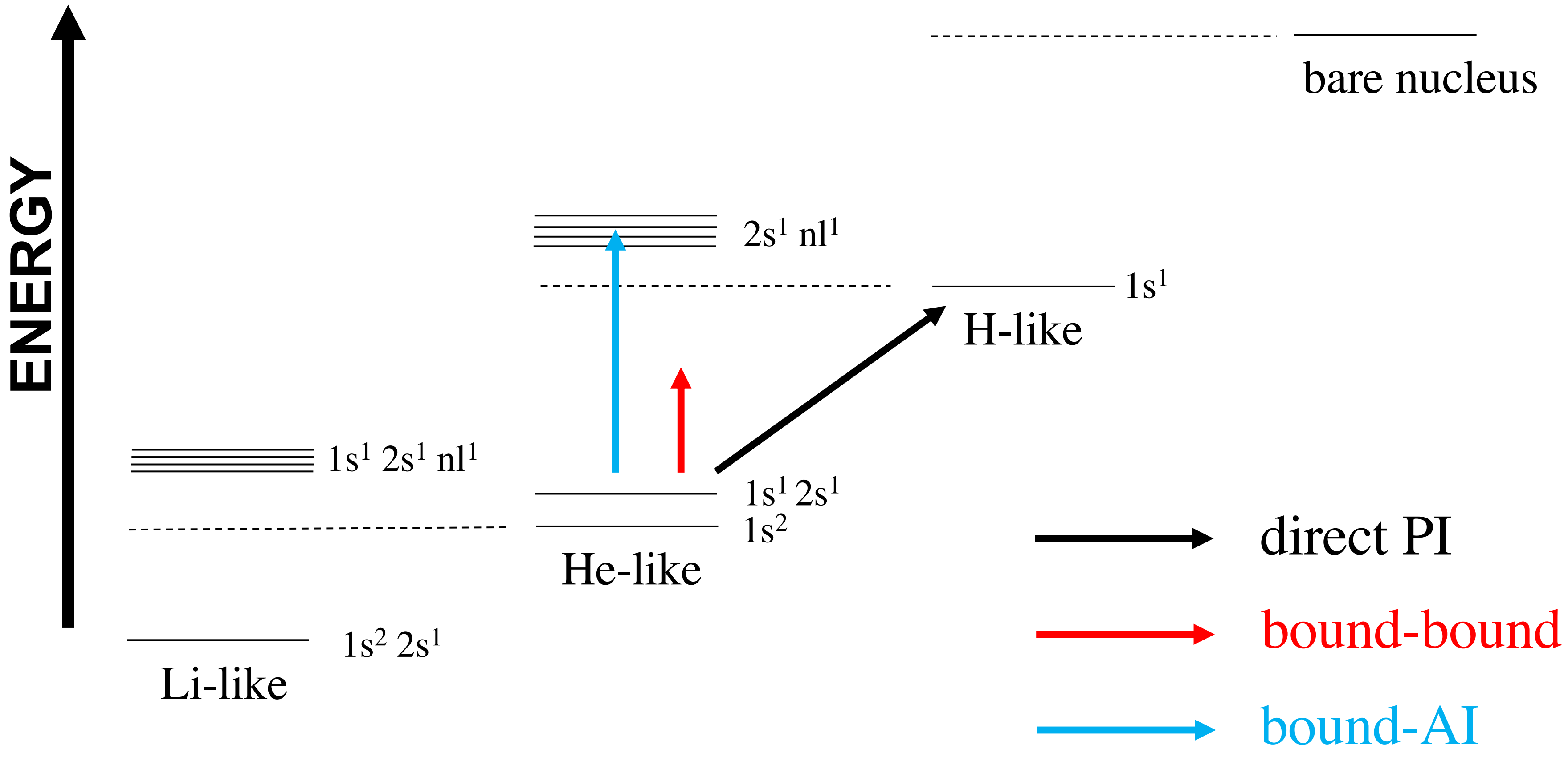
inverse Bremsstrahlung contribution

An illustrative energy level diagram (not drawn to scale)



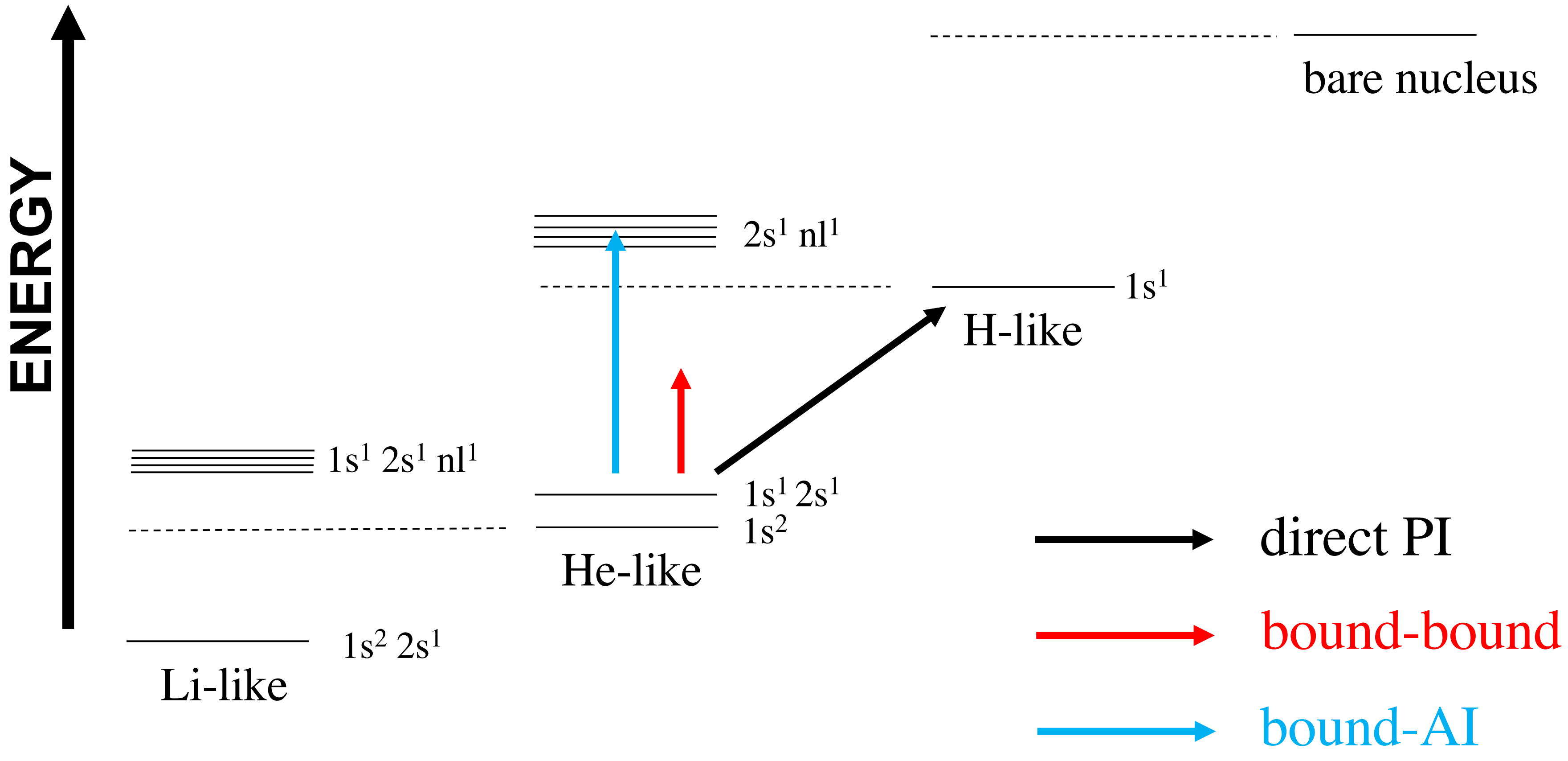
Consider photoionization from the 1s2s $^3S_1$ level of He-like Fe (Fe XXV)

$h\nu + 1s2s\ ^3S_1 \rightarrow 1s + e^-$ (DW PI language)



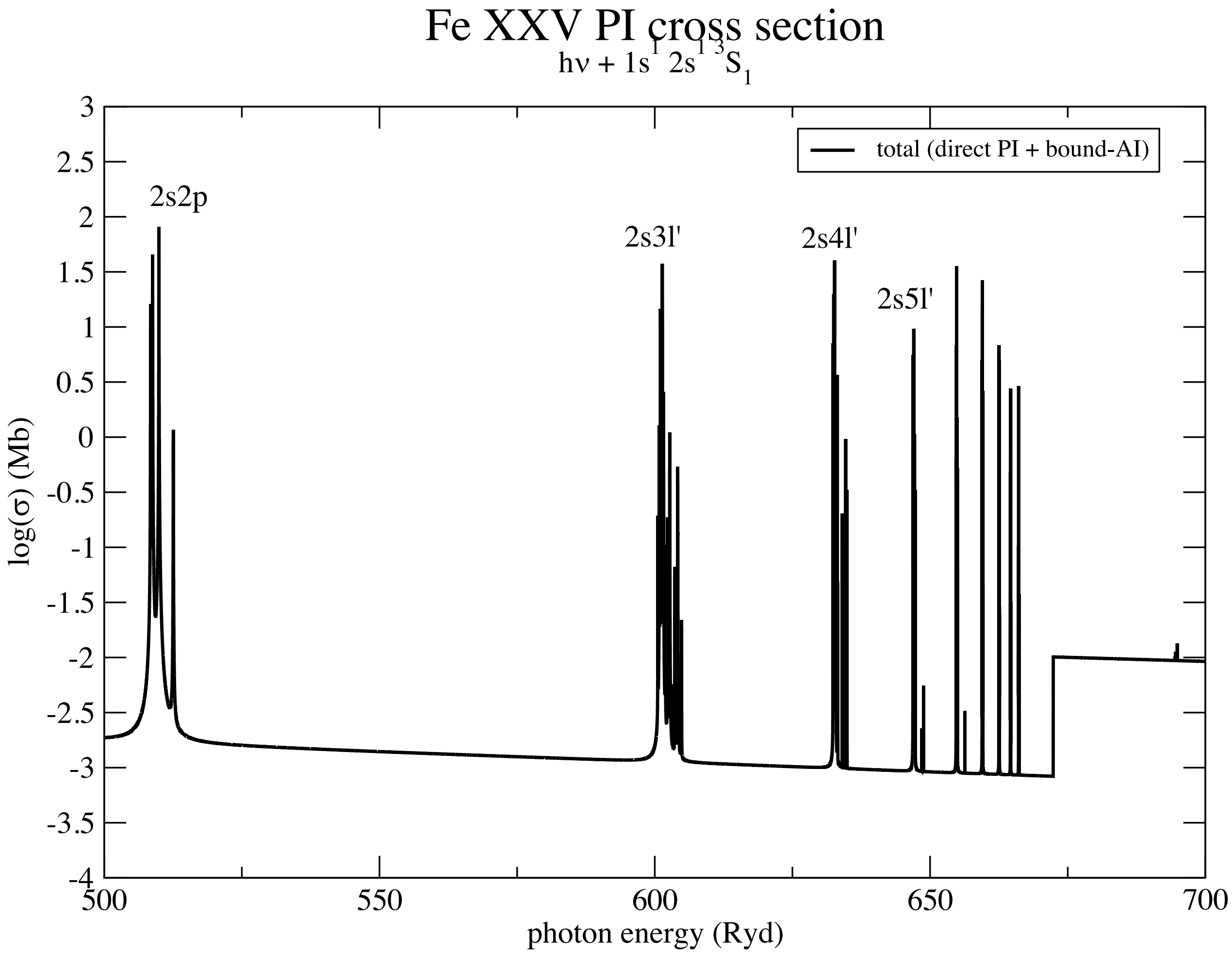
Consider photoionization from the 1s2s $^3S_1$ level of He-like Fe (Fe XXV)

$h\nu + 1s2s\ ^3S_1 \rightarrow 1s + e^-$ (DW PI language)



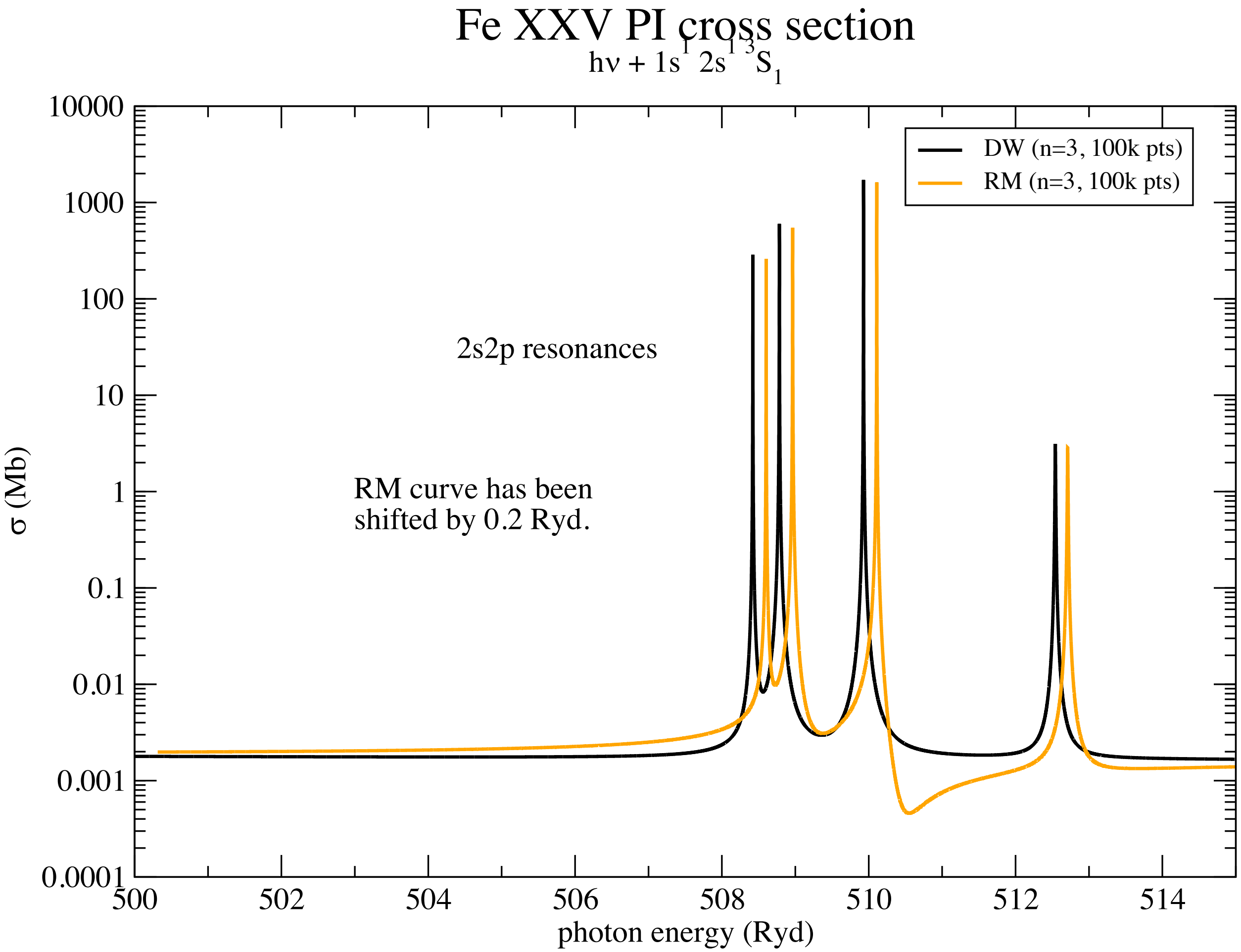
direct PI + bound-AI corresponds to RM PI

Compare DW vs RM PI cross section in a consistent (bookkeeping) manner: DW result

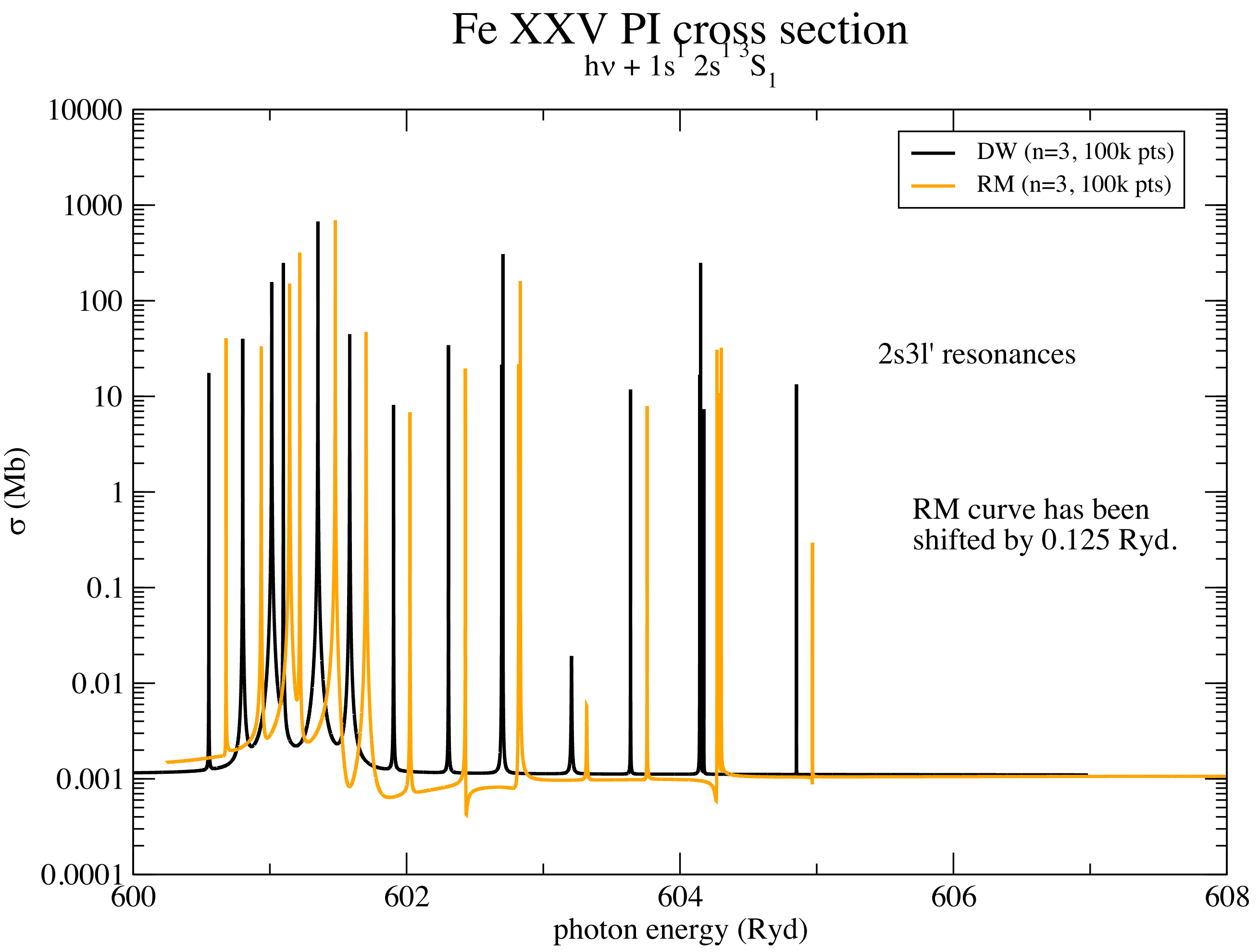


DW calculations: LANL Suite of Atomic Physics Codes;
Fontes et al, JPB 48, 144014 (2015)

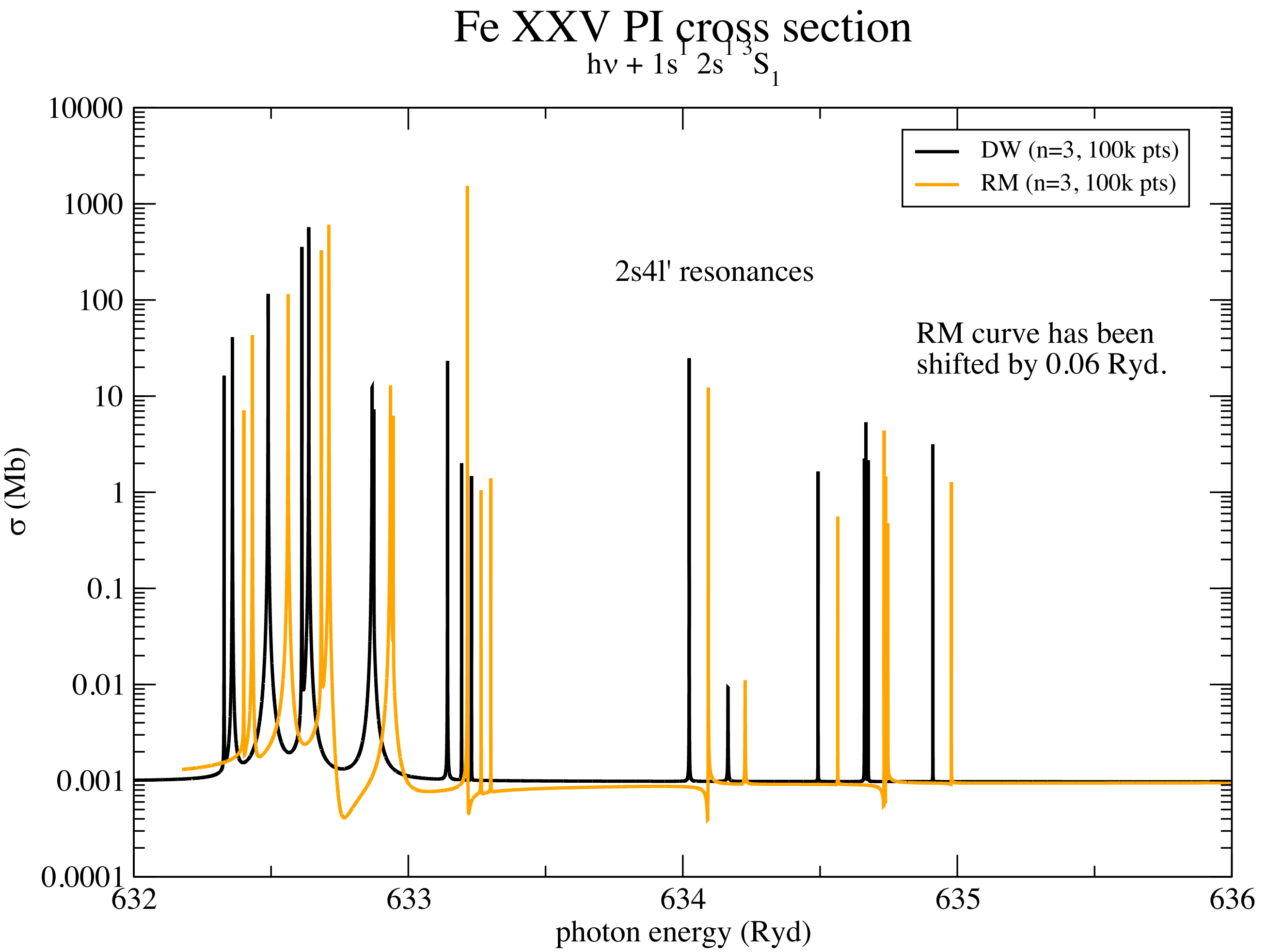
Compare DW vs RM PI cross section: zoom in on 2s2p resonance region



Compare DW vs RM PI cross section: zoom in on 2s3l’ resonance region



Compare DW vs RM PI cross section: zoom in on 2s4l' resonance region



An important conclusion

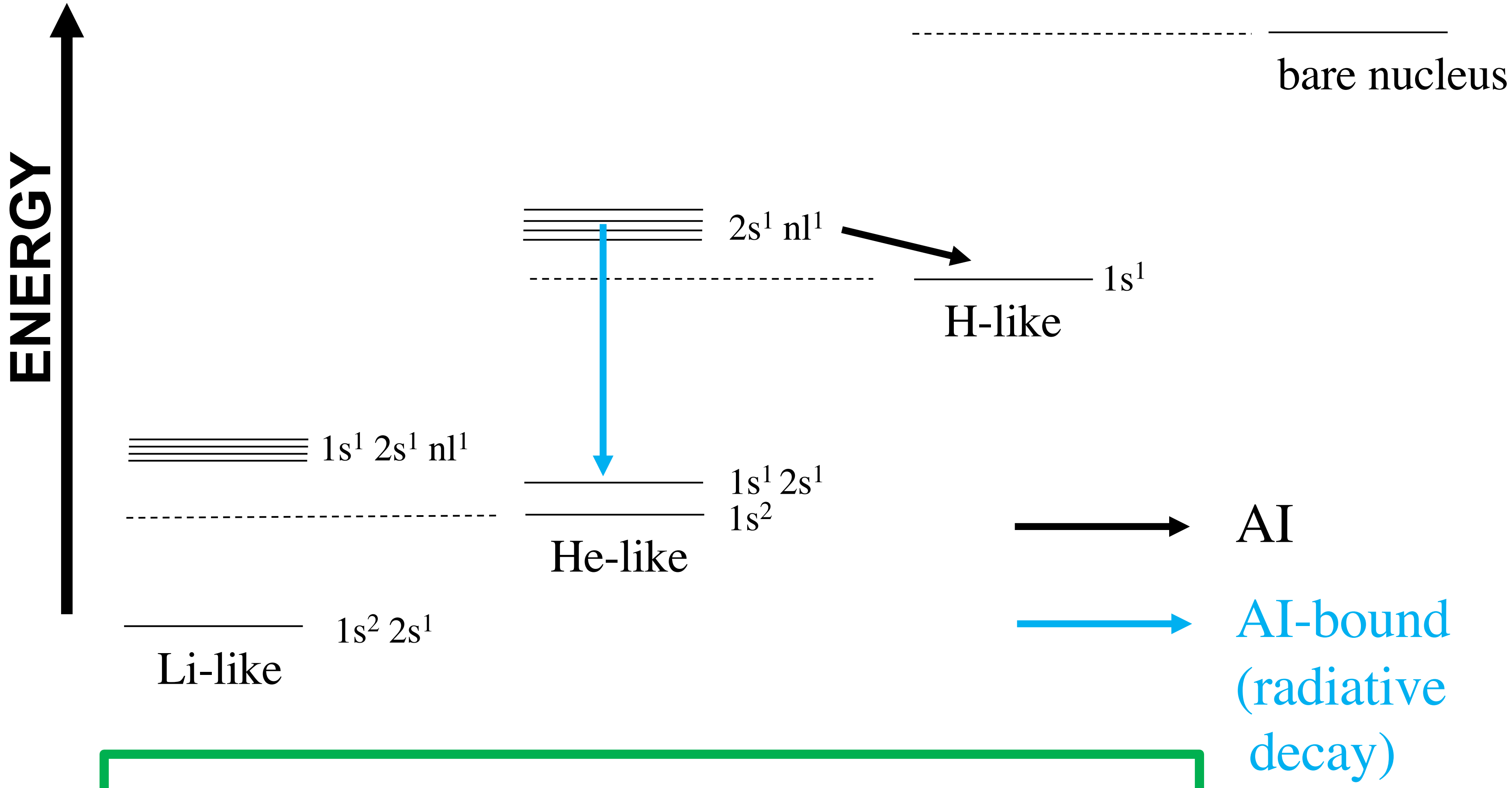
- For highly charged ions, the DW and RM methods produce very similar cross sections if you are consistent in the two calculations, e.g. if you include the same atomic structure, with the same AI levels/resonances
- A similar conclusion was reached in a recent paper by F. Delahaye, C.P. Balance, R.T. Smyth, and N.R. Badnell, MNRAS 508, 421 (2021) for opacities calculated with the DW and RM methods for Fe XVII

Something important that I don’t have time to discuss in detail: branching ratios

- If you care about the production of a photo-electron from the AI levels, i.e. true “resonances” to the photoionization process, then you need to take into account the probability that an AI level will radiative decay versus autoionize → branching ratios = AI / (AI + radiative decay)

Consider photoionization from the 1s2s $^3S_1$ level of He-like Fe (Fe XXV): branching ratios

$h\nu + 1s2s\ ^3S_1 \rightarrow 1s + e^-$ (DW PI language)



ENERGY

bare nucleus

$2s^1\ nl^1$

$1s^1$

H-like

$1s^1\ 2s^1\ nl^1$

$1s^1\ 2s^1$

$1s^2$

He-like

$1s^2\ 2s^1$

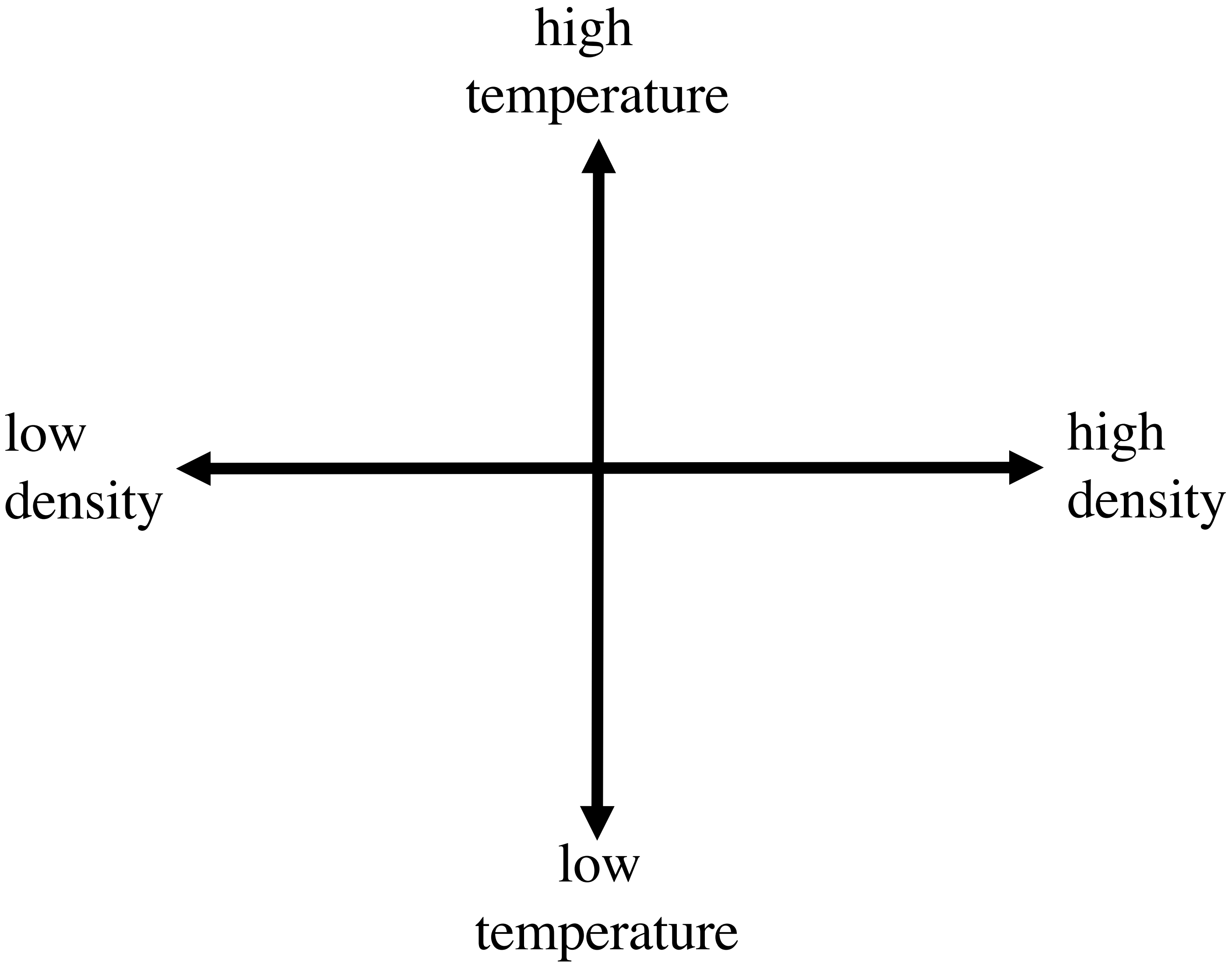
Li-like

AI

AI-bound (radiative decay)

Need branching ratio for AI vs radiative decay

Some basic guidelines for DW and RM cross section calculations



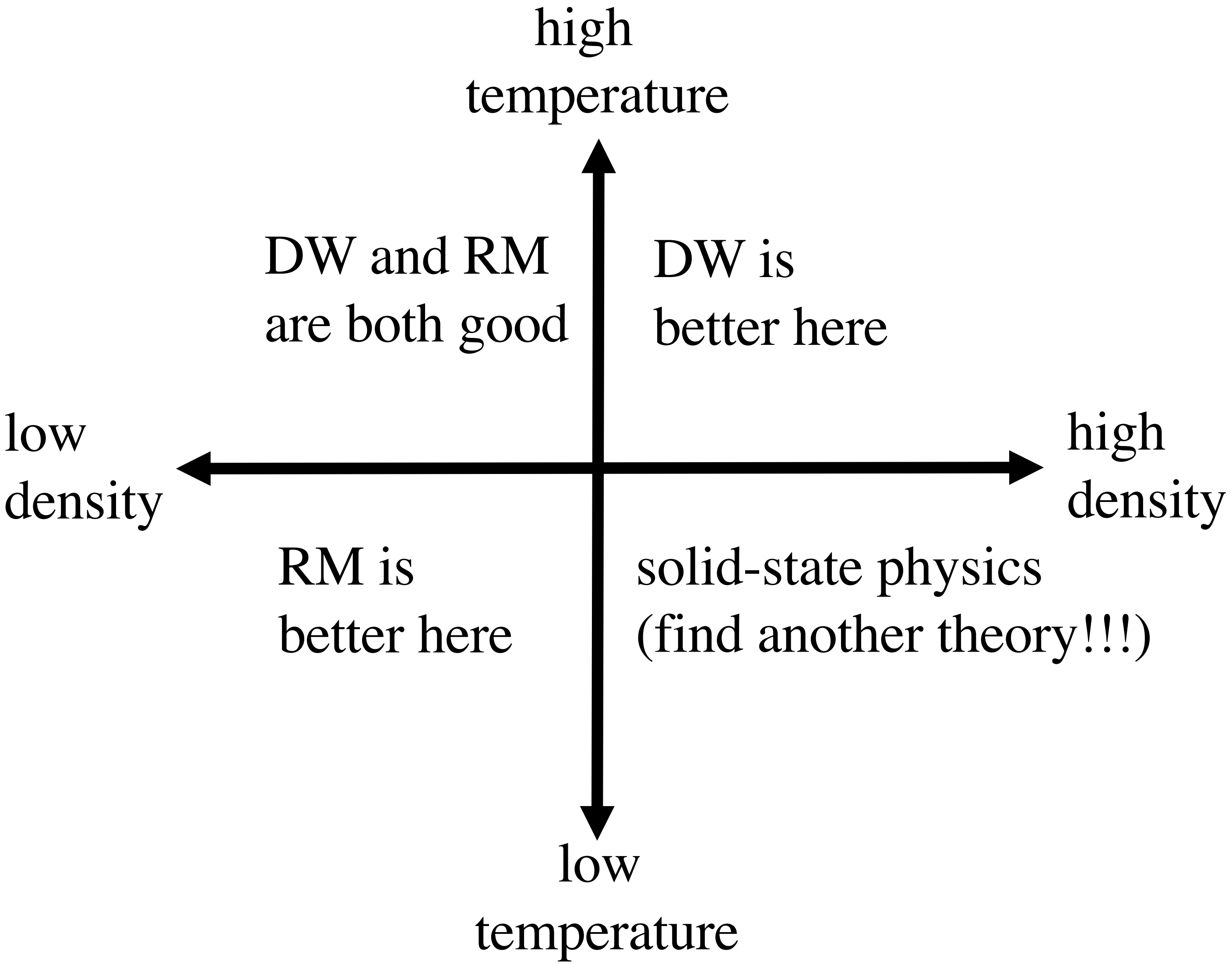
high
temperature

low
density

high
density

low
temperature

Some basic guidelines for DW and RM cross section calculations



high temperature

DW and RM are both good

DW is better here

low density

high density

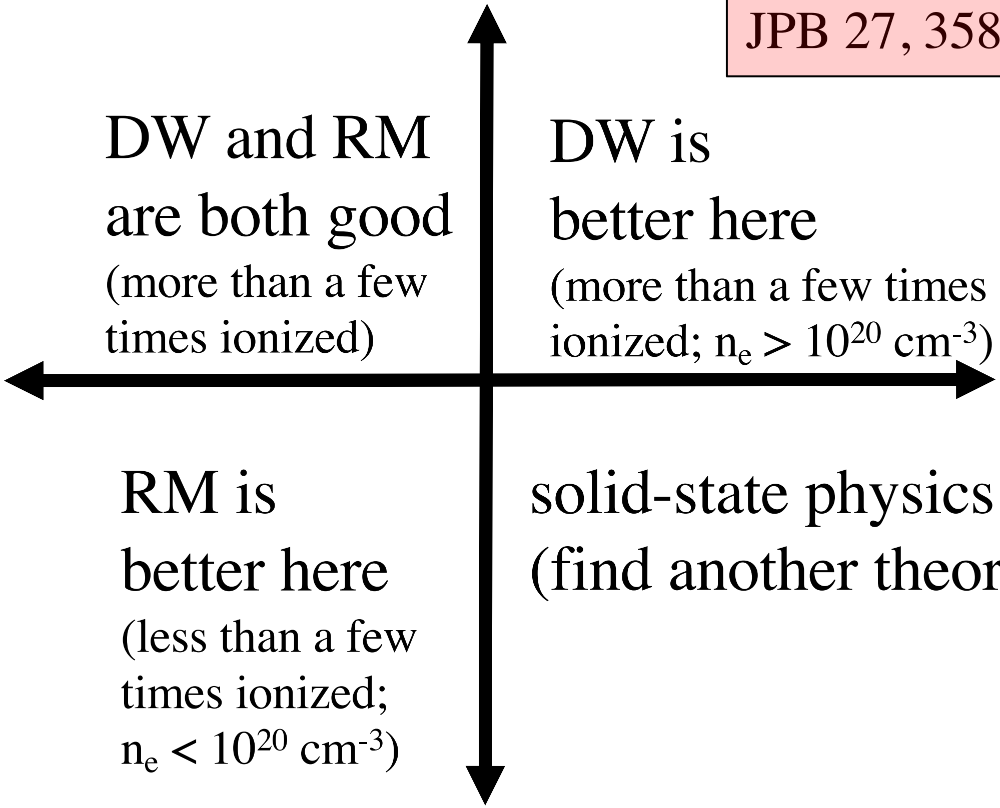
RM is better here

solid-state physics (find another theory!!!)

low temperature

Some basic guidelines for DW and RM cross section calculations

The boundary of $n_e = 10^{20}$ cm^{-3} comes from Abdallah and Clark, JPB 27, 3589 (1994).



high temperature

DW and RM are both good (more than a few times ionized)

DW is better here (more than a few times ionized; $n_e > 10^{20}$ cm^{-3})

low density

high density

RM is better here (less than a few times ionized; $n_e < 10^{20}$ cm^{-3})

solid-state physics (find another theory!!!)

low temperature

Suggested reading (the resonance contribution in distorted-wave calculations)

- D.R. Bates and A. Dalgarno, in *Atomic and Molecular Processes*, Ed. D.R. Bates (New York: Academic) pp. 258-61 (1962)
- A. Burgess, ApJL 39, 776 (1964)
- A.H. Gabriel and C. Jordan, Nature 221, 941 (1969)
- A.H. Gabriel and T.M. Paget, JPB 5, 673 (1972)
- M.J. Seaton, JPB 2, 5 (1969)
- R.D. Cowan, JPB 13, 1471 (1980)
- N.R. Badnell et al, PRA 43, 2250 (1991); PRA 47, 2937 (1993)
- E. Behar et al, PRA 52, 3770 (1995); PRA 54, 3070 (1996)
- D.H. Sampson, H.L. Zhang, C.J. Fontes, Phys. Rep. 477, 111 (2009) (this review article contains a discussion of resonances for all of the major processes)