Understanding Solar Opacity: Fundamentals, Theoretical Foundations, and Experimental Validation

Taisuke Nagayama

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U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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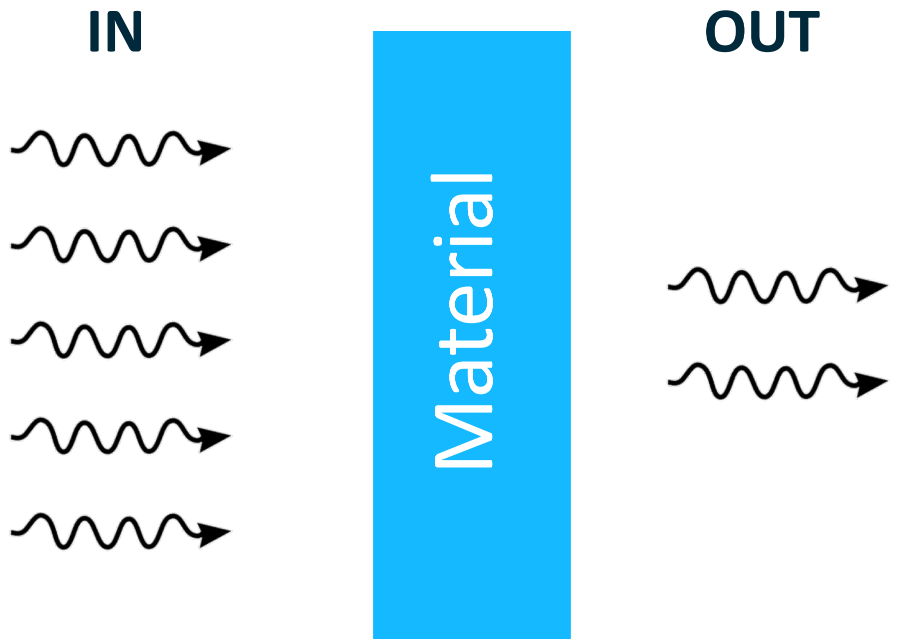
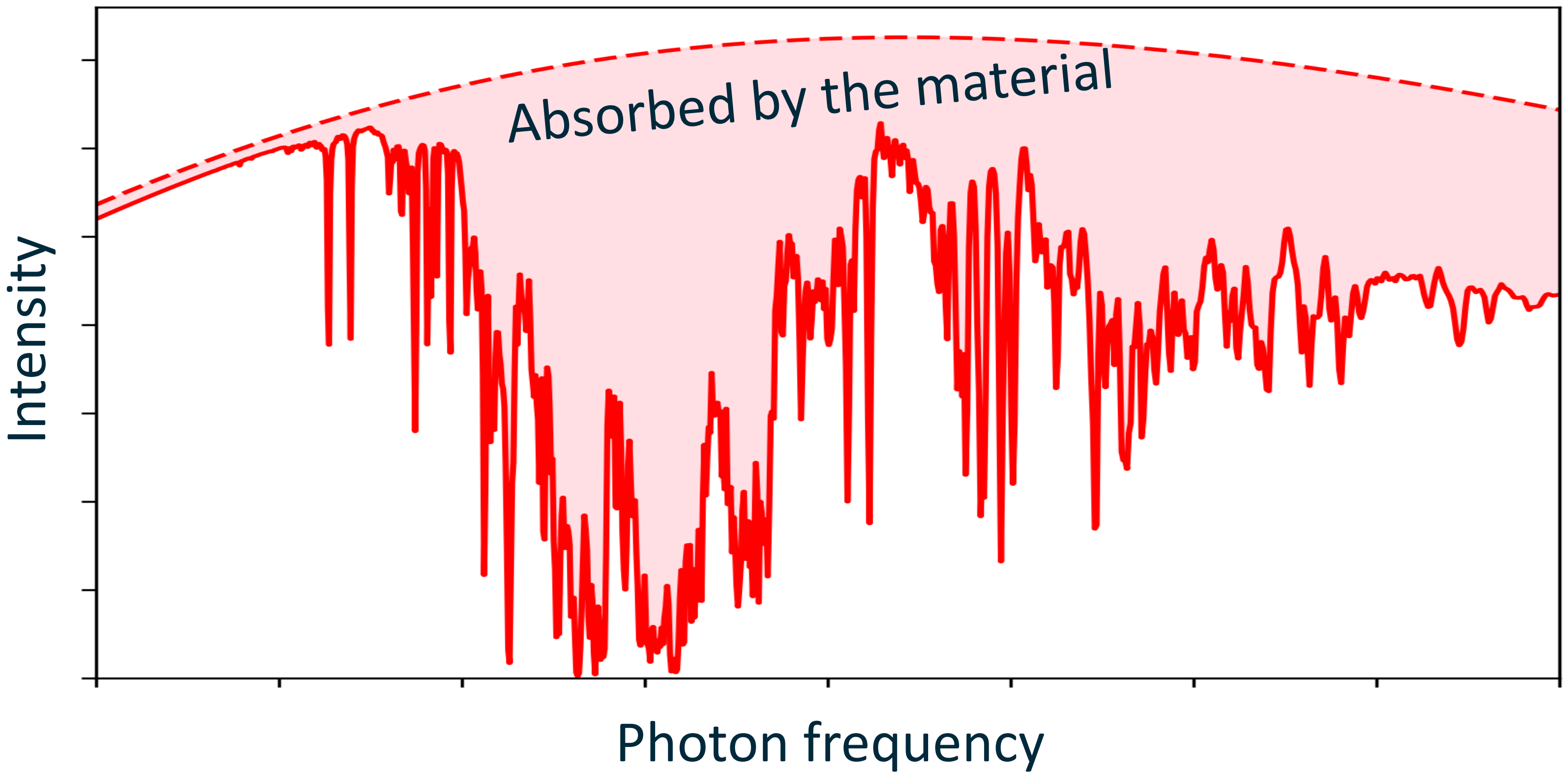
Opacity quantifies photon absorption in matter



$$Transmission = \frac{\text{2 photons}}{\text{5 photons}} = 40\%$$

3 photons are *absorbed* due to its *opacity*, κ.

Opacity (thus transmission) depends on photon frequency



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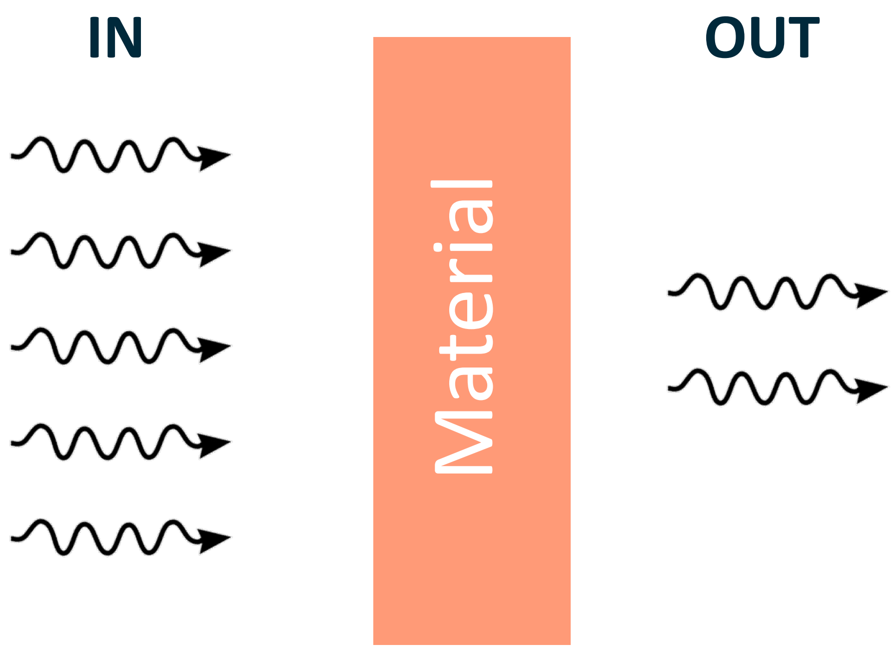

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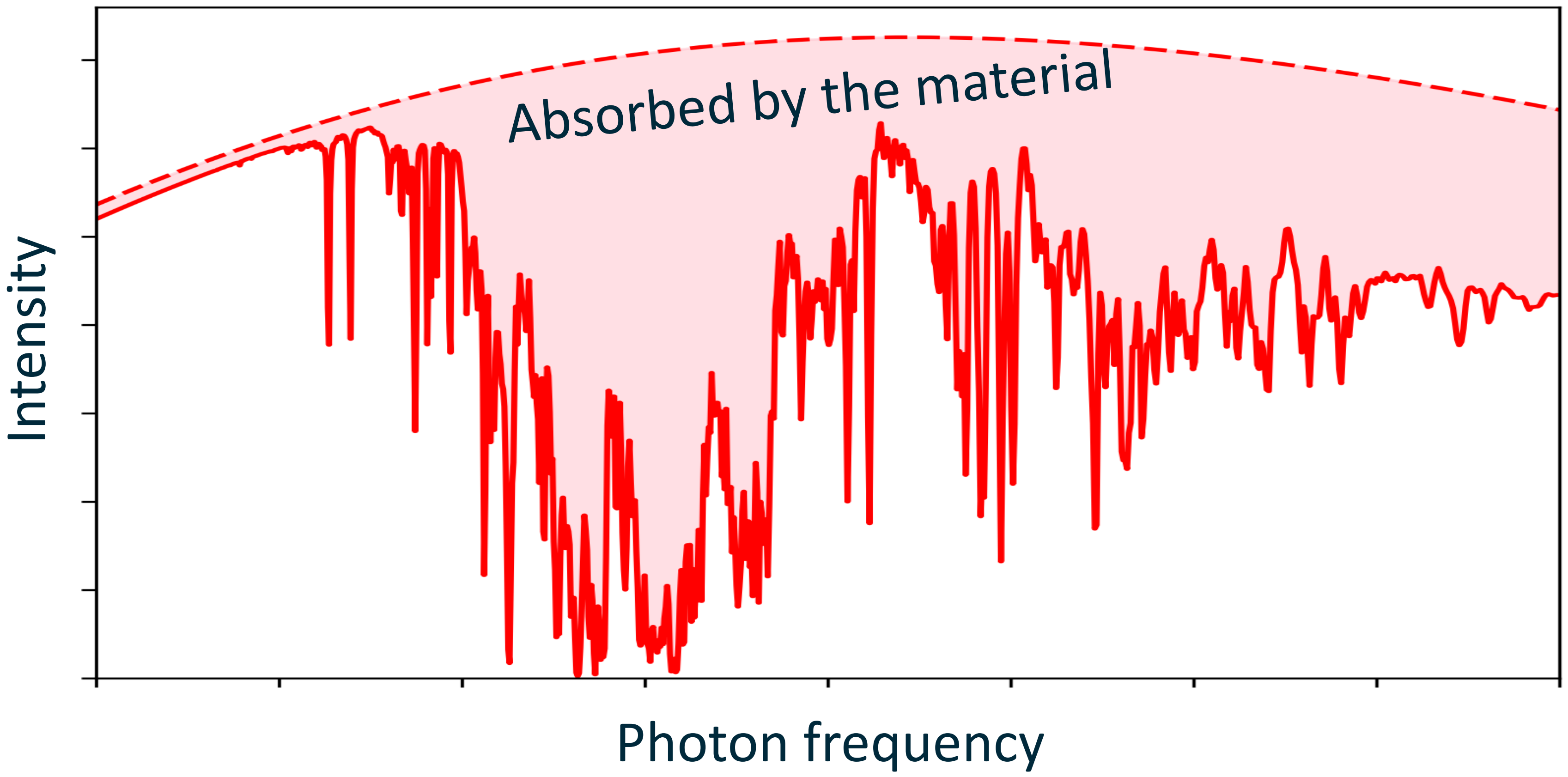

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2. **Opacity is essential for understanding how energy is transported via radiation**

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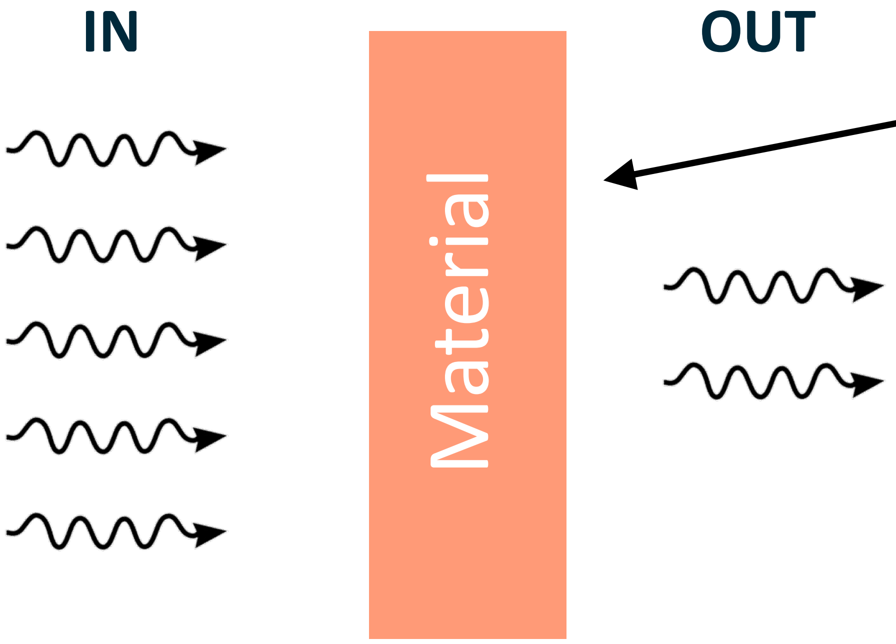

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3 photons are *absorbed* due to its *opacity*, κ.

Radiative Heat Flux q_R

$$q_R = -\frac{16\sigma T^3}{3\kappa_R}\nabla T$$ (LTE, diffusion limit)

Rosseland-mean opacity

$$\frac{1}{\kappa_R} = \int \frac{1}{\kappa_\nu} w_\nu d\nu \quad \text{where} \quad w_\nu = \frac{\frac{dB_\nu}{dT}}{\int \frac{dB_\nu}{dT} d\nu}$$

1. **Opacity is a complex function of photon frequency**
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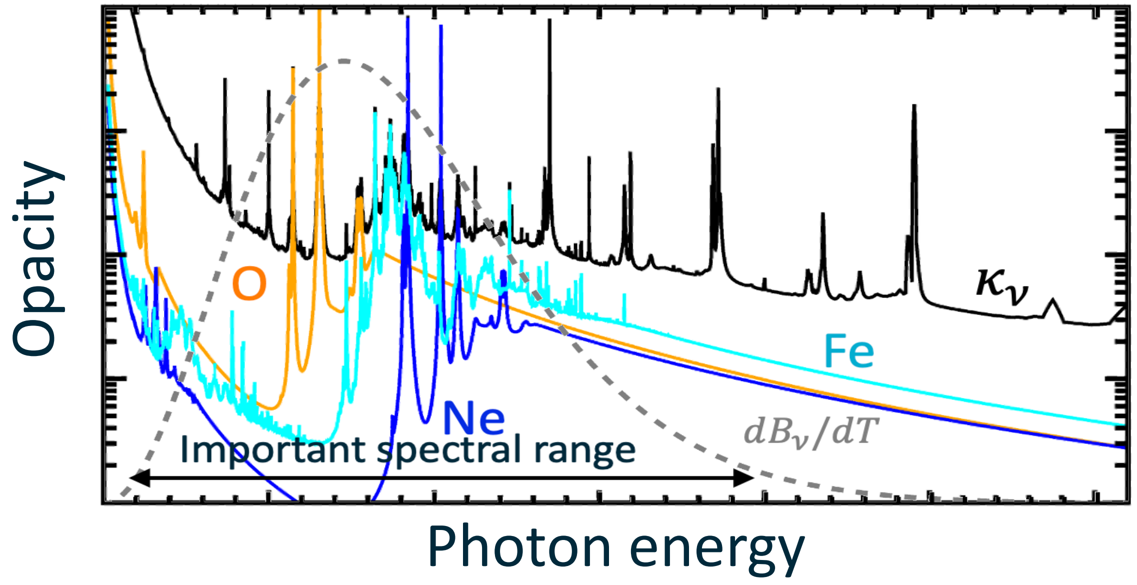
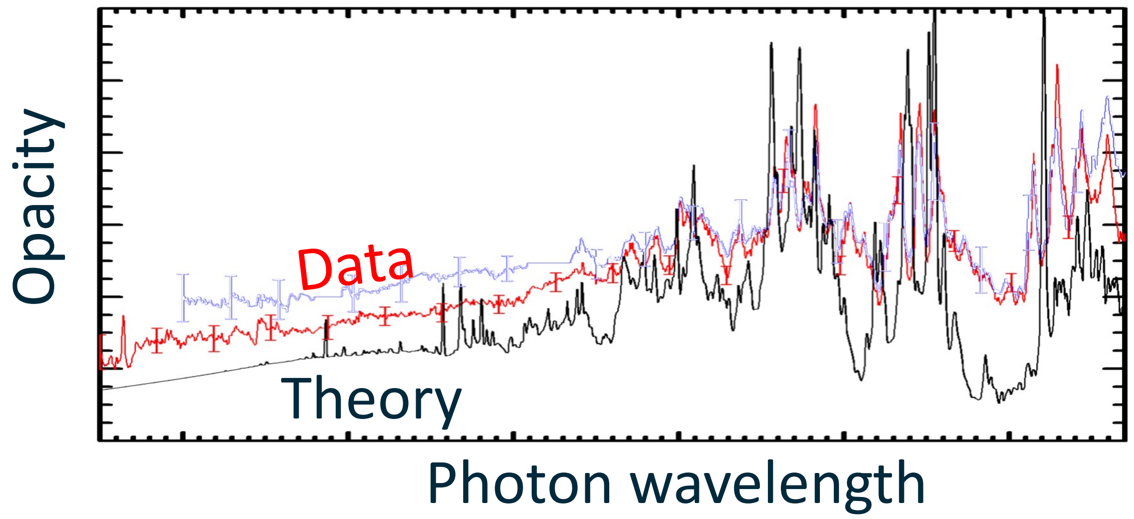
Understanding solar opacity is challenging due to complex nature of Rosseland mean opacity

1. **Basics:** Rosseland mean opacity
   - Derivations, assumptions, and complexity
   - If RMO is wrong:
     → (1) Abundance and/or
     → (2) Calculated element opacity.
2. **Theory:** How element opacity is computed.
   - Opacity is computed by "first principle"
   - Models contain "untested" approximations
3. **Experiments:** experiments and future perspective
   - Experimental challenges
   - Z and NIF experiments





Worldwide opacity collaborations will soon help quantify the true accuracy of calculated element opacities

Caution1: When I say "opacity," I often mean "absorption coefficient".

Absorption coefficient

κ_ν (1/cm)

→

Opacity

$$\kappa_\nu^{op} = \frac{\kappa_\nu}{\rho} \quad (\text{cm}^2/\text{g})$$

More fundamental quantity for photon absorption.

e.g., $q_R = -\frac{16\sigma T^3}{3\kappa_R}\nabla T$

Convenient quantity for plasma simulations

$$q_R = -\frac{16\sigma T^3}{3\kappa_R^{op}\rho}\nabla T$$

Caution2: I use photon frequency, energy, and wavelength interchangeably

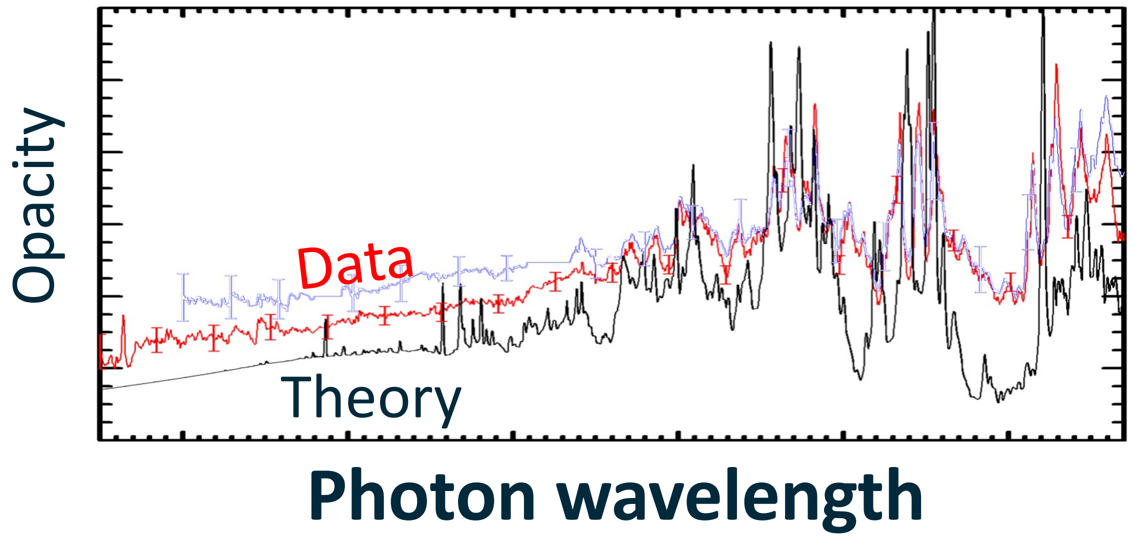
Photon wavelength, photon frequency, and photon energy are all related:

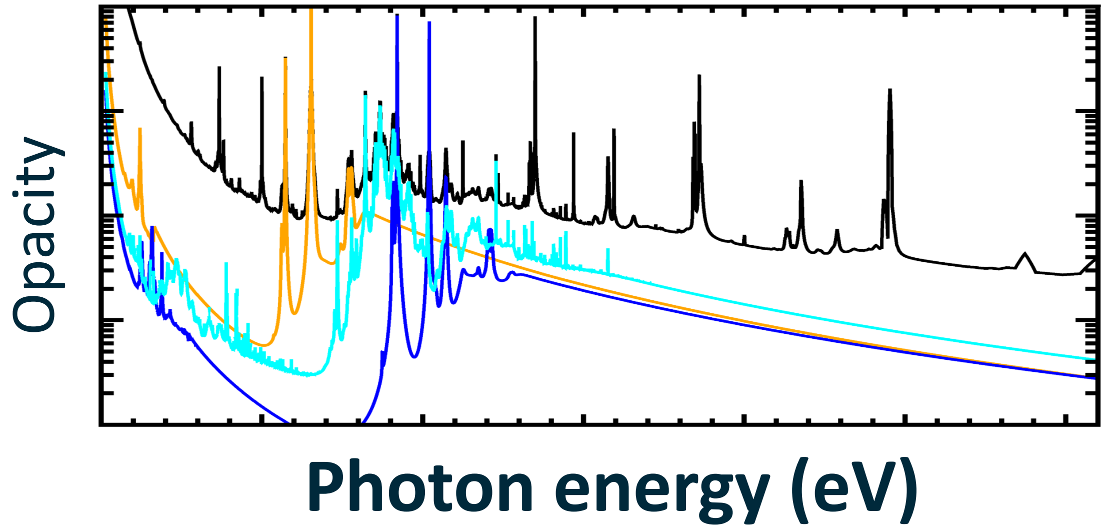
$$\lambda = \frac{12398}{h\nu}$$

Wavelength [Å]

Frequency [Hz]

Energy [eV]





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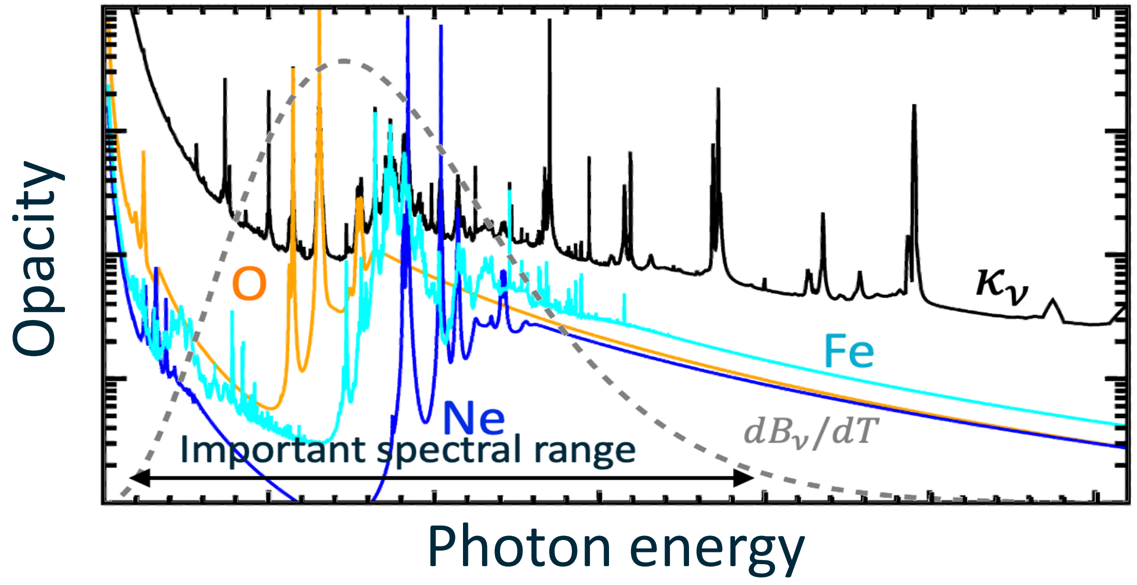

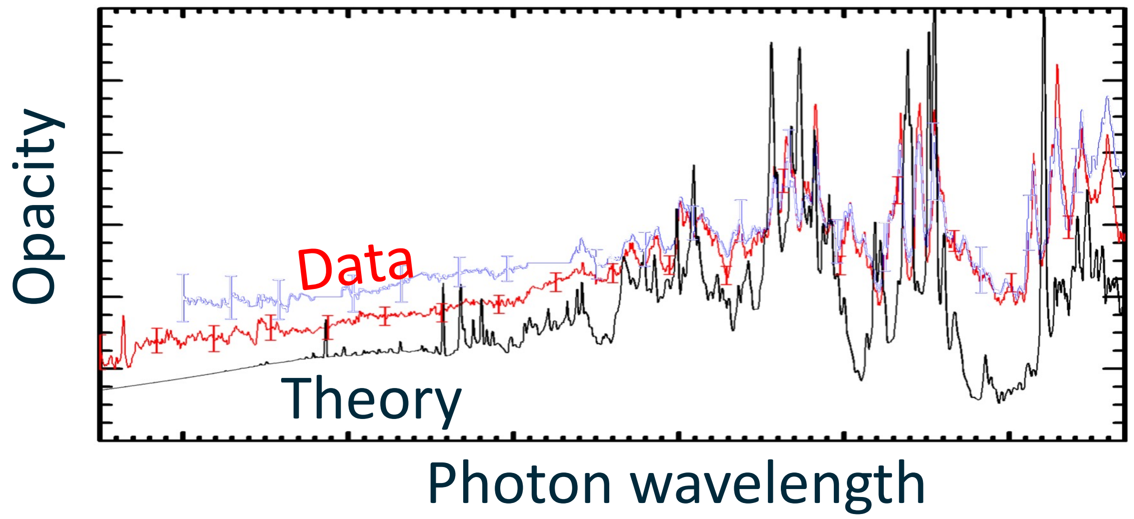

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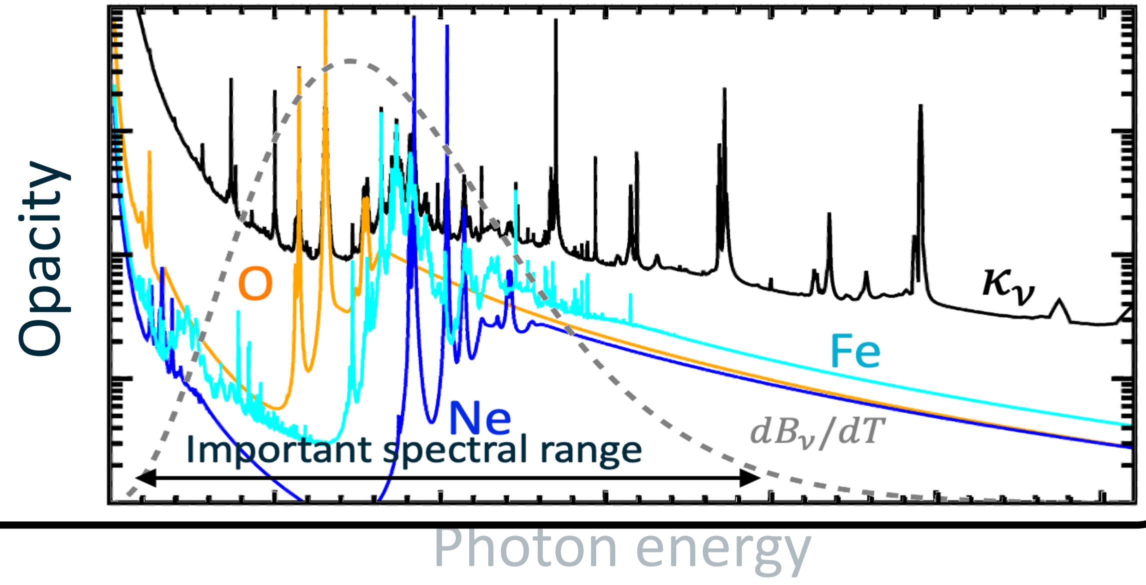

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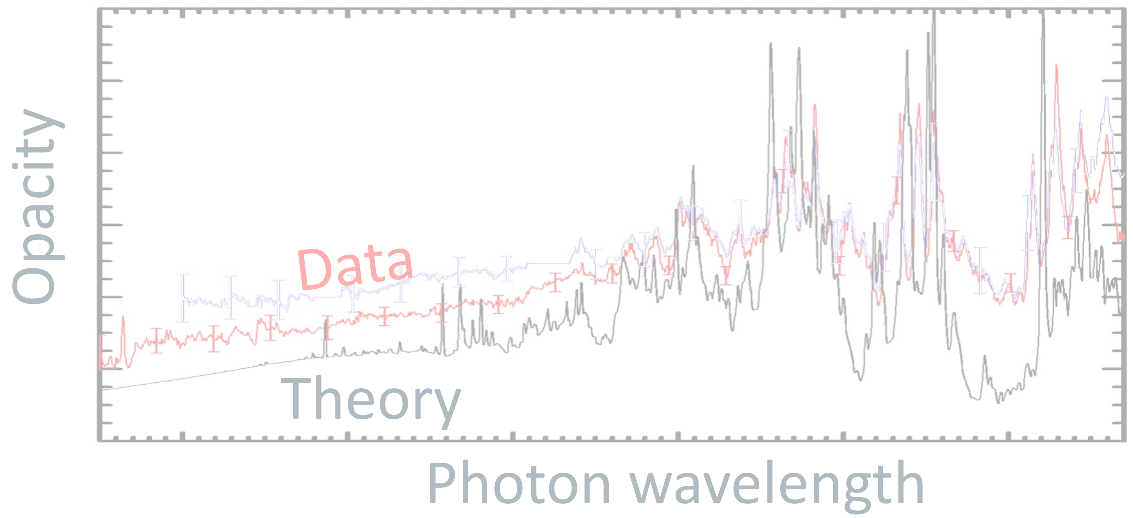

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Why can we approximate radiative heat flux q_R using Rossleand-mean opacity κ_R*

Why ?

$$q_R = -\frac{16\sigma T^3}{3\kappa_R}\nabla T$$

Necessary steps for computing $\boldsymbol{q_R}$

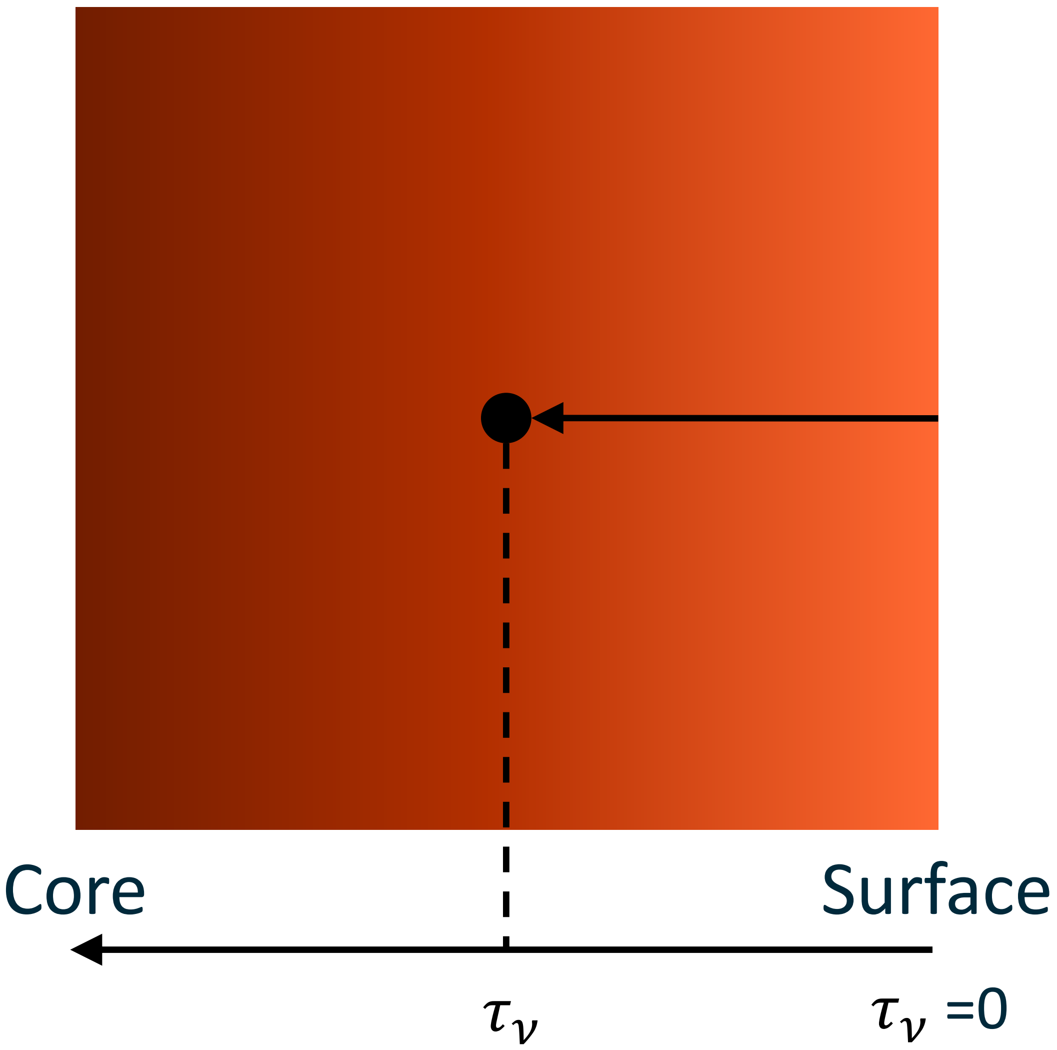
1. Line integration (or radiation transport) → I_ν
2. Angular integration → q_ν
3. **Spectral integration → $\boldsymbol{q_R}$**

$$q_R = \int q_\nu \, dh\nu$$

*In this presentation, opacity has a unit of 1/cm.

Step1. Solving radiation transport equation

$B_\nu = \frac{\epsilon_\nu}{\kappa_\nu}$ ... Blackbody



Radiation transport equation

$$I_\nu(\tau_\nu, \mu) \approx B_\nu(\tau_\nu) - \mu \frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$$

Step1. Change of variable: $x \rightarrow \tau_\nu$ $(d\tau_\nu = \kappa_\nu dx)$

Distance from surface → Optical depth from surface

Step2. Solve for $I_\nu(\tau_\nu)$

Step3. Diffusion limit ($\tau_\nu \gg 1$)

Step4. Change of variable: $s = \tau_\nu - t$

Step5. First order Taylor expansion on $B_\nu(\tau_\nu - s)$

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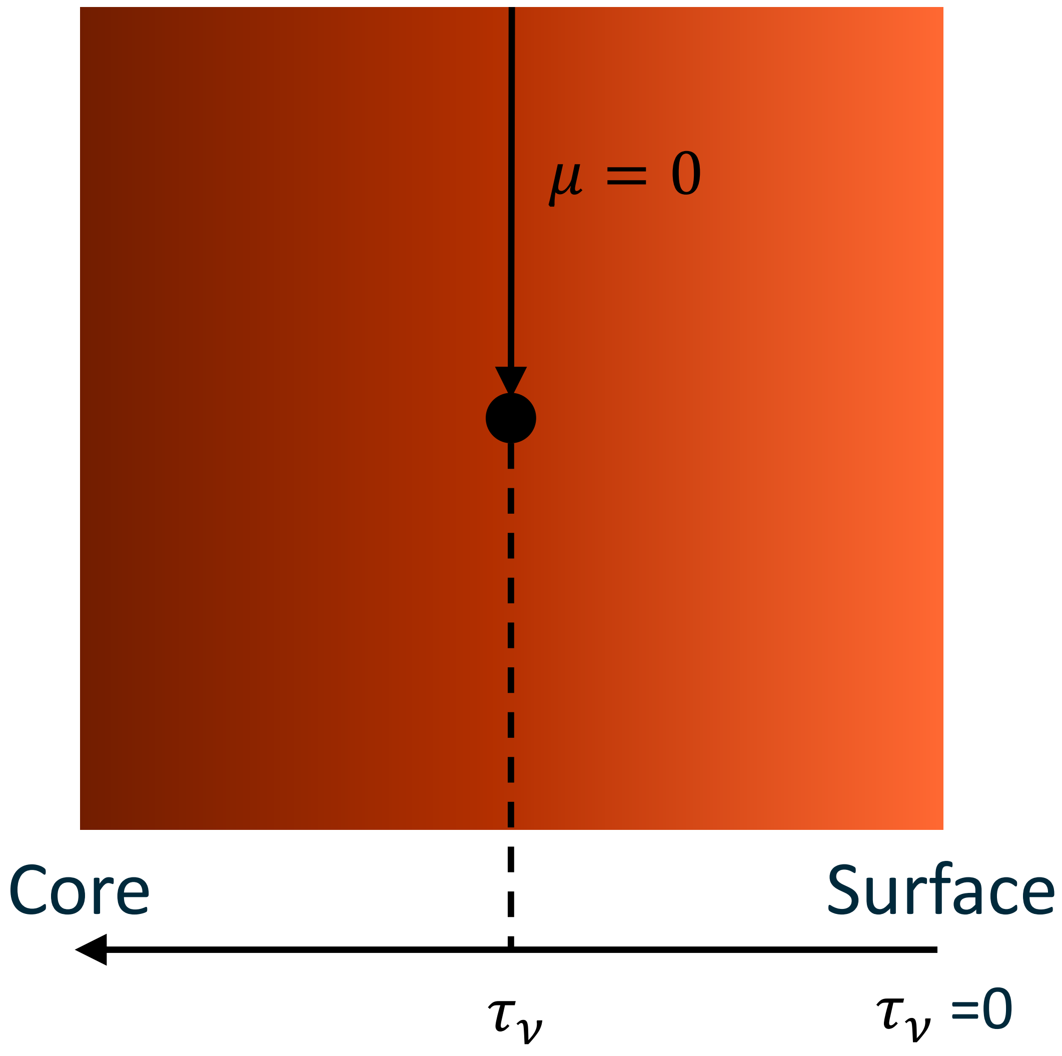

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$$I_\nu(\tau_\nu, \mu) \approx B_\nu(\tau_\nu) - \mu \frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$$

This provides angle (μ) dependent emergent intensity.

From surface: μ=1 → $I_\nu(\tau_\nu) \approx B_\nu(\tau_\nu) - \frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$

From core: μ=-1 → $I_\nu(\tau_\nu) \approx B_\nu(\tau_\nu) + \frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$

From top: μ=0 → $I_\nu(\tau_\nu) \approx B_\nu(\tau_\nu)$

Step2. Compute spectral flux by integrate it over all solid angle

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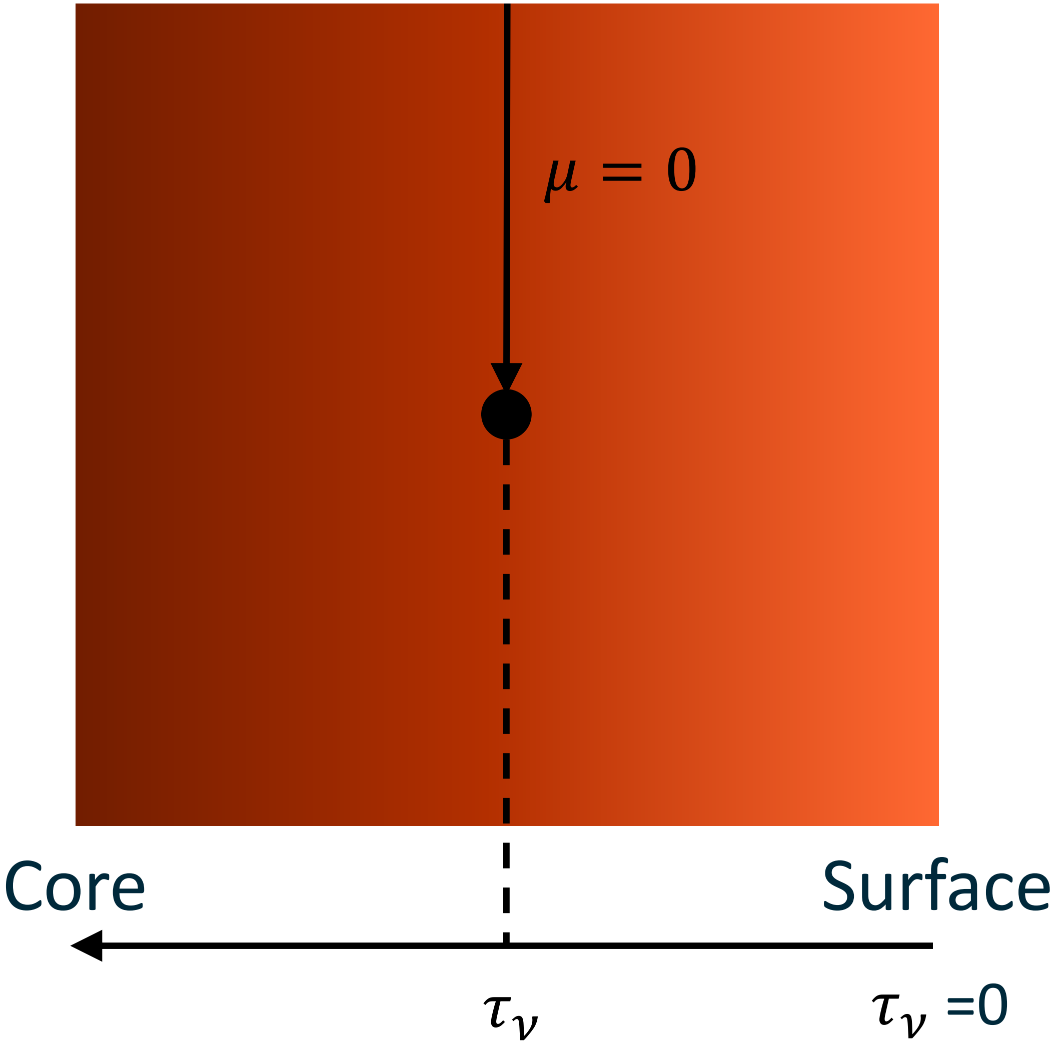

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Compute spectral flux:

$$q_\nu = \int_{4\pi} I_\nu(\tau_\nu, \hat{n})\, \hat{n}\, d\Omega$$

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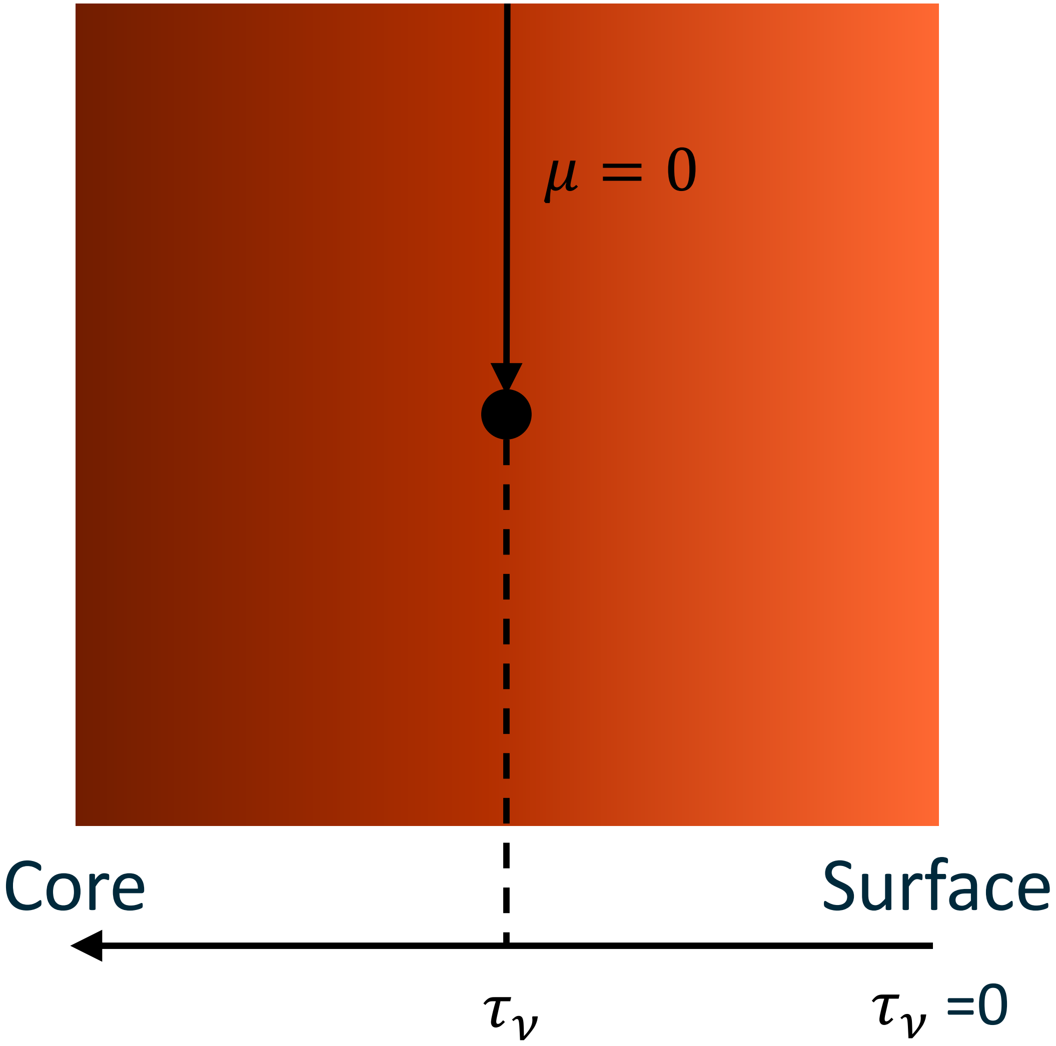

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Compute spectral flux:

$$q_\nu = 2\pi \int_{-1}^{1} \mu \left[B_\nu - \mu \frac{dB_\nu(\tau_\nu)}{d\tau_\nu} \right] d\mu$$

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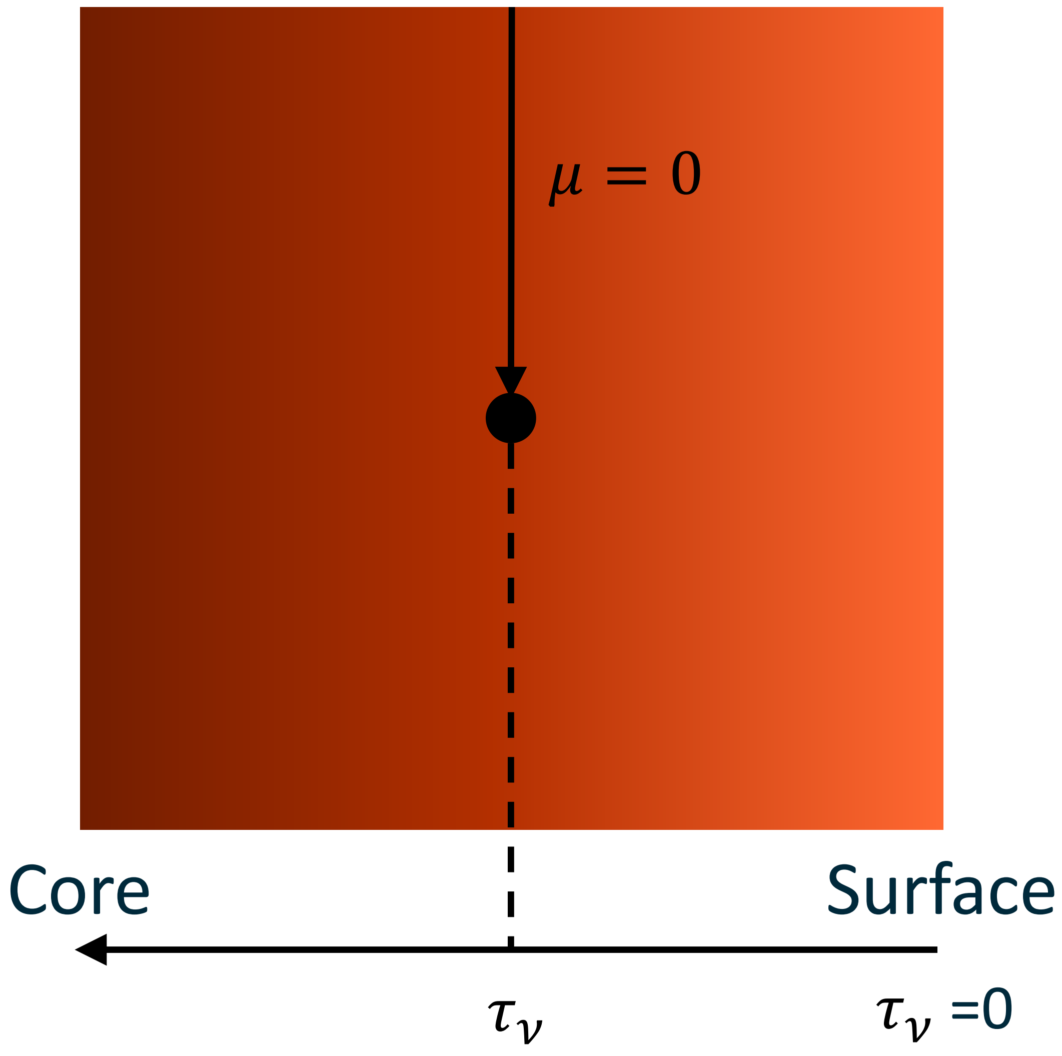

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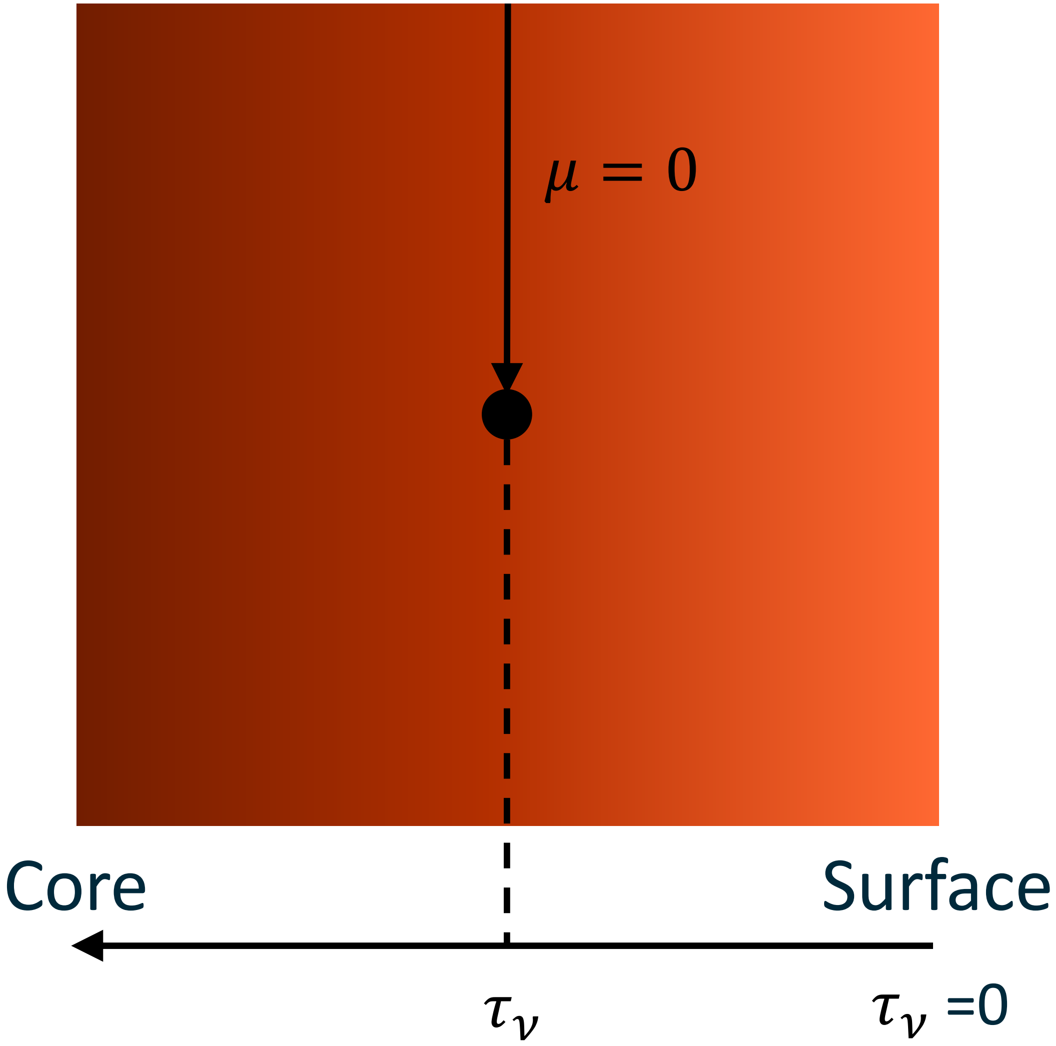

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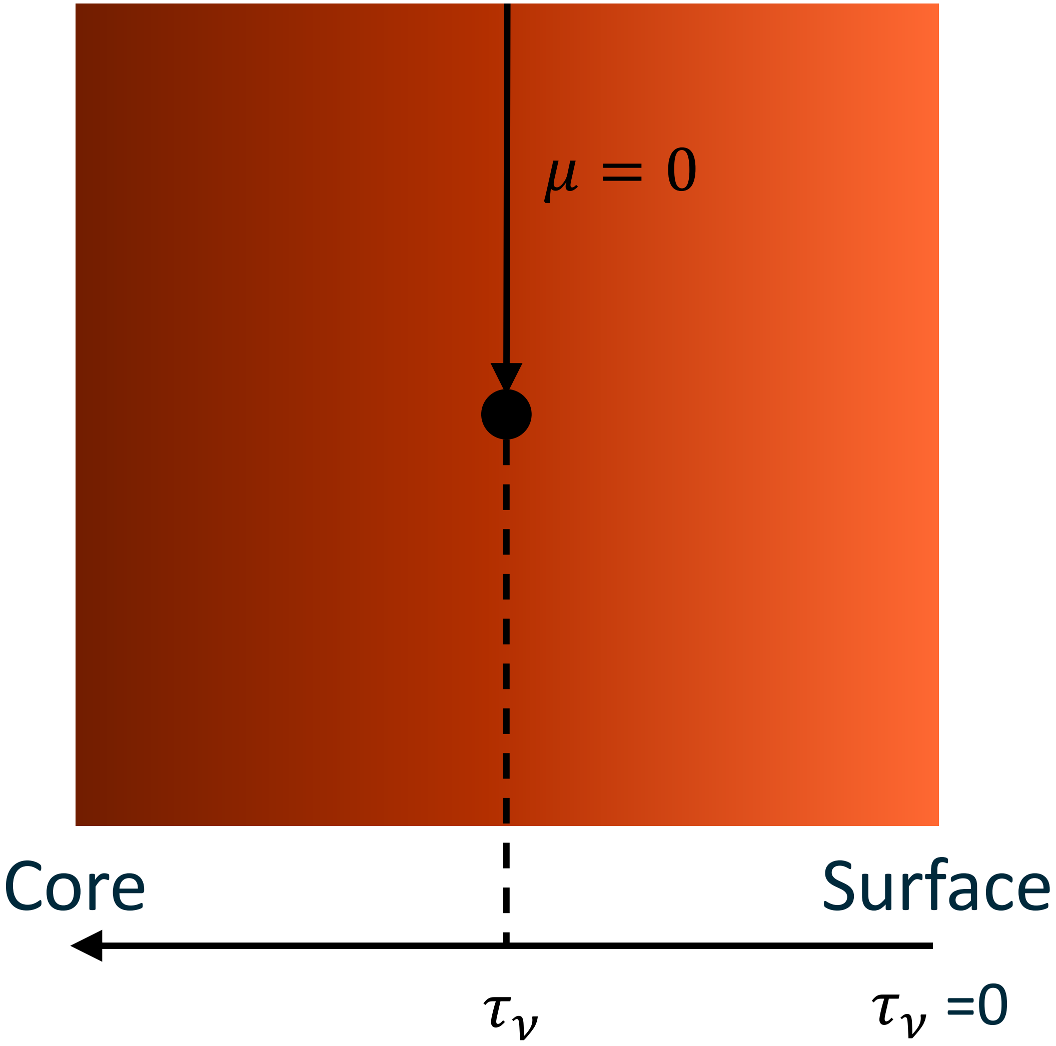

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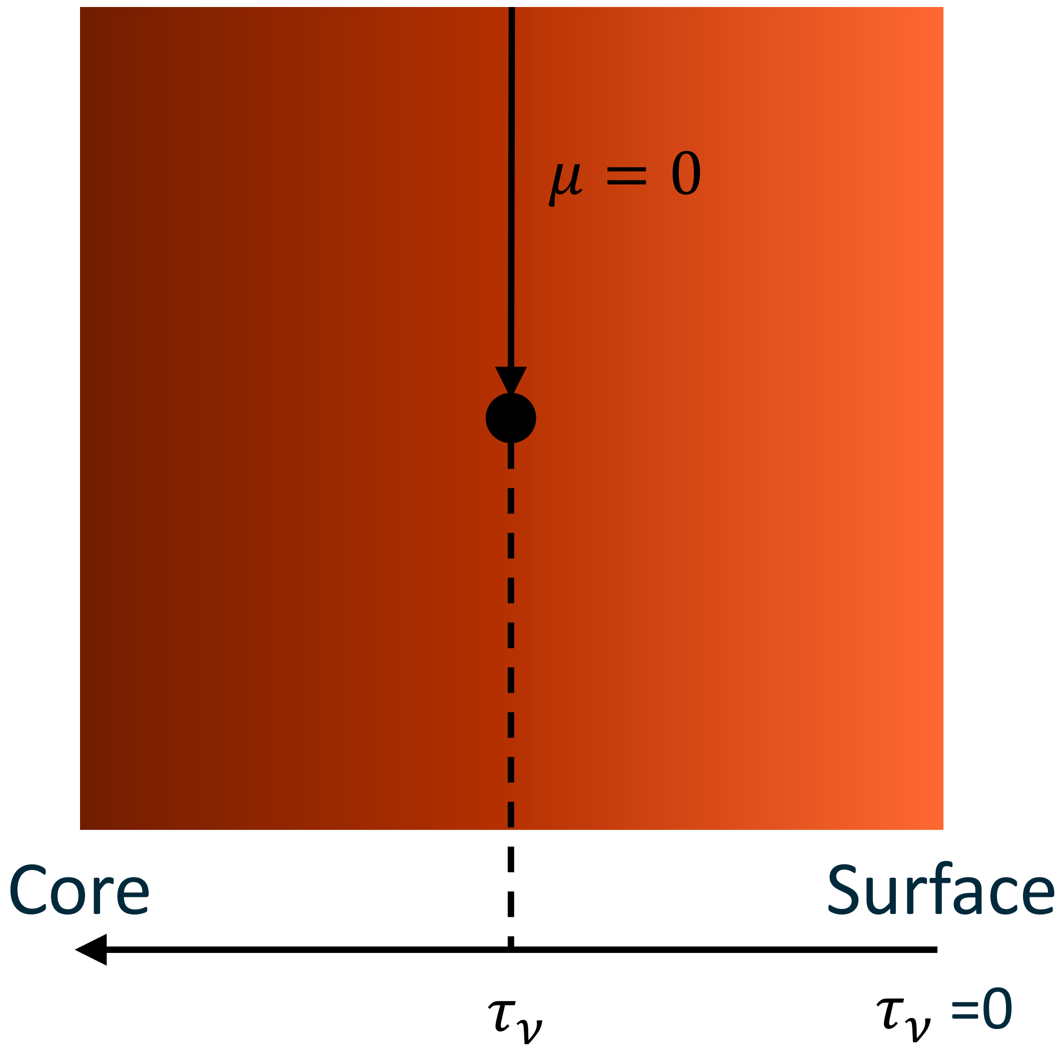

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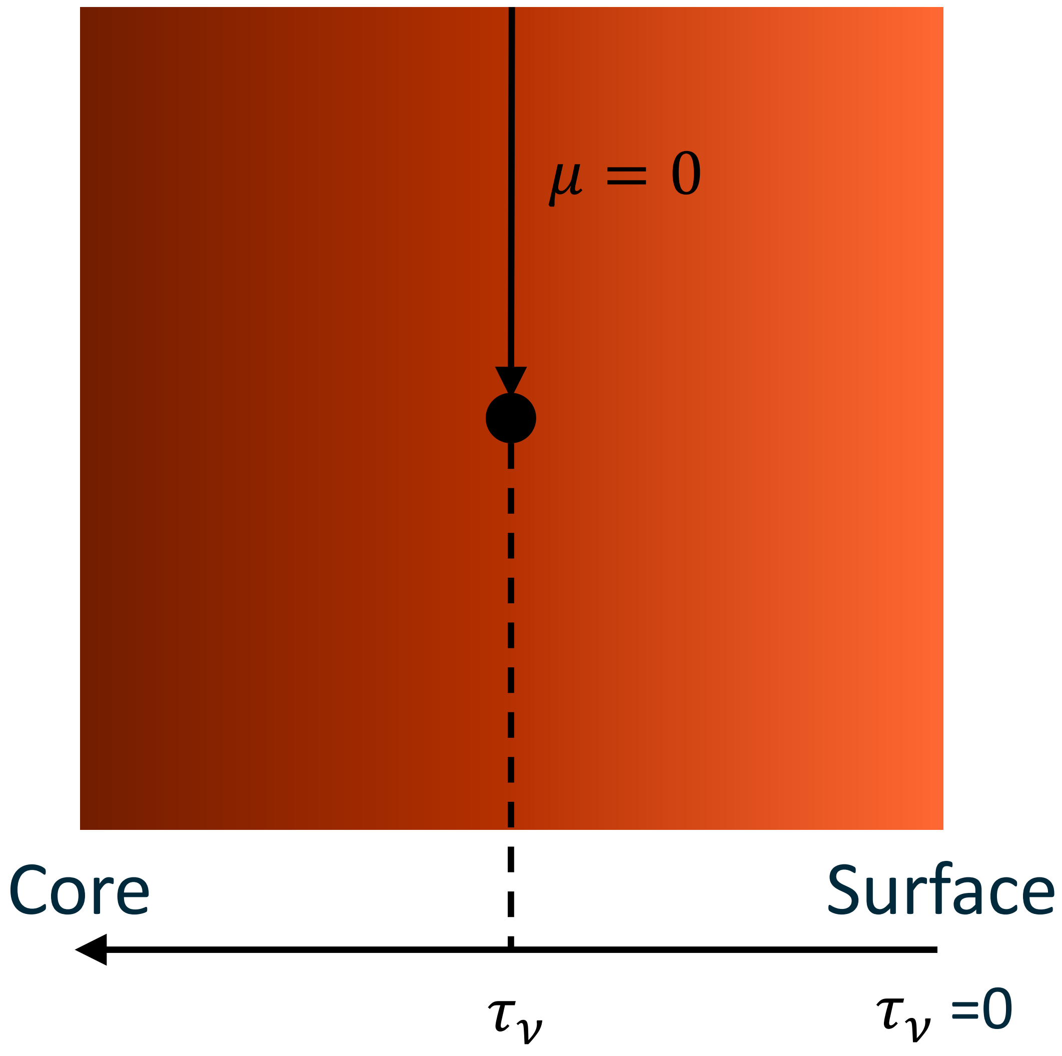

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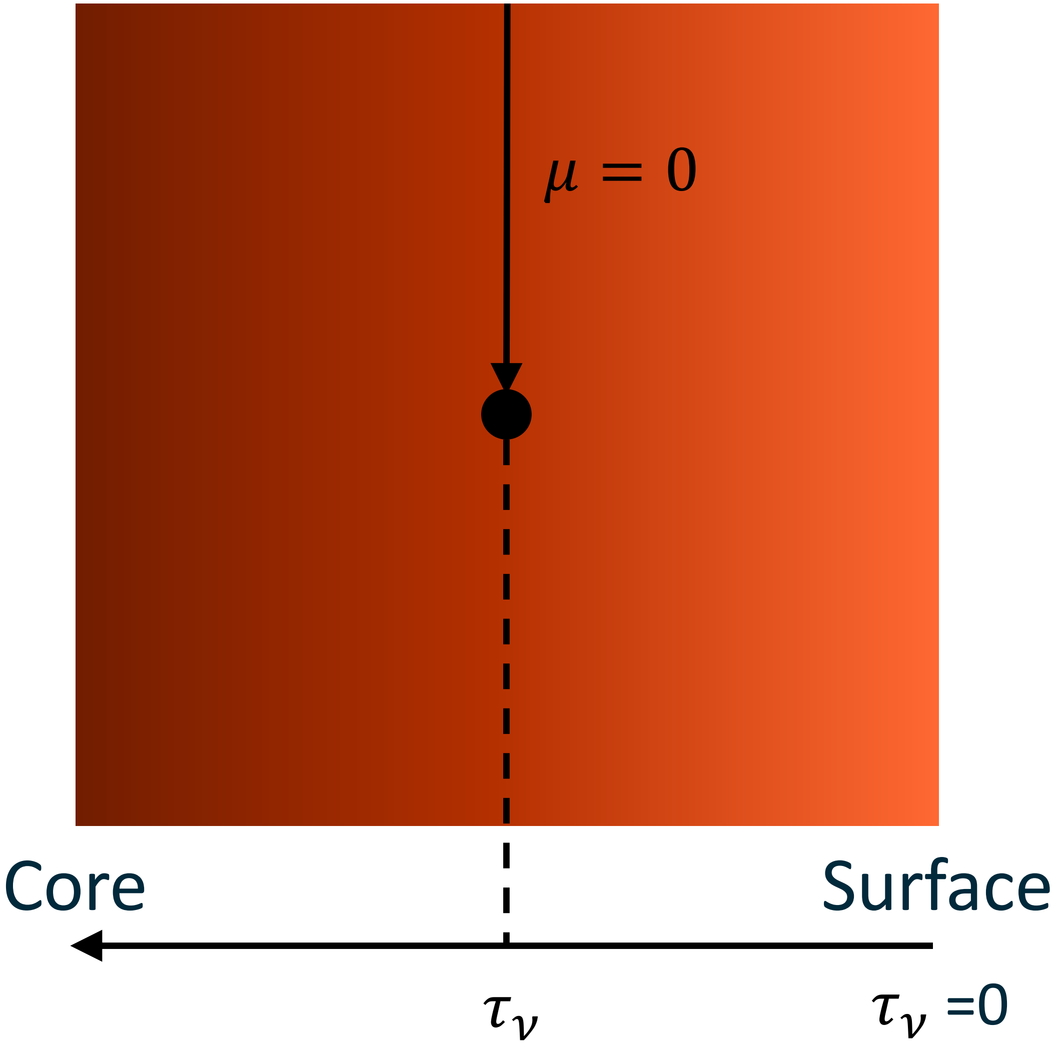

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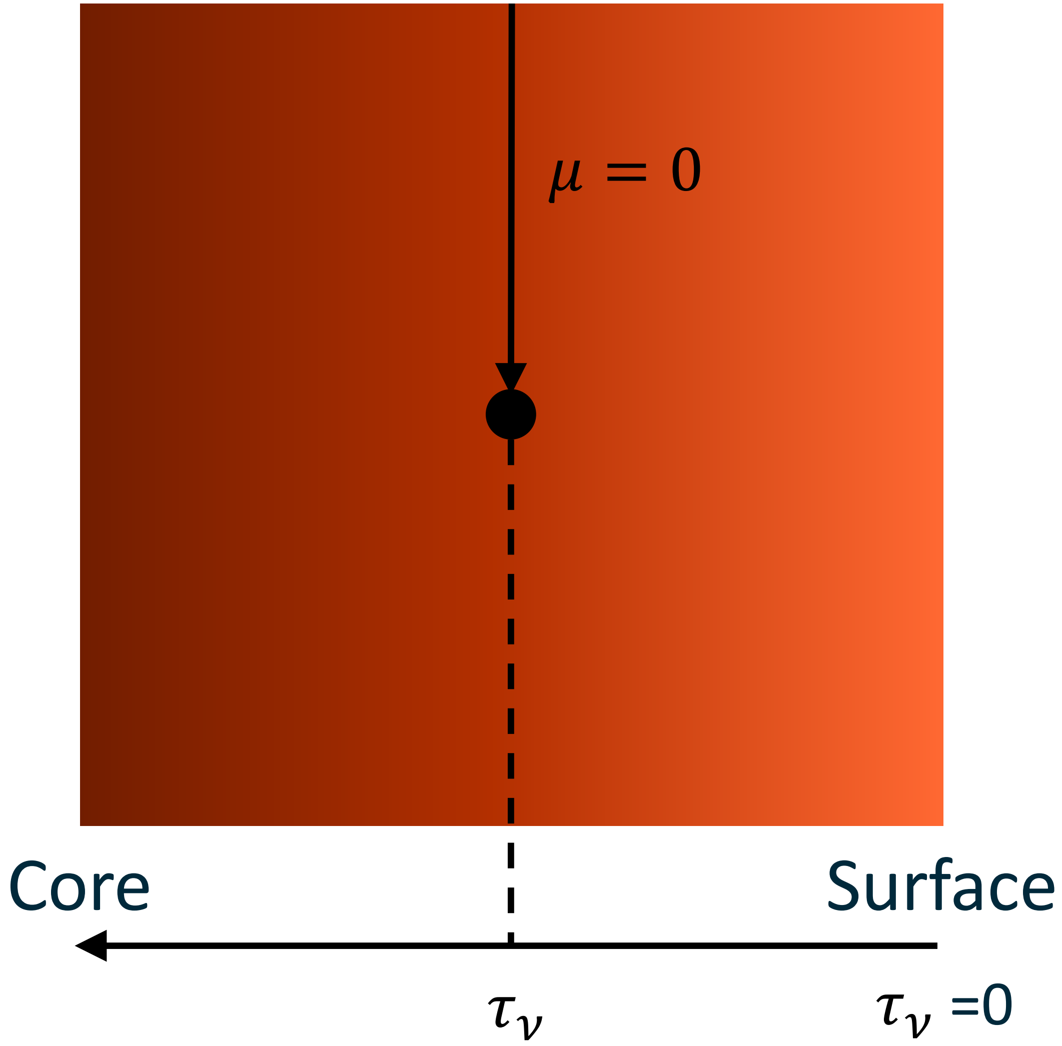

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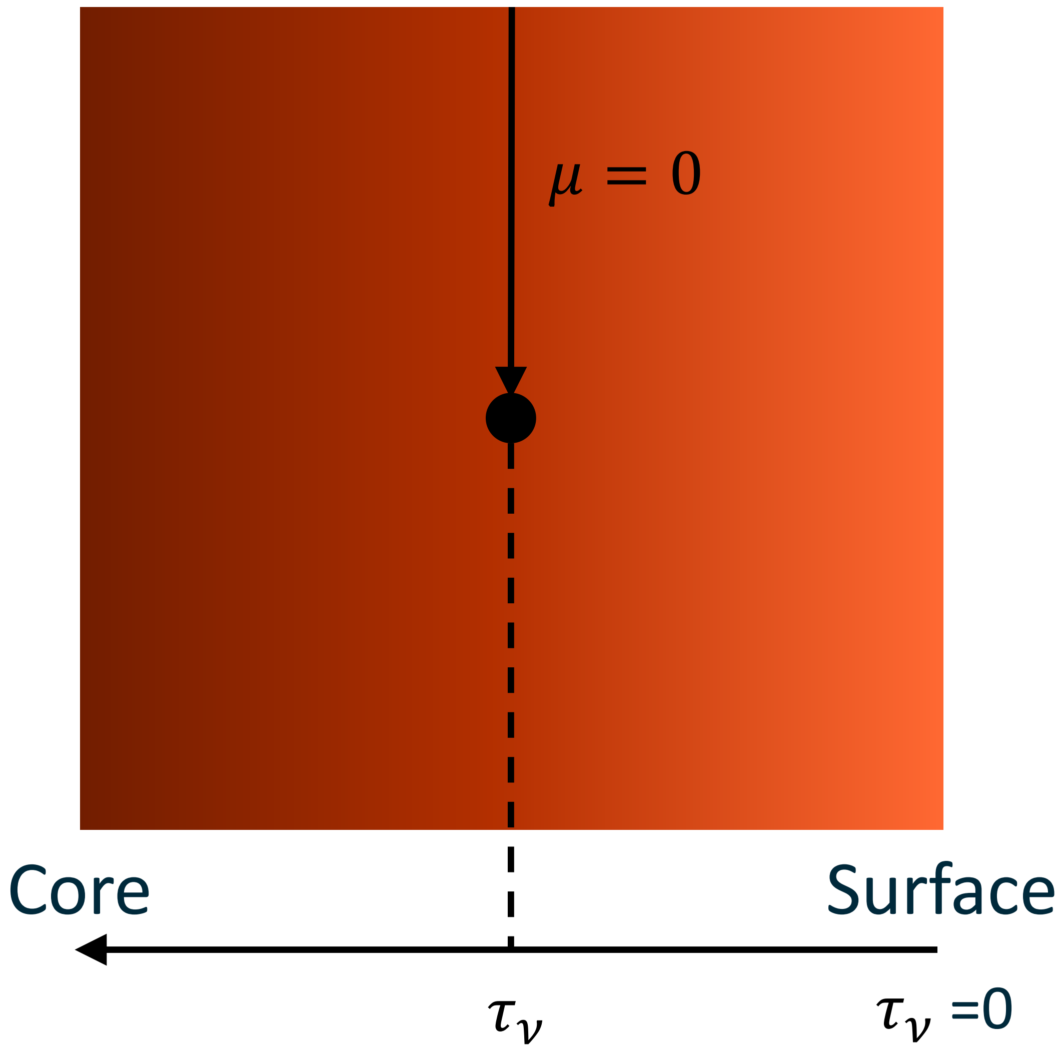

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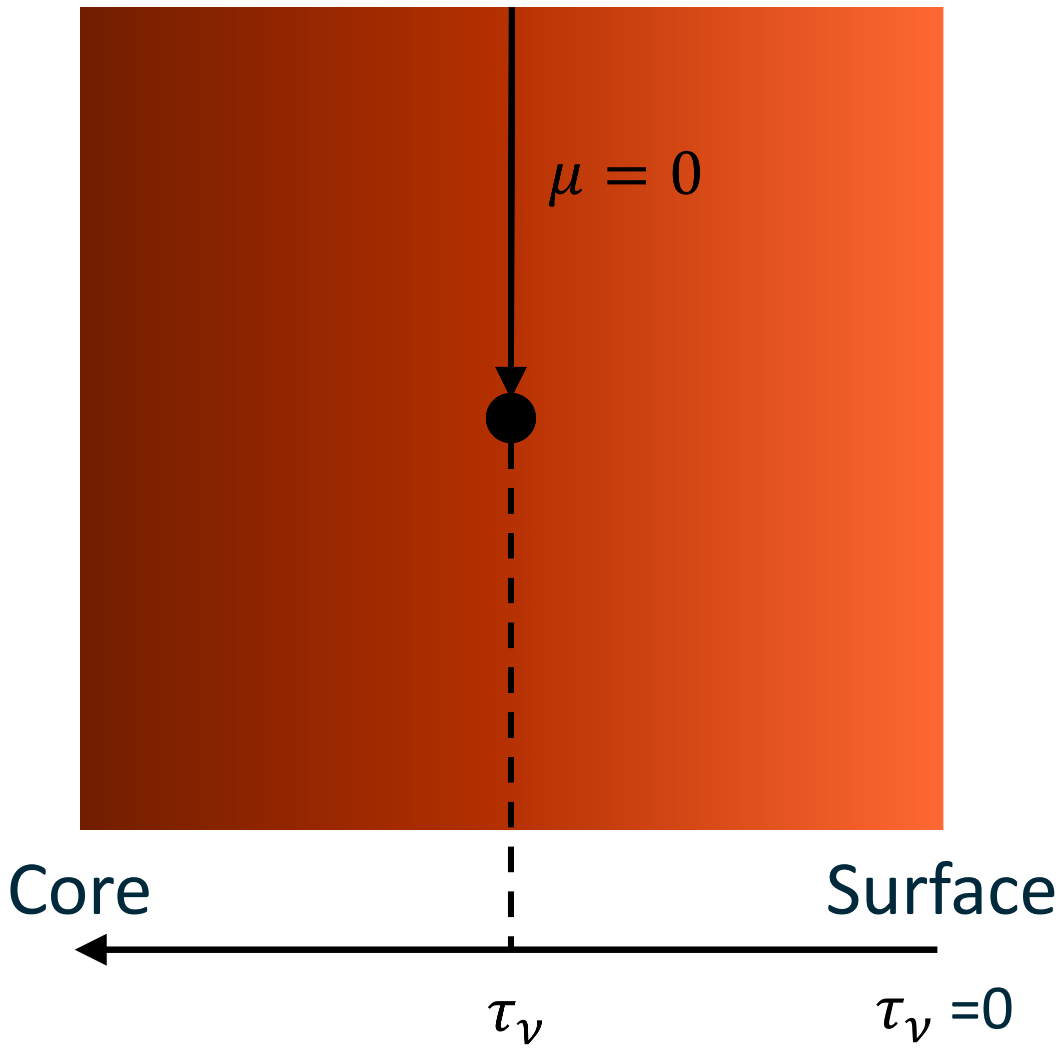

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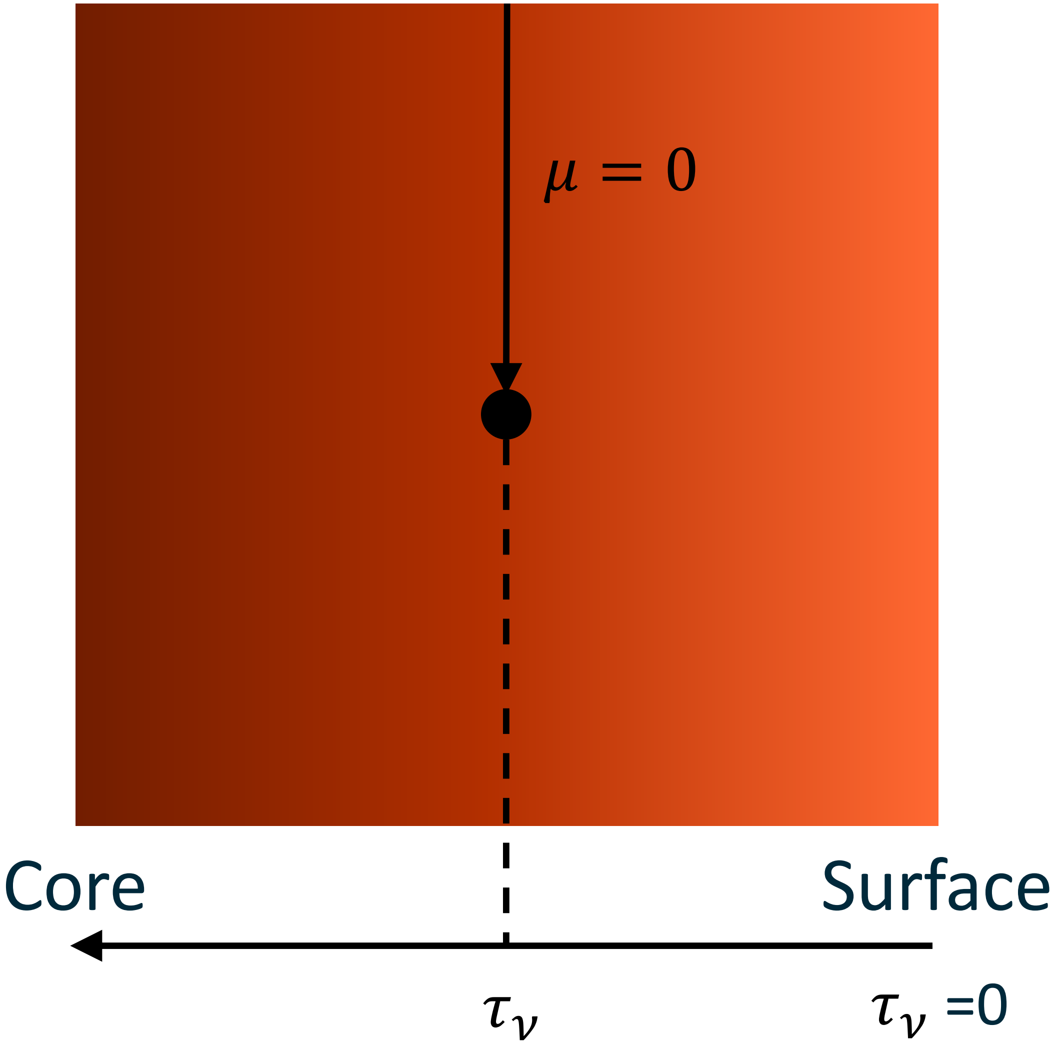

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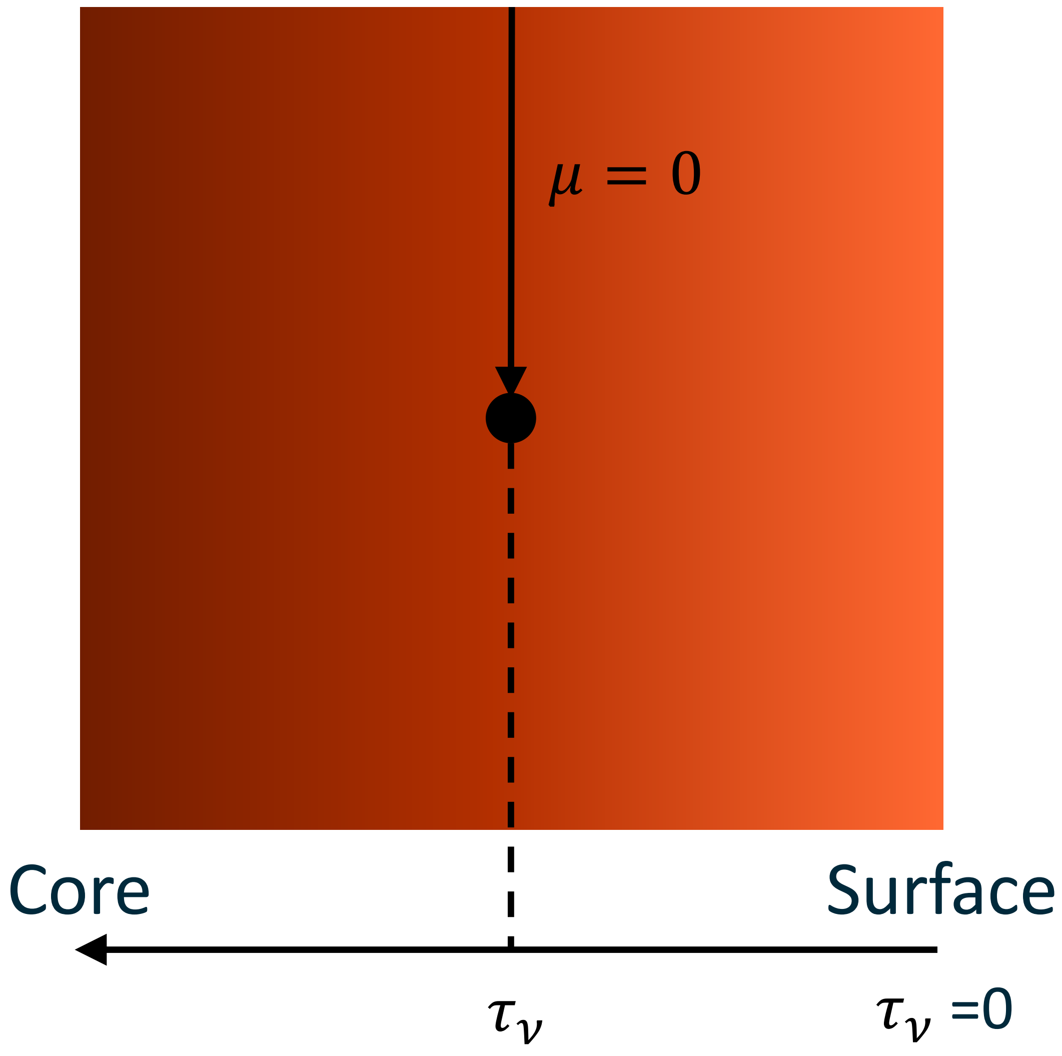

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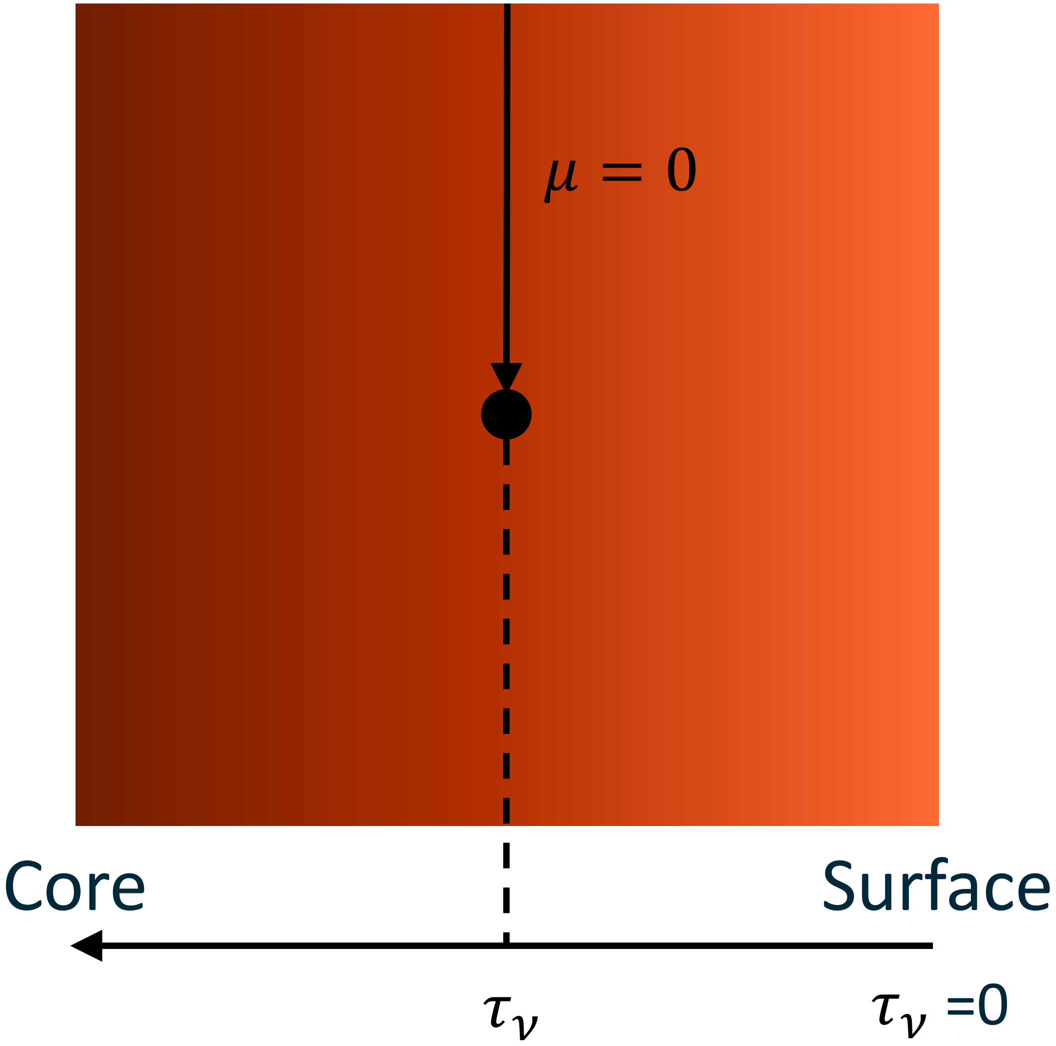

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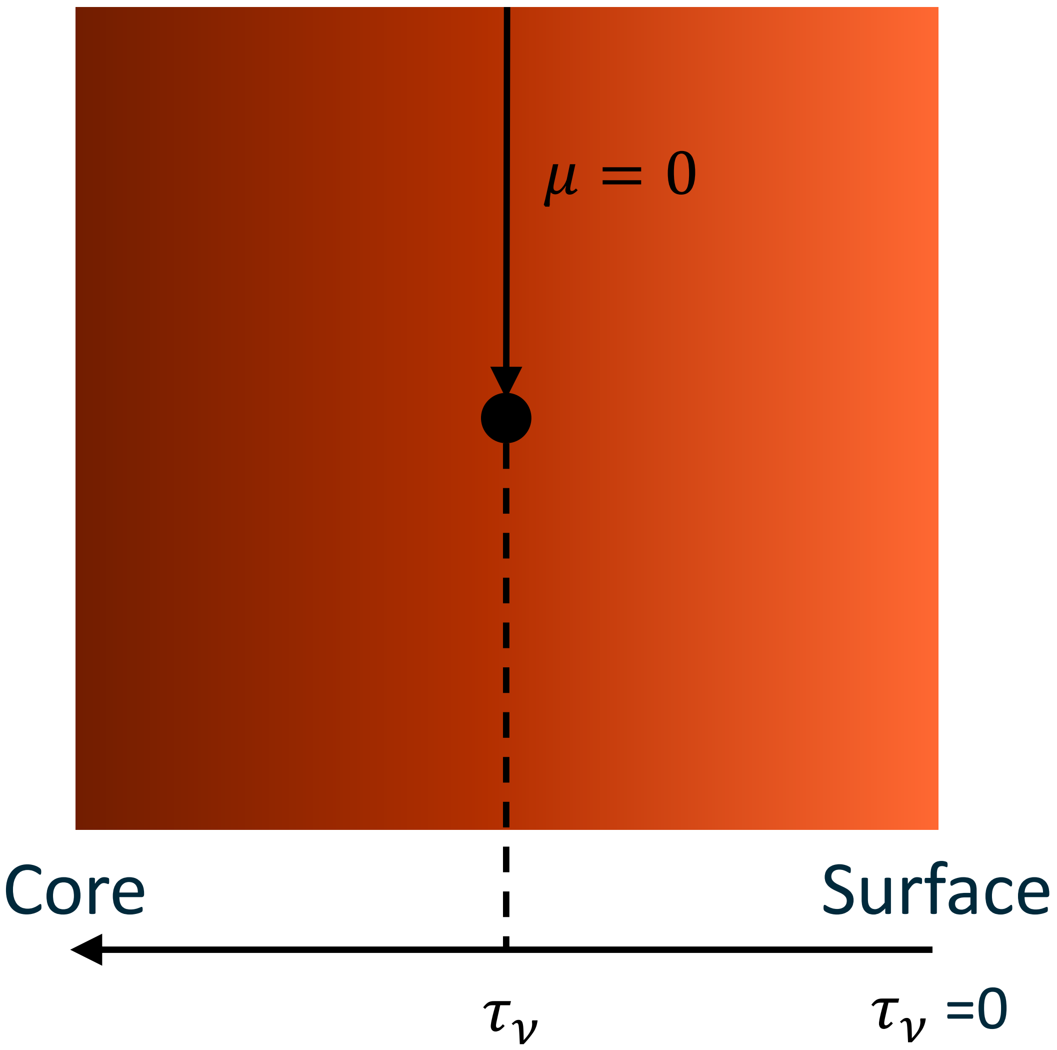

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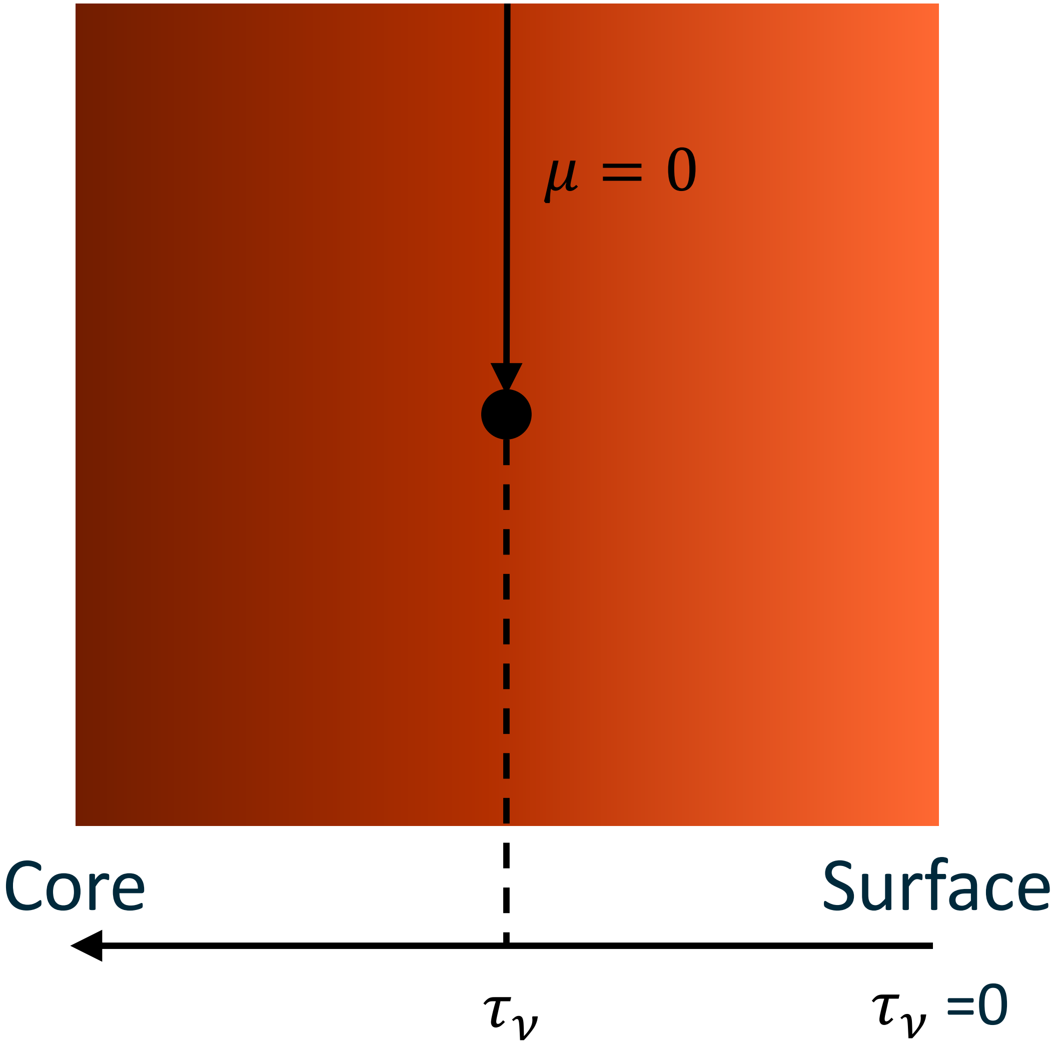

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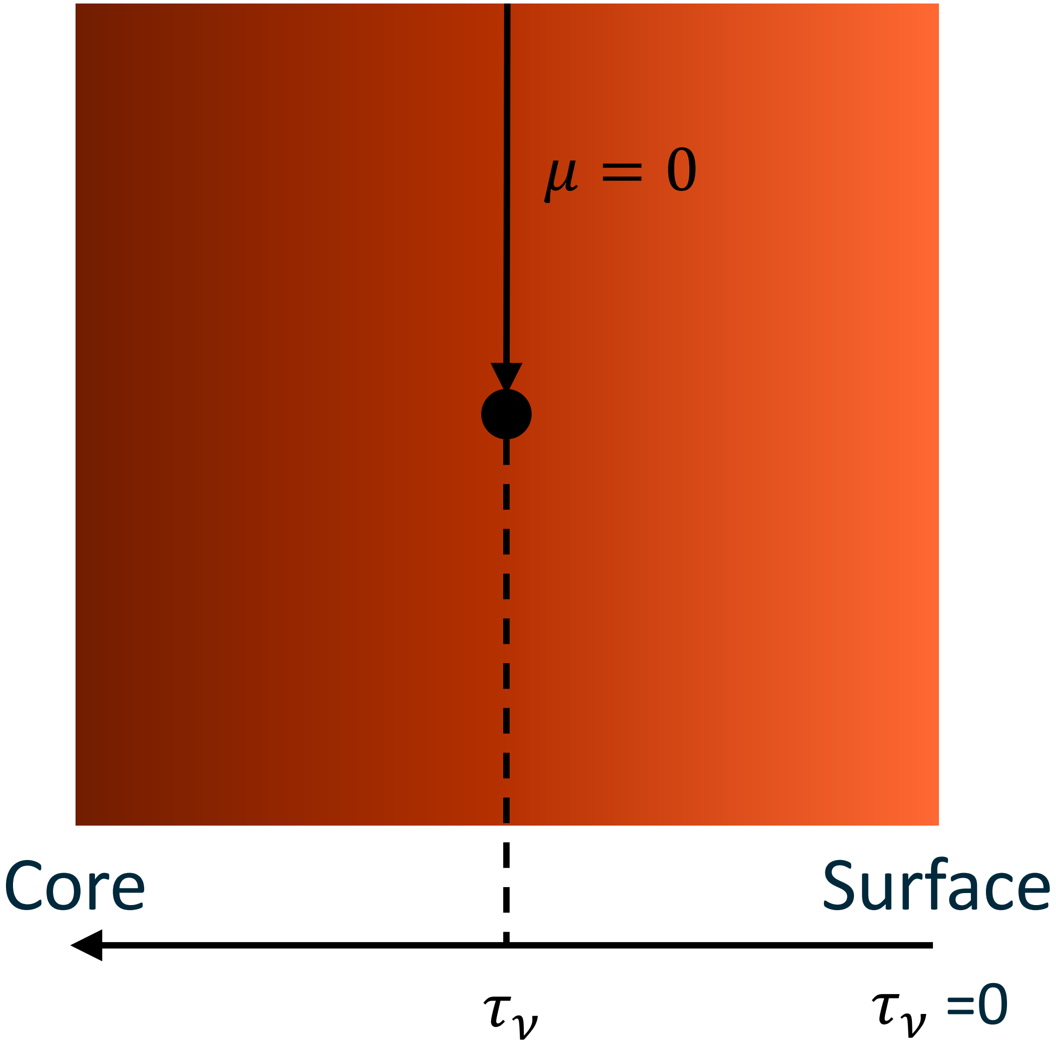

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Integrate over all frequency

$$q_R = -\frac{4\pi}{3} \frac{\left[\int \frac{1}{\kappa_\nu} \frac{dB_\nu}{dT} d\nu\right]}{\int \frac{dB_\nu}{dT} d\nu} \int \frac{dB_\nu}{dT} d\nu \frac{dT}{dx}$$

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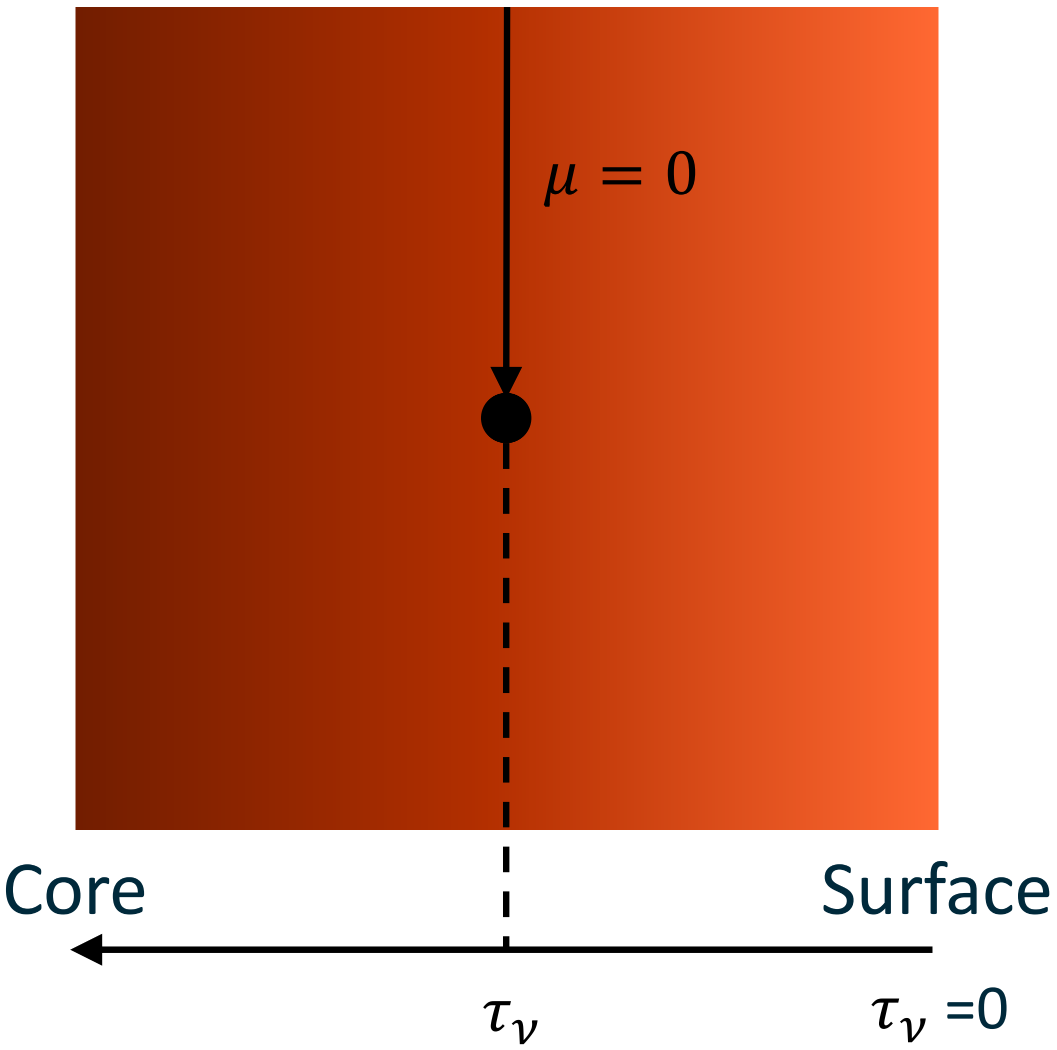

Radiation transport equation

$$I_\nu(\tau_\nu, \mu) \approx B_\nu(\tau_\nu) - \mu \frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$$

Compute spectral flux:

$$q_\nu = -\frac{4\pi}{3}\frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$$

Integrate over all frequency

$$q_R = -\frac{4\pi}{3}\frac{\left[\int \frac{1}{\kappa_\nu}\frac{dB_\nu}{dT}d\nu\right]}{\int \frac{dB_\nu}{dT}d\nu}\int \frac{dB_\nu}{dT}d\nu \frac{dT}{dx}$$

$4\sigma T^3/\pi$

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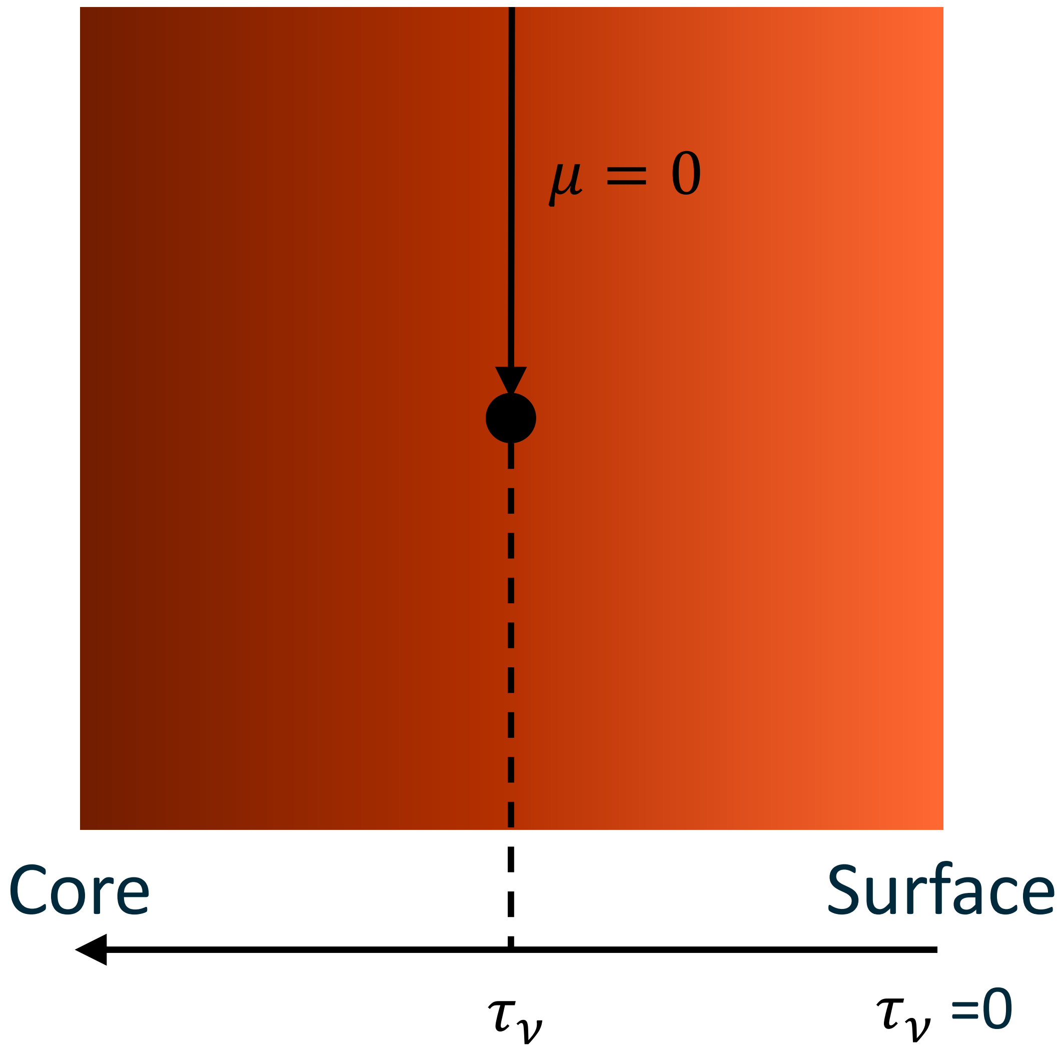

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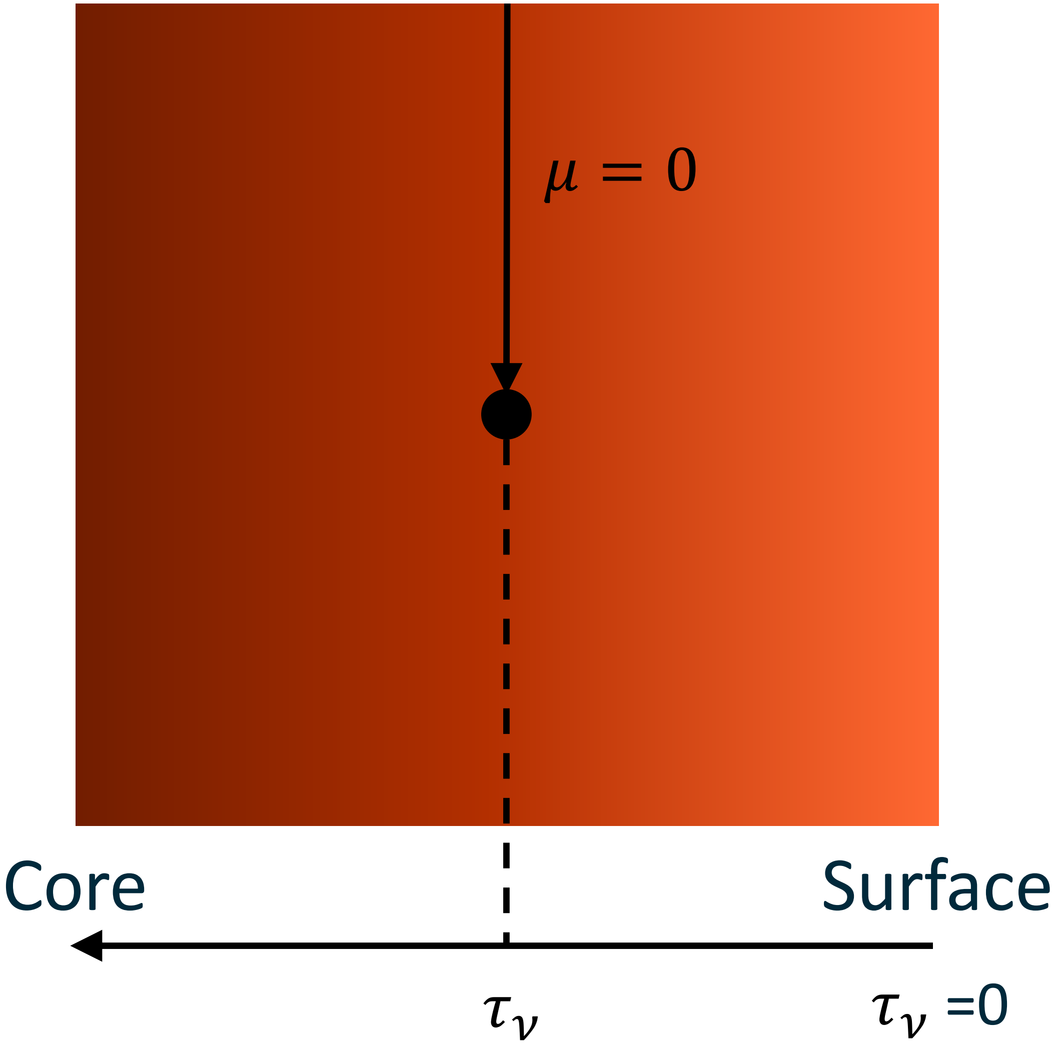

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$1/\kappa_R$ $\quad$ $4\sigma T^3/\pi$

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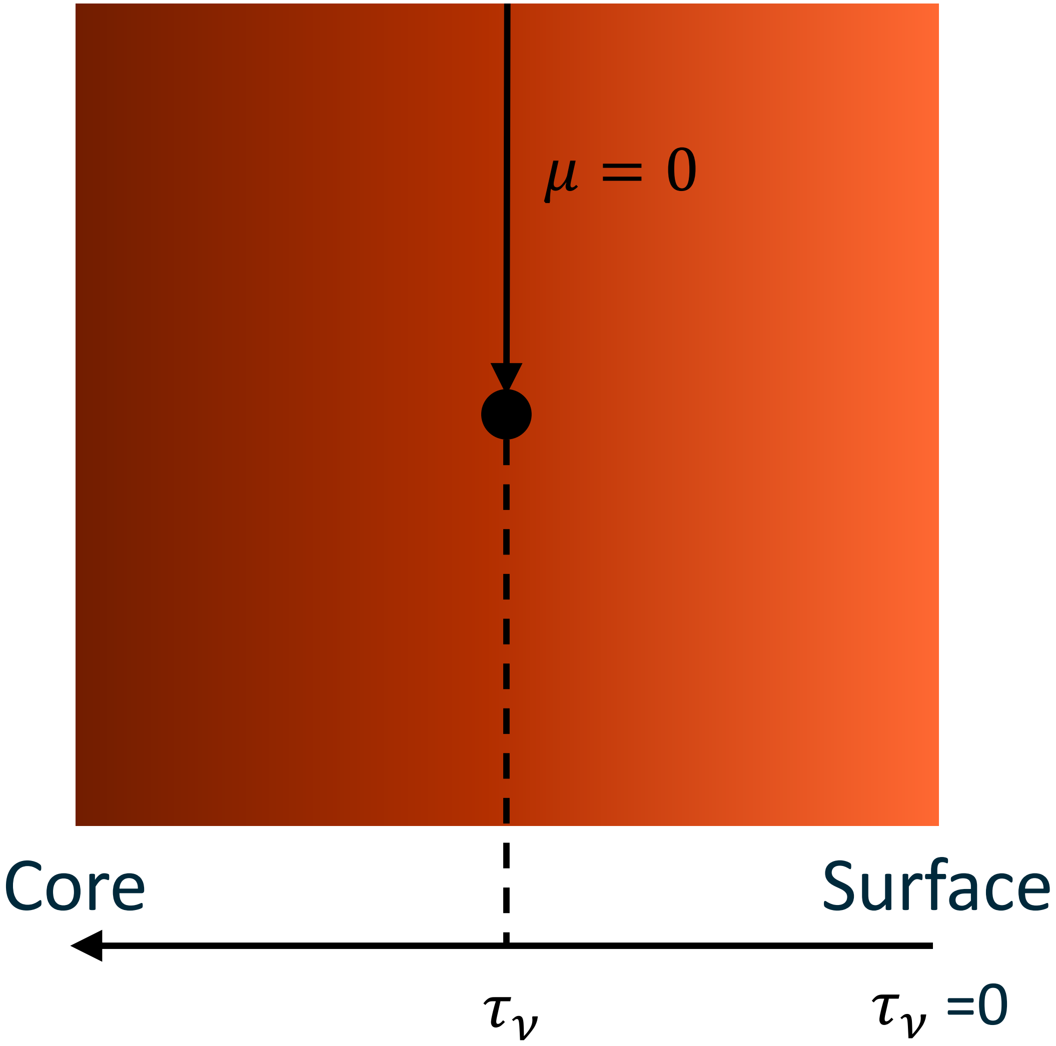

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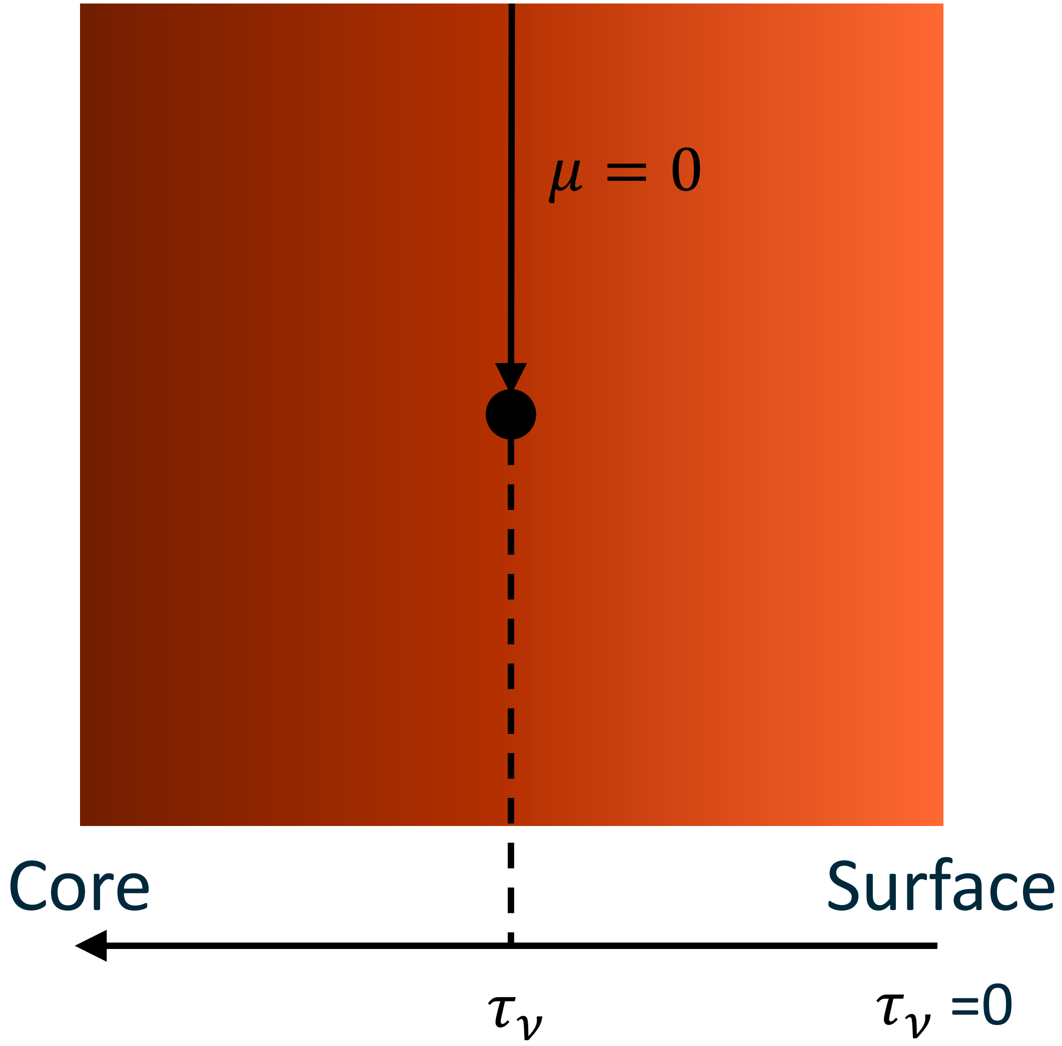

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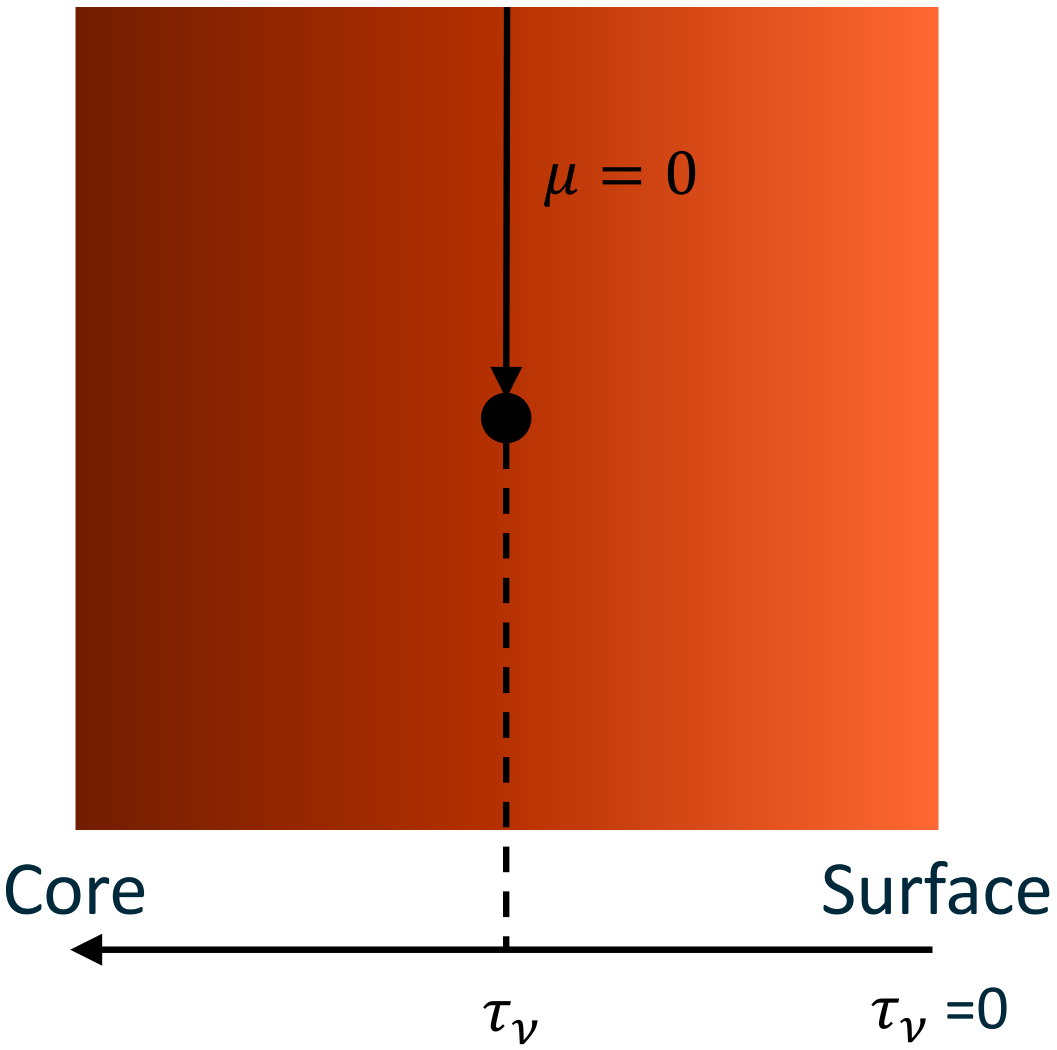

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Radiative heat flux with Rosseland-mean opacity is accurate at solar interior

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Assumptions:

- $S_\nu \equiv \epsilon_\nu / \kappa_\nu \approx B_\nu$

  → LTE
- $I_\nu(\tau_\nu, \mu) \approx B_\nu(\tau_\nu) - \mu \frac{dB_\nu(\tau_\nu)}{d\tau_\nu}$

  → Far enough from surface ($\tau_\nu \gg 1$)

  → The gradient is linear over the photon absorption length

These are valid assumptions at solar interior

Radiative heat flux with Rosseland-mean opacity is accurate at solar interior

Correct for solar interior

$$q_R = -\frac{16\sigma T^3}{3\kappa_R}\nabla T$$

where $\frac{1}{\kappa_R} \equiv \int \frac{1}{\kappa_\nu} w_\nu d\nu$ and $w_\nu \propto \frac{dB_\nu}{dT}$

Assumptions:

- $S_\nu \equiv \epsilon_\nu / \kappa_\nu \approx B_\nu$

  → LTE

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Can this be wrong? … Yes

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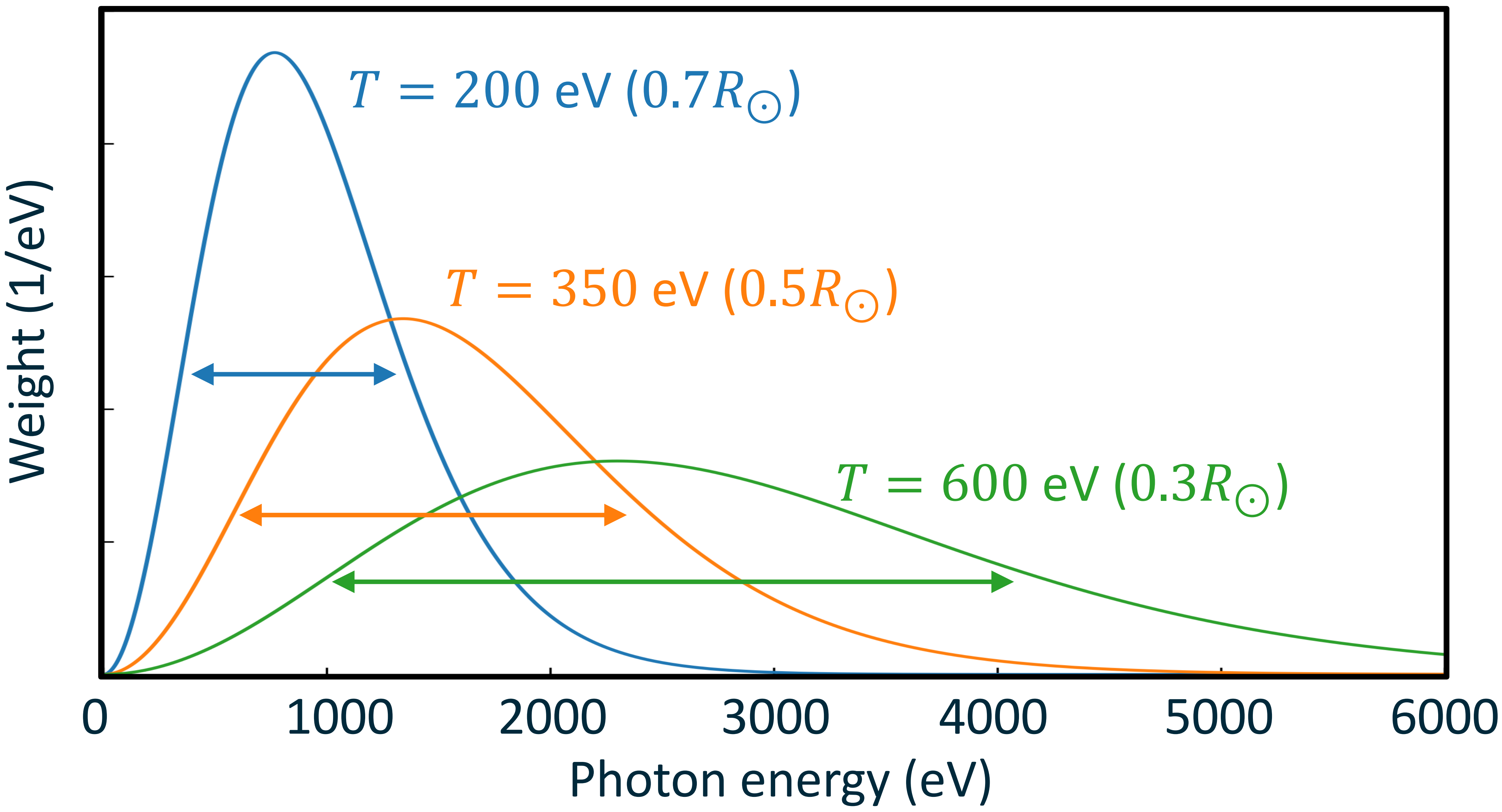
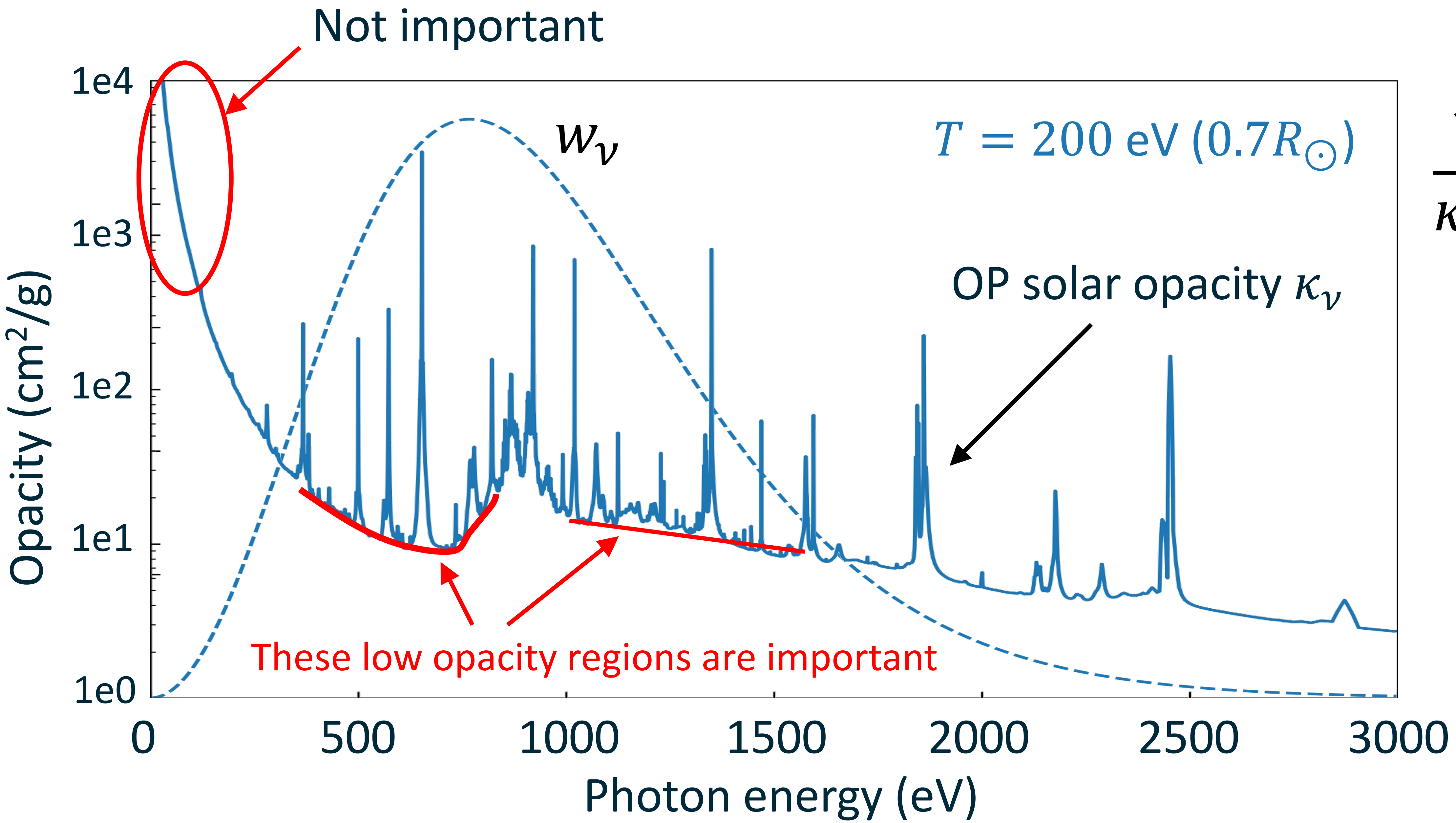
When κ_R is wrong, what exactly is wrong?
➔ Tough question to answer!

These are valid assumptions at solar interior

Challenge #1: Important spectral range depends on radius



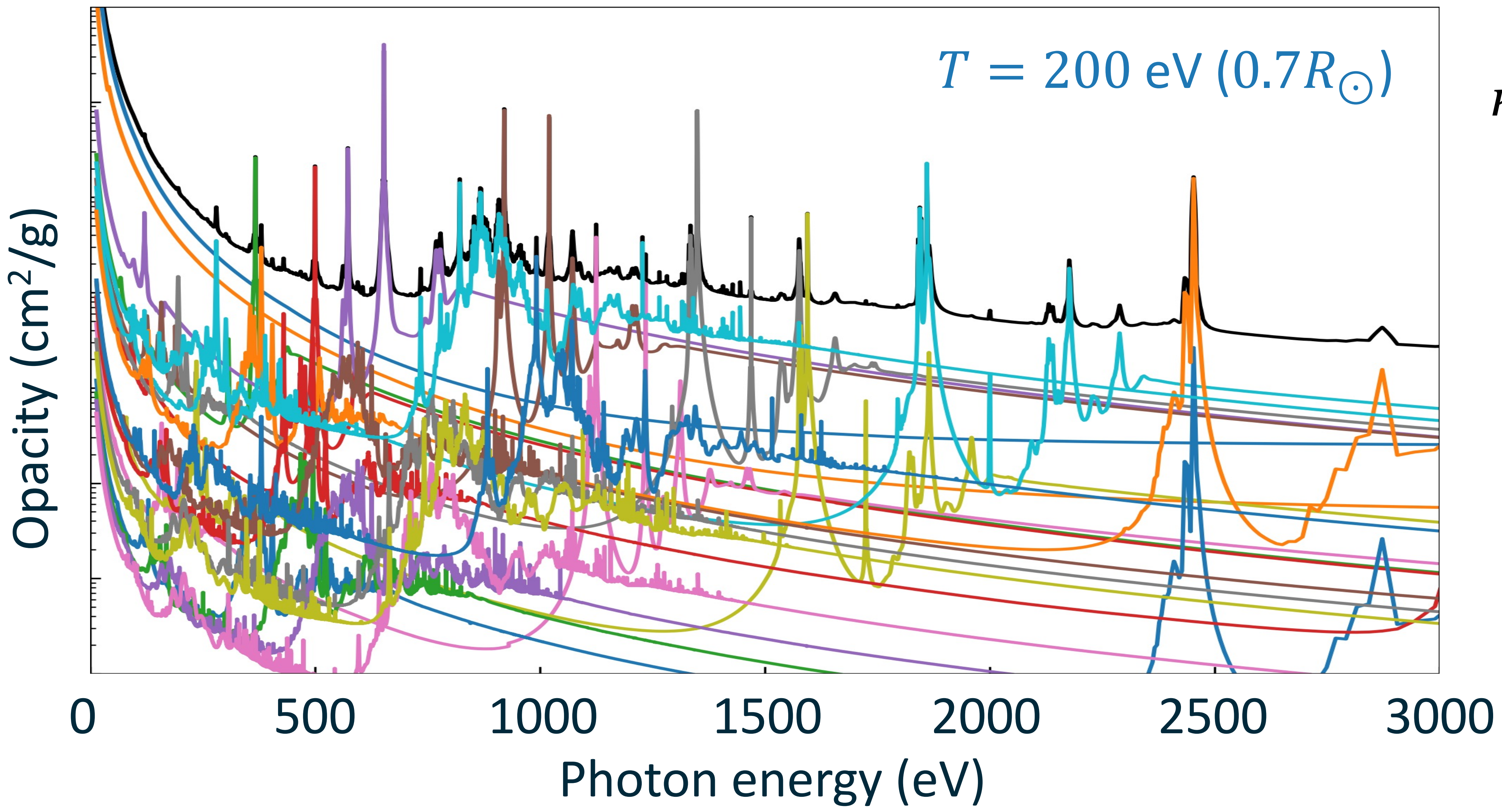
Challenge #2: Low opacity regions are important



$$\frac{1}{\kappa_R} \equiv \int \left(\frac{1}{\kappa_\nu}\right) w_\nu d\nu$$

Low opacity is important

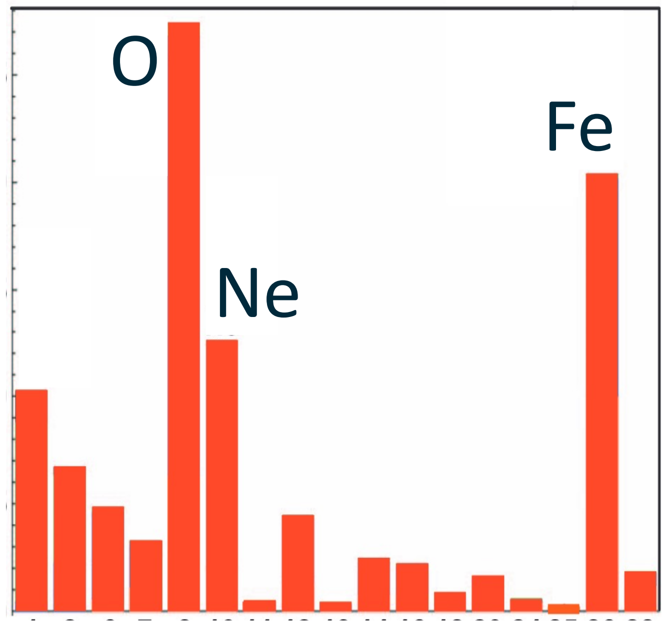
Challenge #3: Solar opacity depends on abundance and element opacity.



$$\kappa_\nu \equiv \sum_i f_i \, \kappa_{i,\nu}$$

abundance

element opacity



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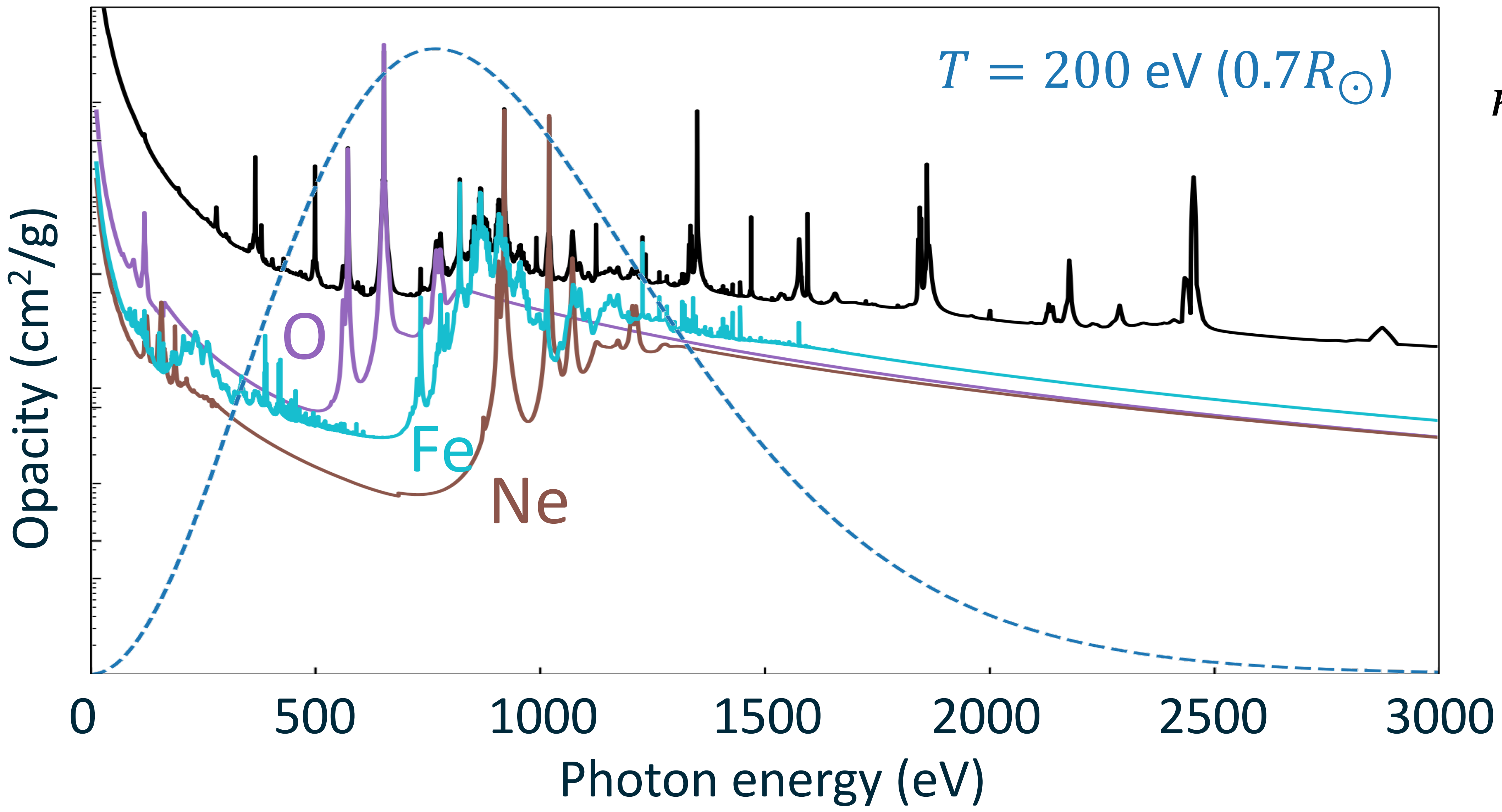

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abundance

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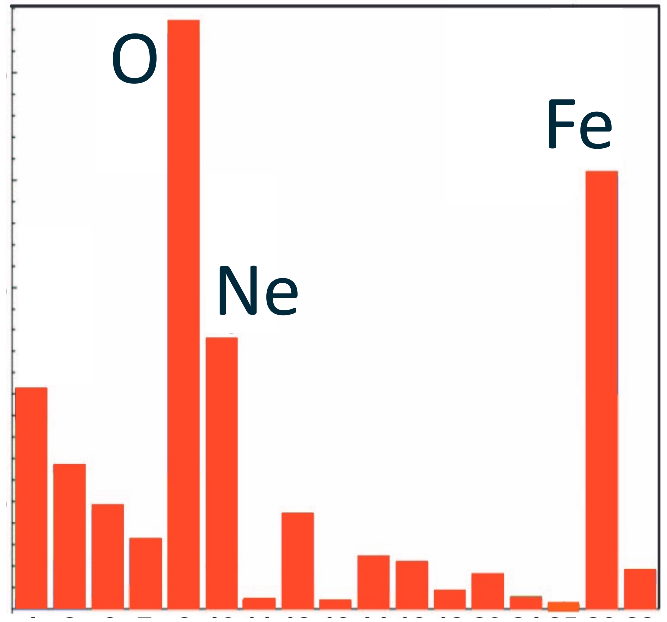
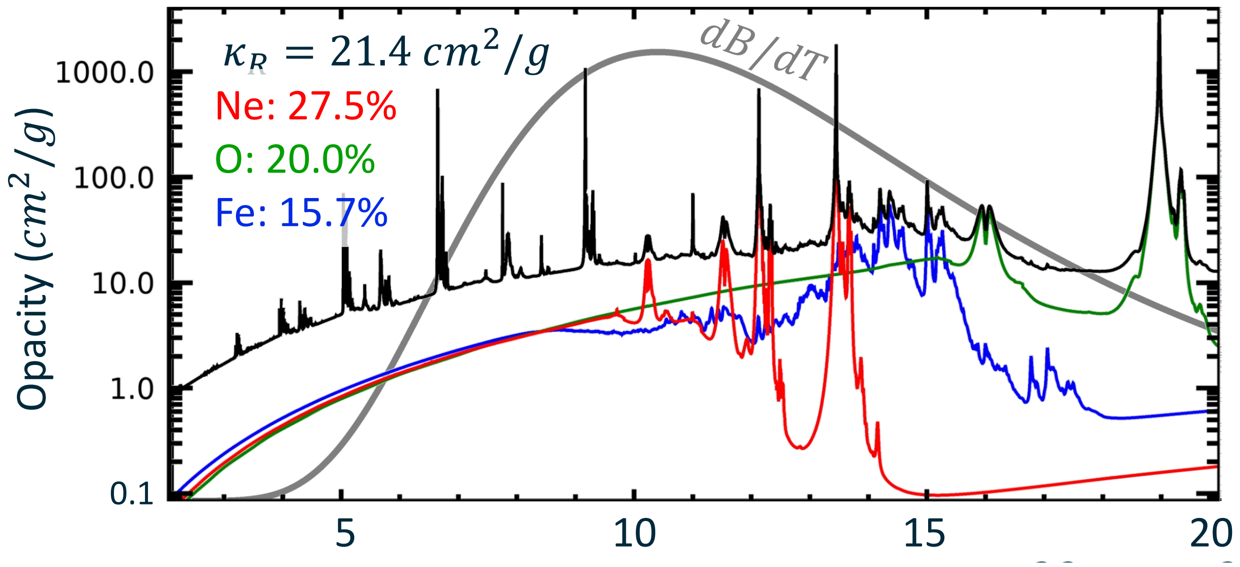
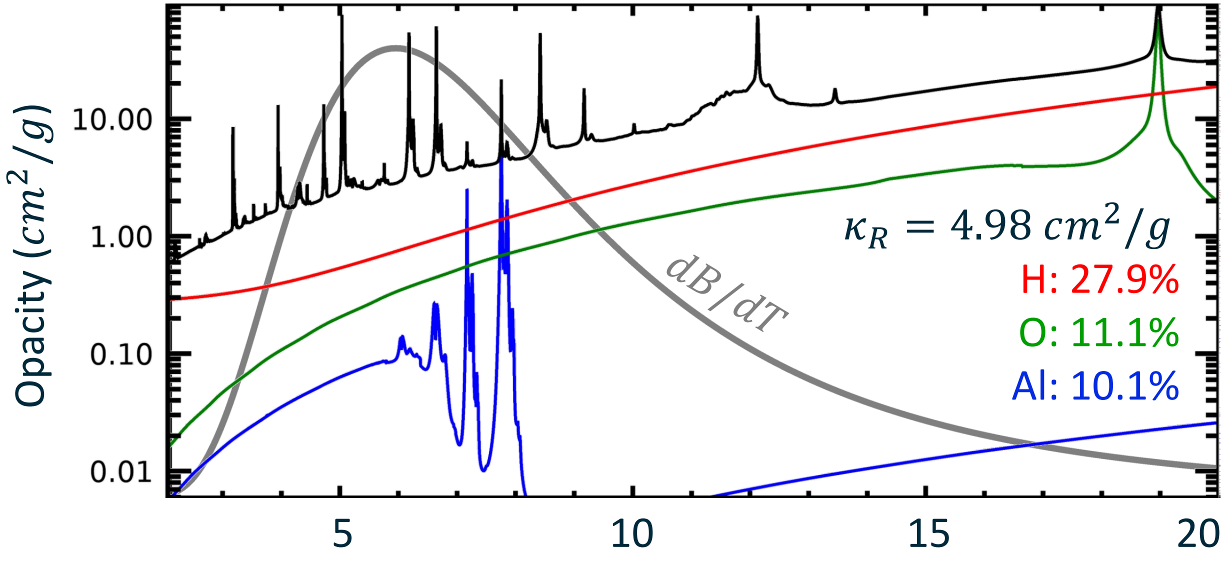


Challenge: Conditions, elements, spectral ranges, and important physics depend on radii

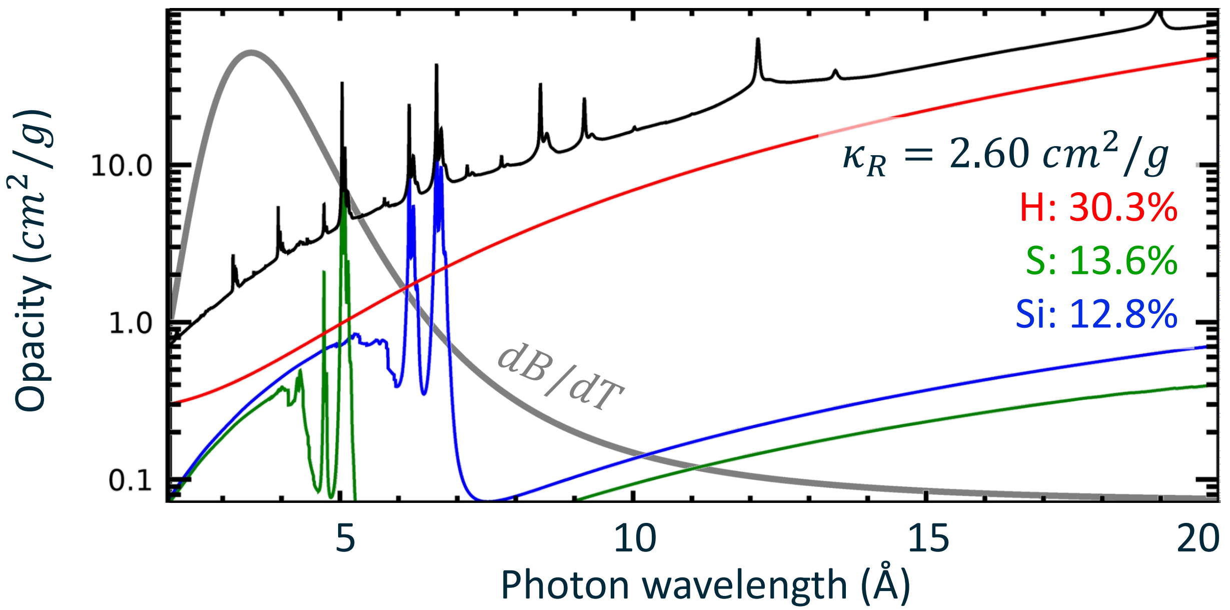
(a) $0.7R_{\odot}, T_e = 200\ eV, n_e = 1.14\times10^{23}\ cm^{-3}$



(b) $0.5R_{\odot}, T_e = 350\ eV, n_e = 7.19\times10^{23}\ cm^{-3}$



(c) $0.3R_{\odot}, T_e = 600\ eV, n_e = 4.34\times10^{24}\ cm^{-3}$



$$\frac{1}{\kappa_R} \equiv \int \frac{1}{\kappa_\nu} w_\nu d\nu$$

$$\kappa_\nu \equiv \sum_i \underline{f_i}\ \underline{\kappa_{i,\nu}}$$

abundance

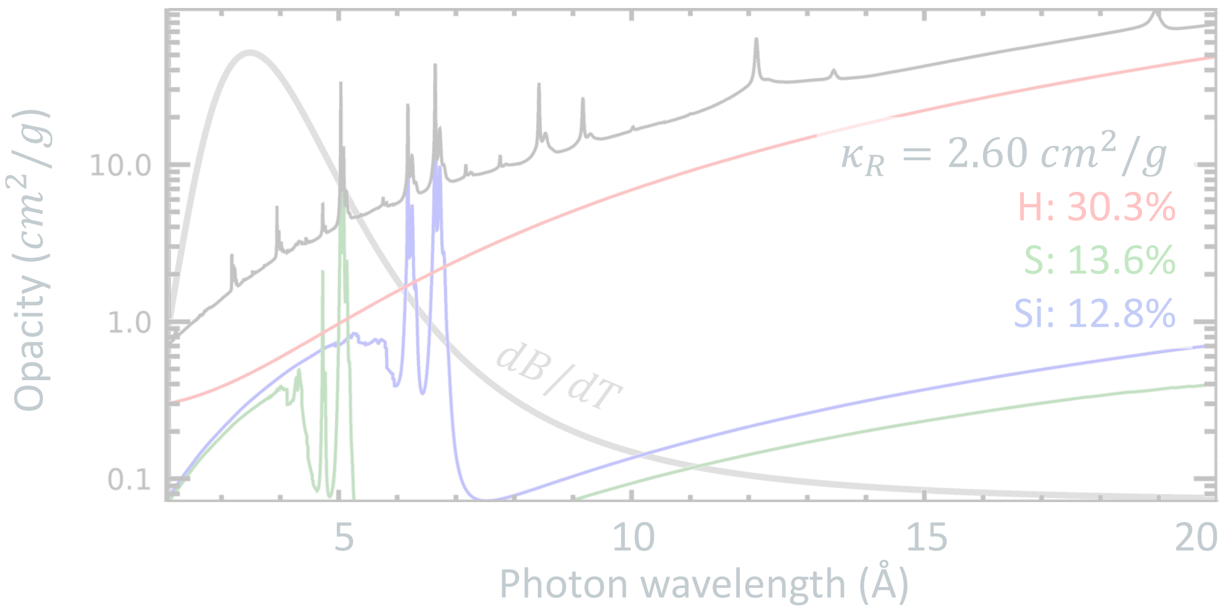
element opacity

Challenge: Conditions, elements, spectral ranges, and important physics depend on radii

(a)

- Solar Rosseland mean opacity is complex
  - Correction is condition-, frequency-, and element-dependent
  - We ***cannot*** introduce a simple correction factor
- **What we need = Experimentally validated opacity models**

(c) $0.3R_{\odot}, T_e = 600\ eV, n_e = 4.34\times10^{24}\ cm^{-3}$



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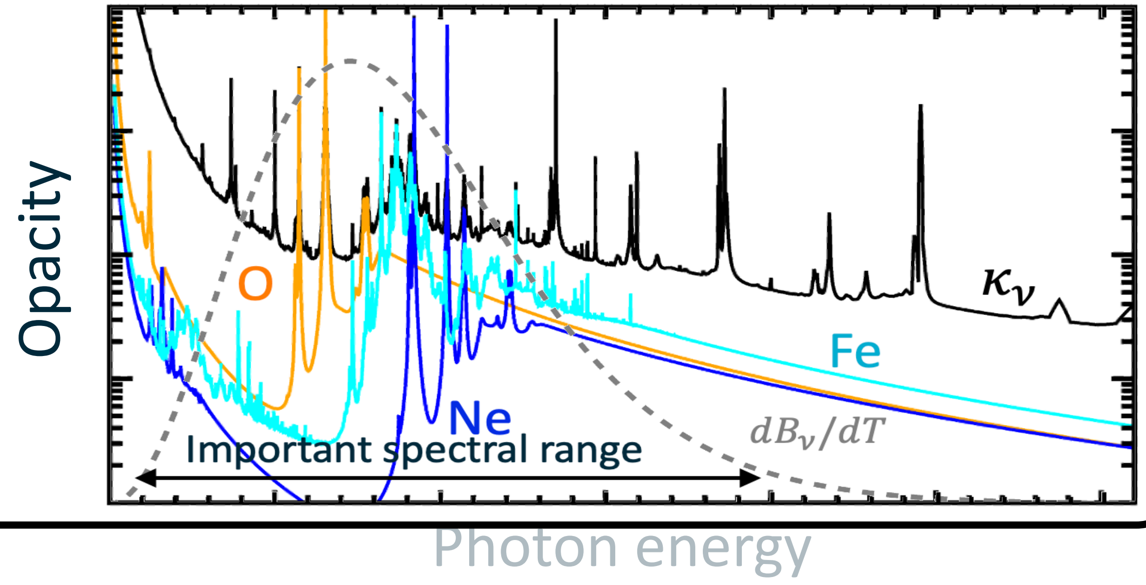
abundance

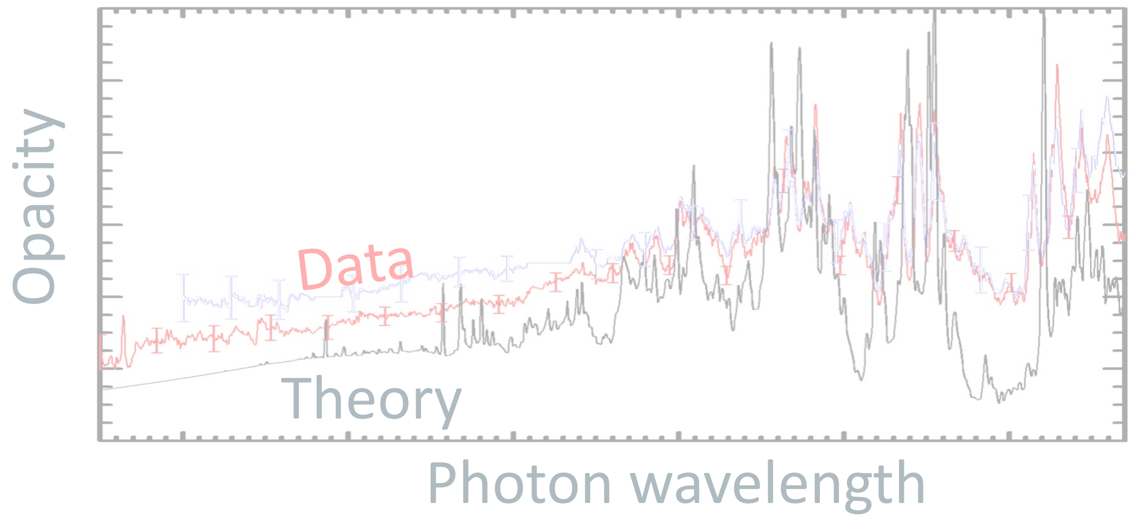
element opacity

Understanding solar opacity is challenging due to complex nature of Rosseland mean opacity

1. **Basics:** Rosseland mean opacity
   - Derivations, assumptions, and complexity
   - If RMO is wrong:
     → (1) Abundance and/or
     → (2) Calculated element opacity.



2. **Theory:** How element opacity is computed.
   - Opacity is computed by "first principle"
   - Models contain "untested" approximations



3. **Experiments:** experiments and future perspective
   - Experimental challenges
   - Z and NIF experiments

Worldwide opacity collaborations will soon help quantify the true accuracy of calculated element opacities

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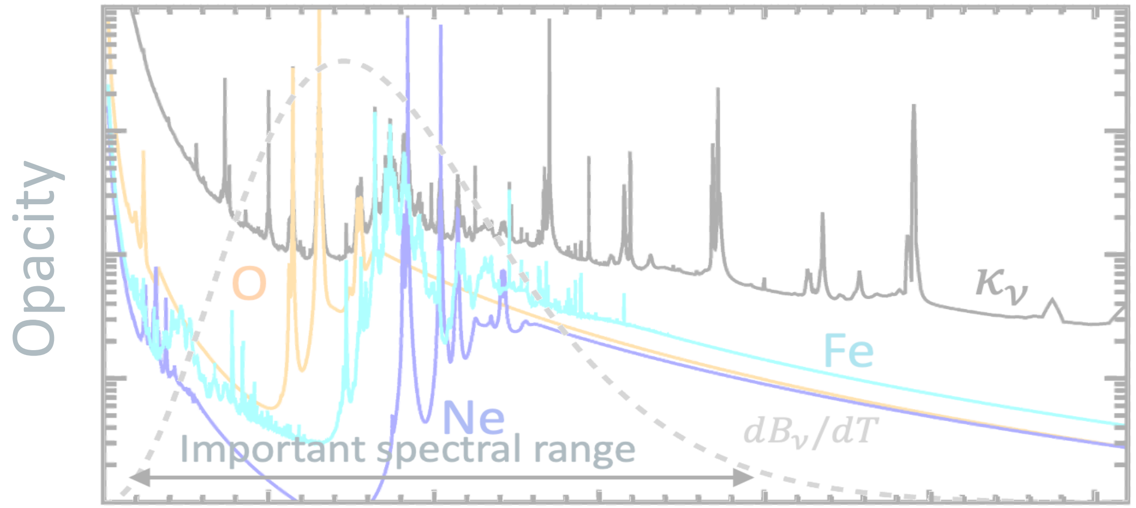

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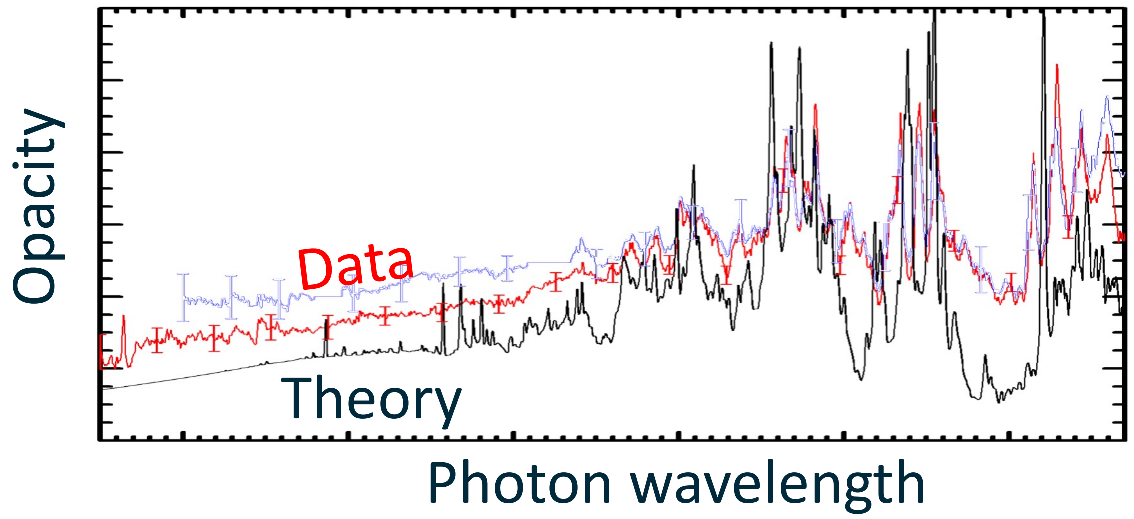

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Let's take a closer look at a couple of opacity spectra …

What are:

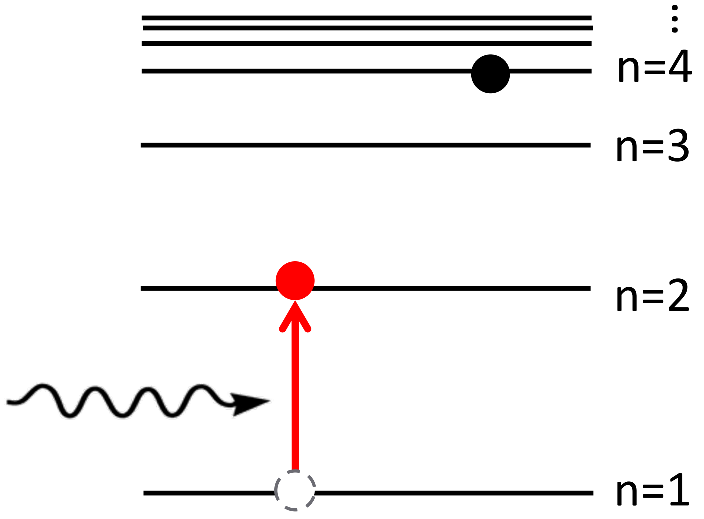
- K-shell, L-shell?
- Bound-bound, bound-free?

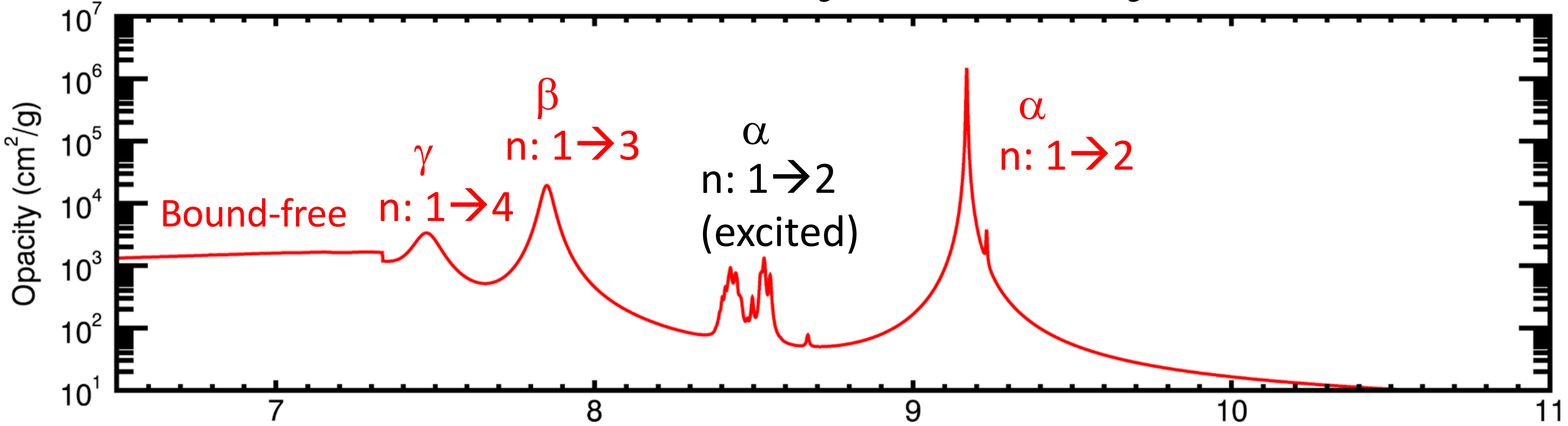
Why is opacity calculation difficult with many bound electrons?

Opacity calculation becomes more challenging as the number of bound electrons increases

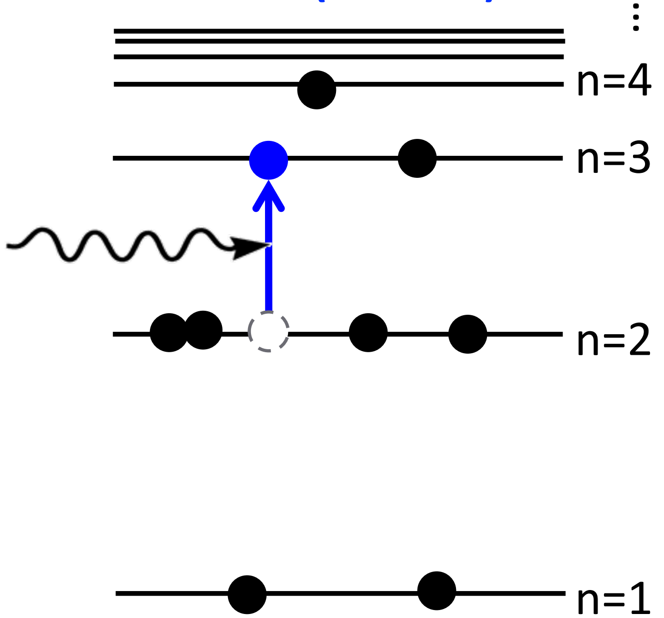
CZB = Convection Zone Base ($T_e = 182$ eV, $n_e = 9\times10^{22}\ cm^{-3}$)

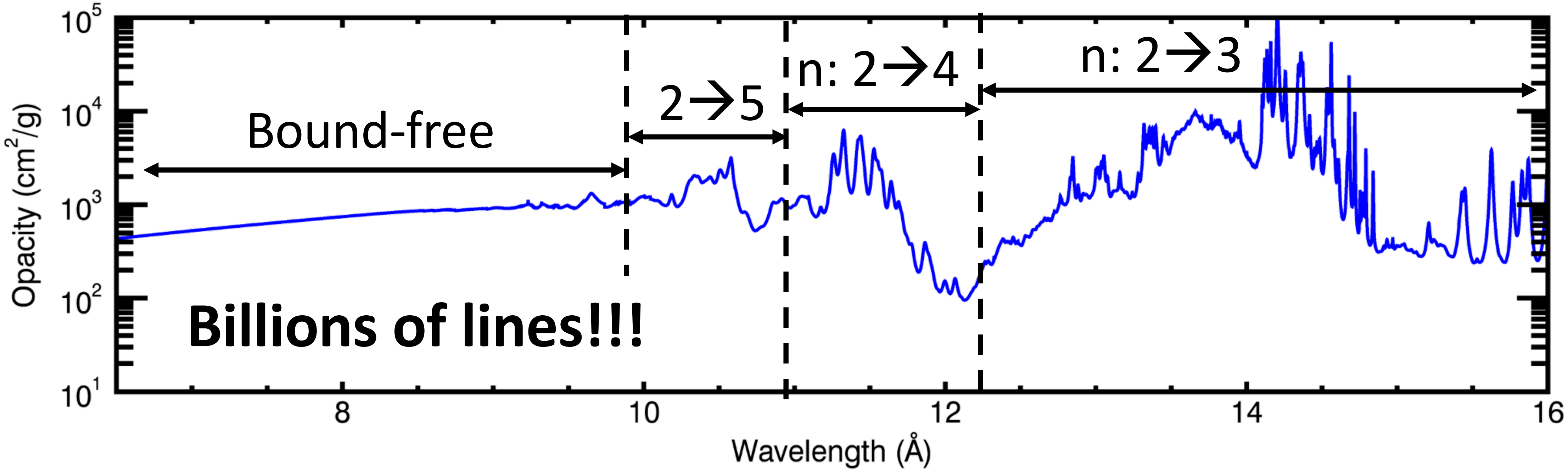
Mg at CZB (Z=12)





Fe at CZB (Z=26)

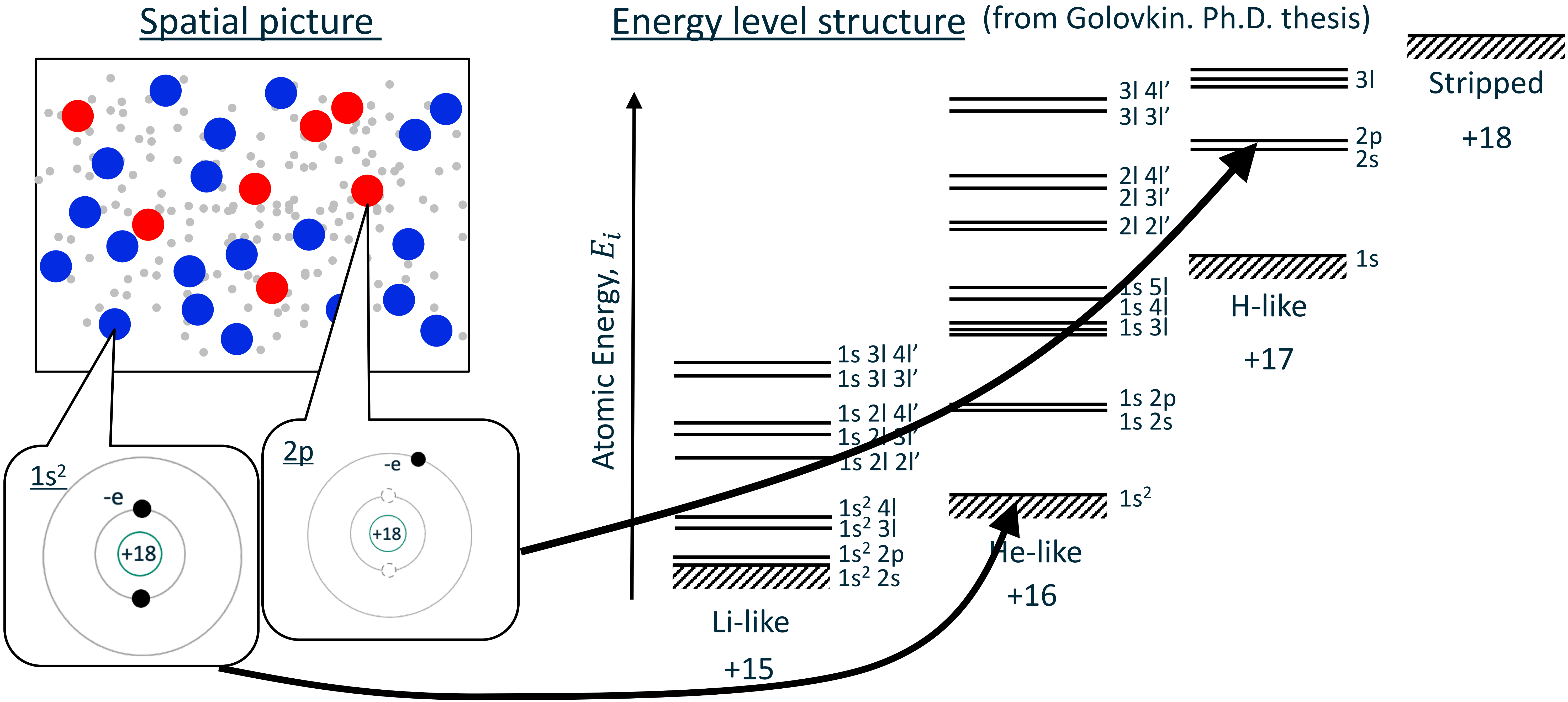




How is opacity computed?

Let’s start with a general picture and elaborate it a little more …

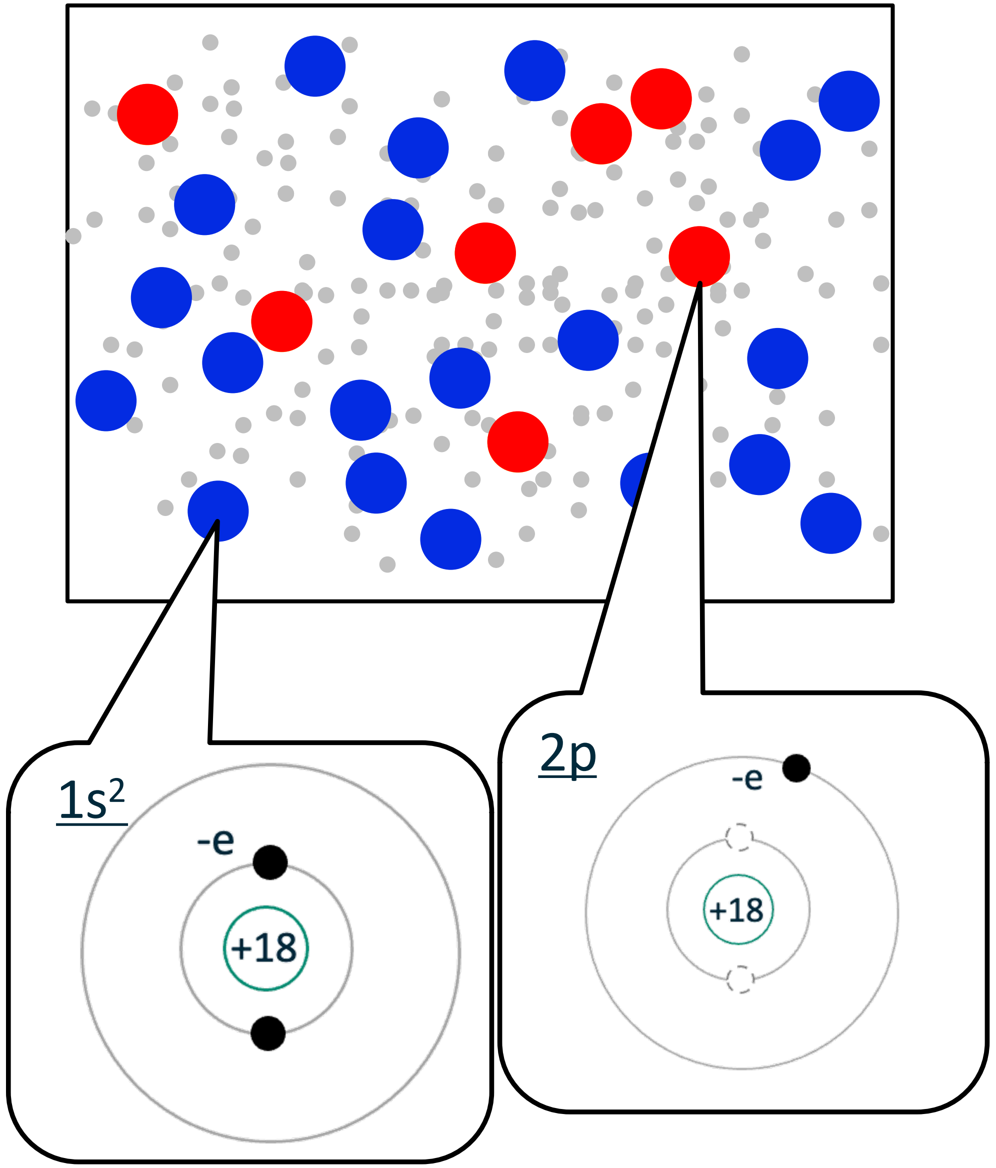
Spectrum is the result of the *energy level structure*, *rates of atomic processes*, and *population*



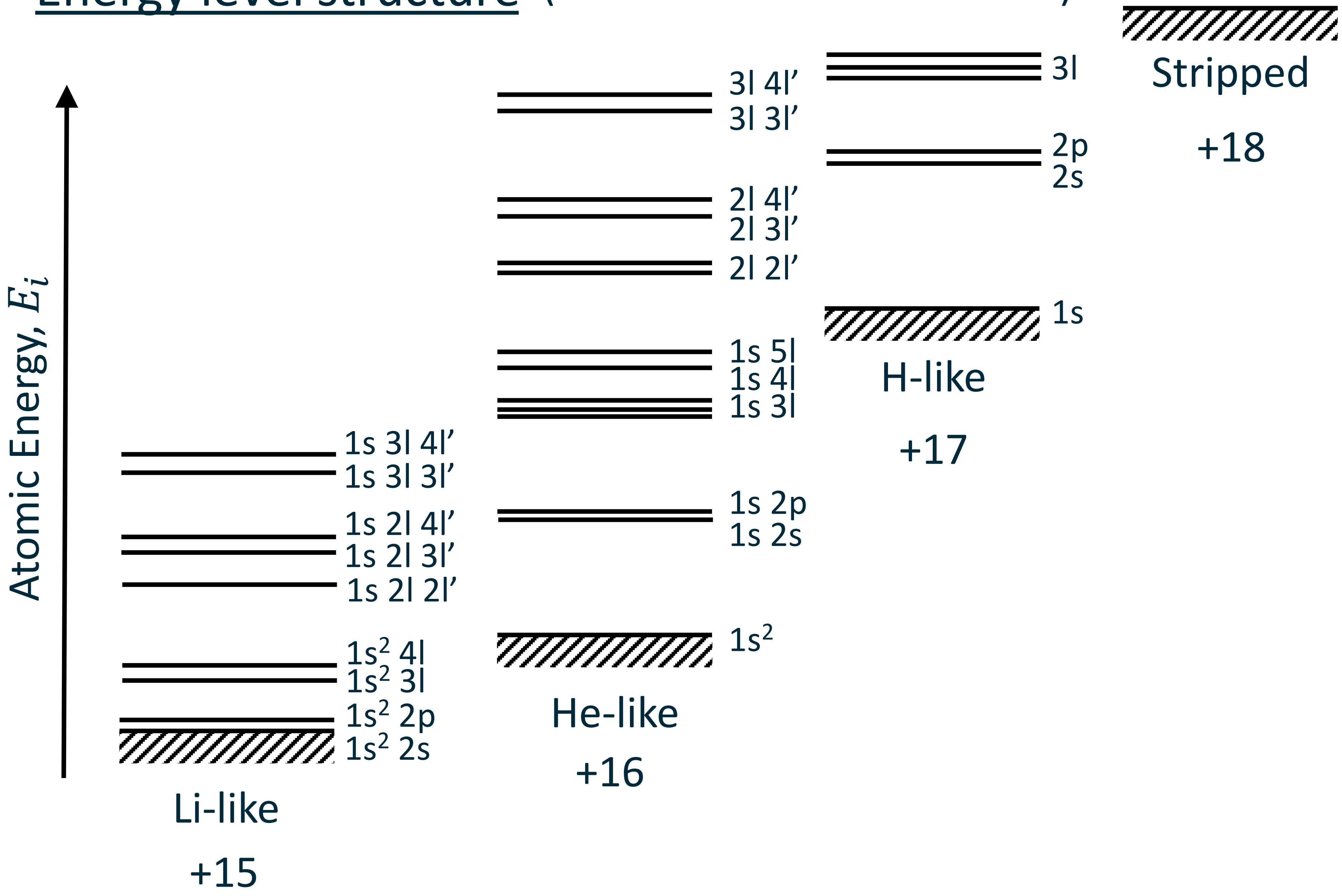
ChatGPT: What is electronic configuration?

Spectrum is the result of the *energy level structure*, *rates of atomic processes*, and *population*

Spatial picture



Energy level structure (from Golovkin. Ph.D. thesis)



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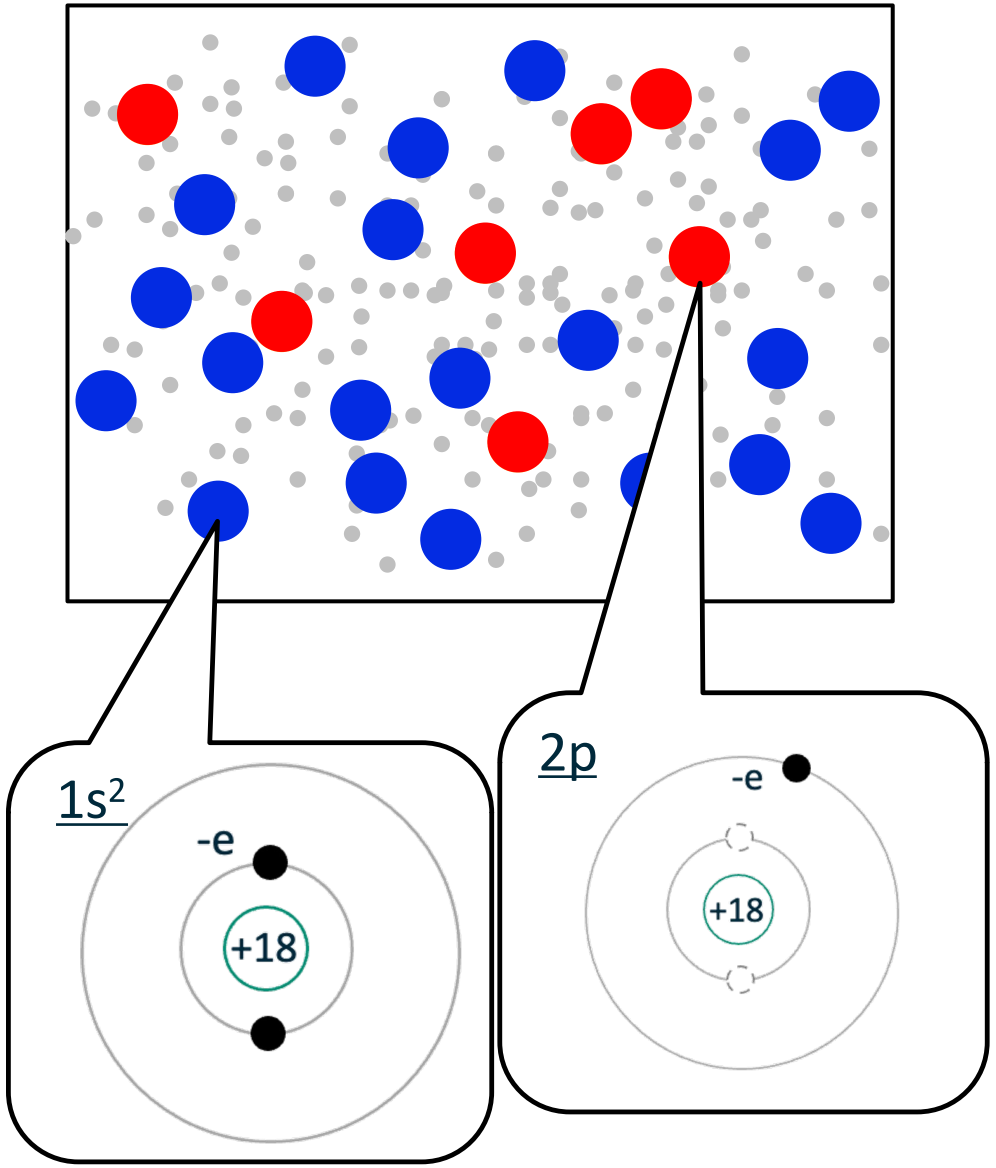

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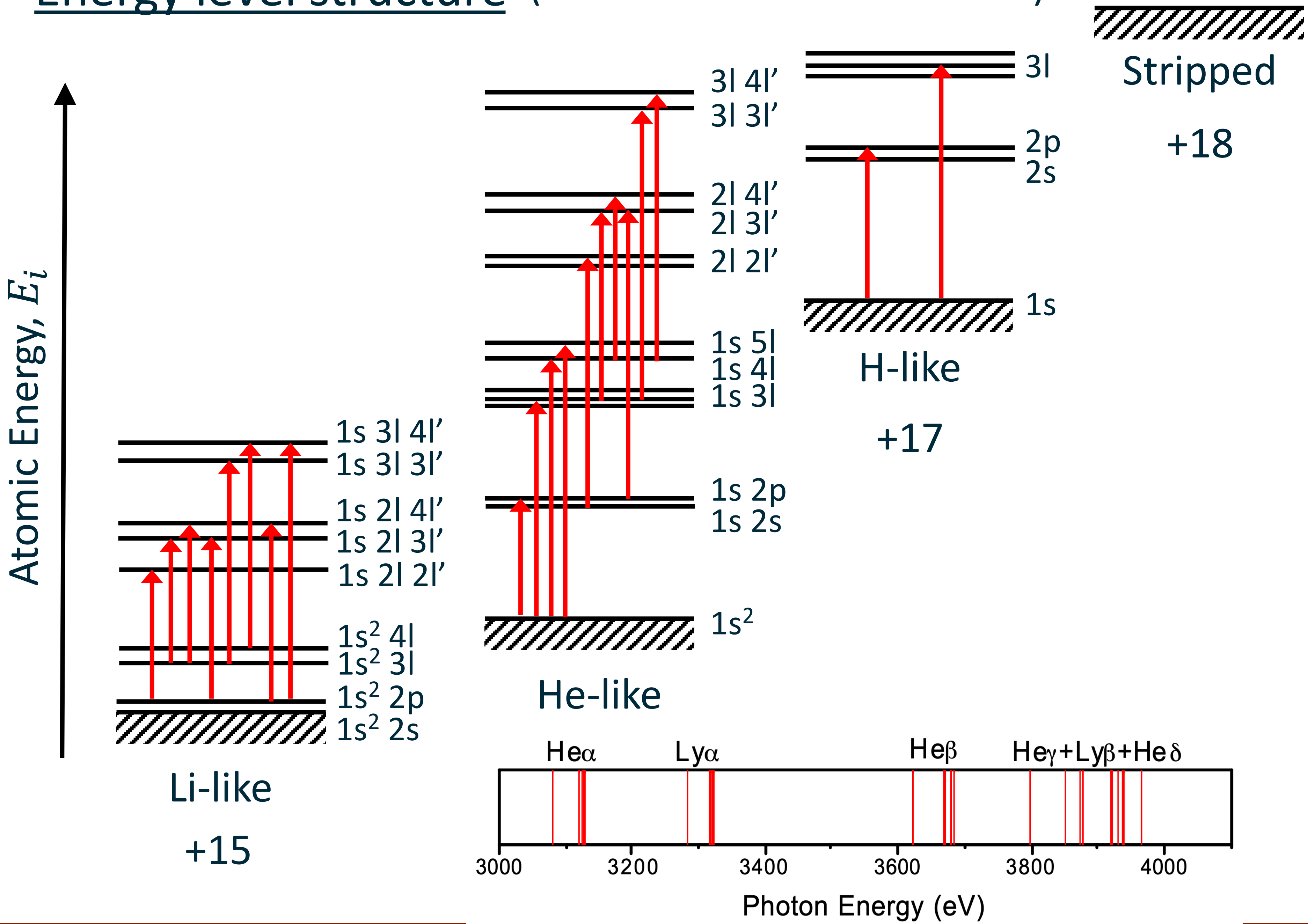

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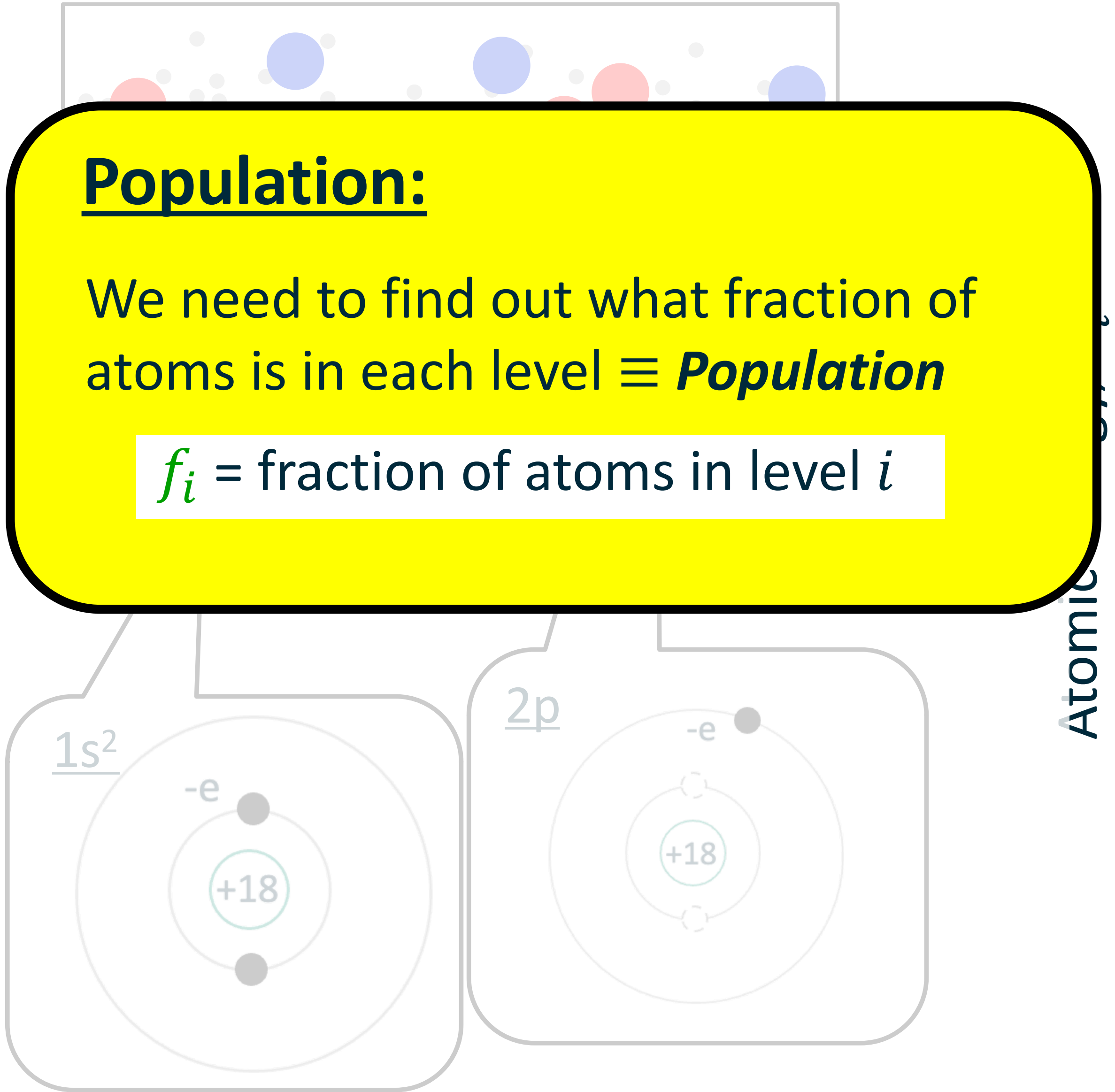
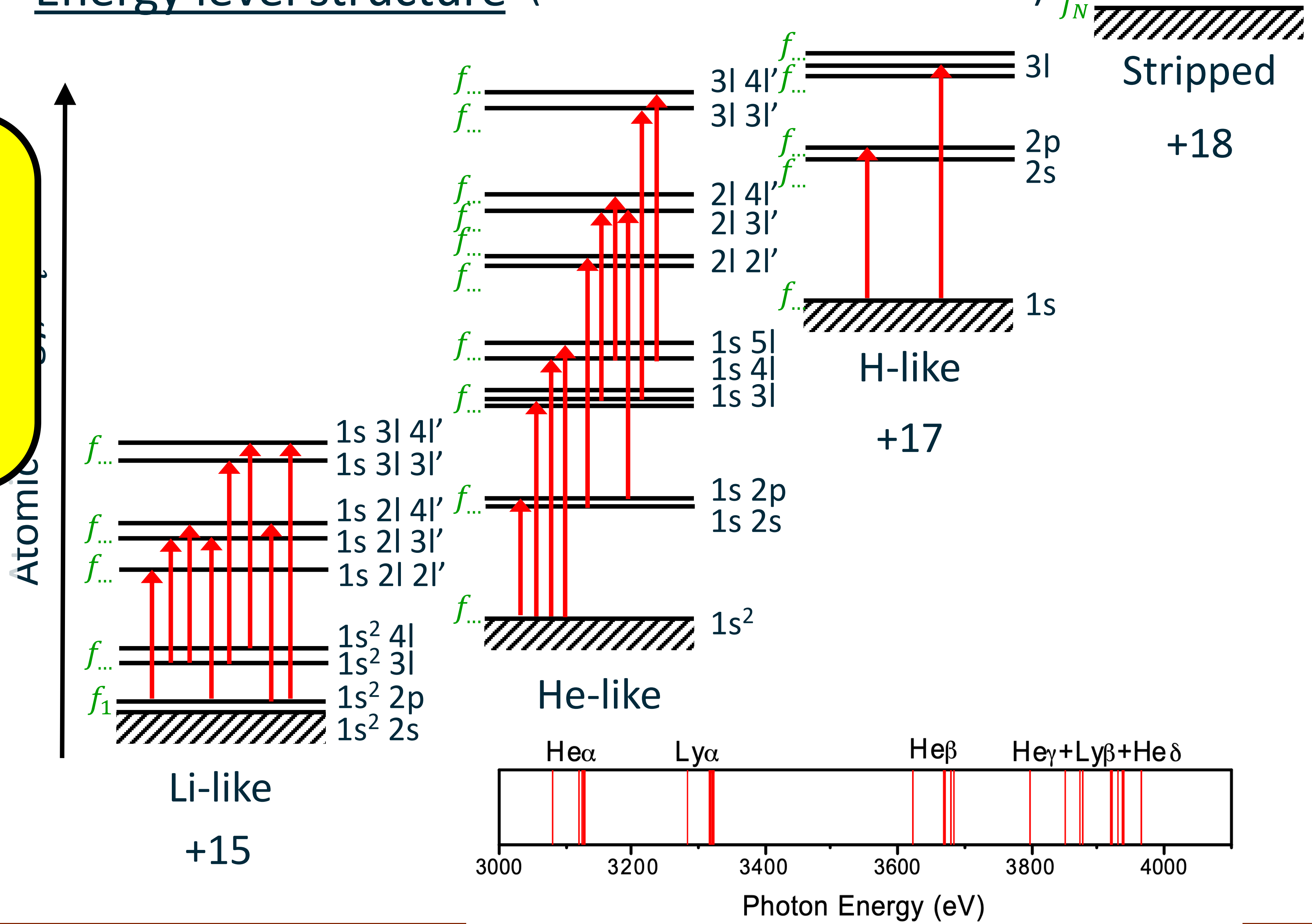


Population:

We need to find out what fraction of atoms is in each level ≡ ***Population***

f_i = fraction of atoms in level i

Energy level structure (from Golovkin. Ph.D. thesis)



ChatGPT: What is electronic configuration?

How is opacity computed?

Opacity is computed from first principle …

Three ingredients:

1: Atomic physics ($\epsilon_i, \psi_i, f_{ij}, \sigma_{ij}$)
2: Spectral line shapes (ϕ_{ij})
3: Equation of state (f_i)

(1–2) Atomic absorption cross-section

(2–3) What atomic states are populated?

→ Combine them all to get element spectral opacity

Ingredient 1: Compute atomic data ϵ_i, ψ_i, f_{bb}, and $\sigma_{bf}(E)$

Atomic structure code*

(1) Solve Schrödinger equation for each atomic state i

$$H_i\psi_i = \epsilon_i\psi_i$$

ϵ_i = state energy
ψ_i = state wavefunction

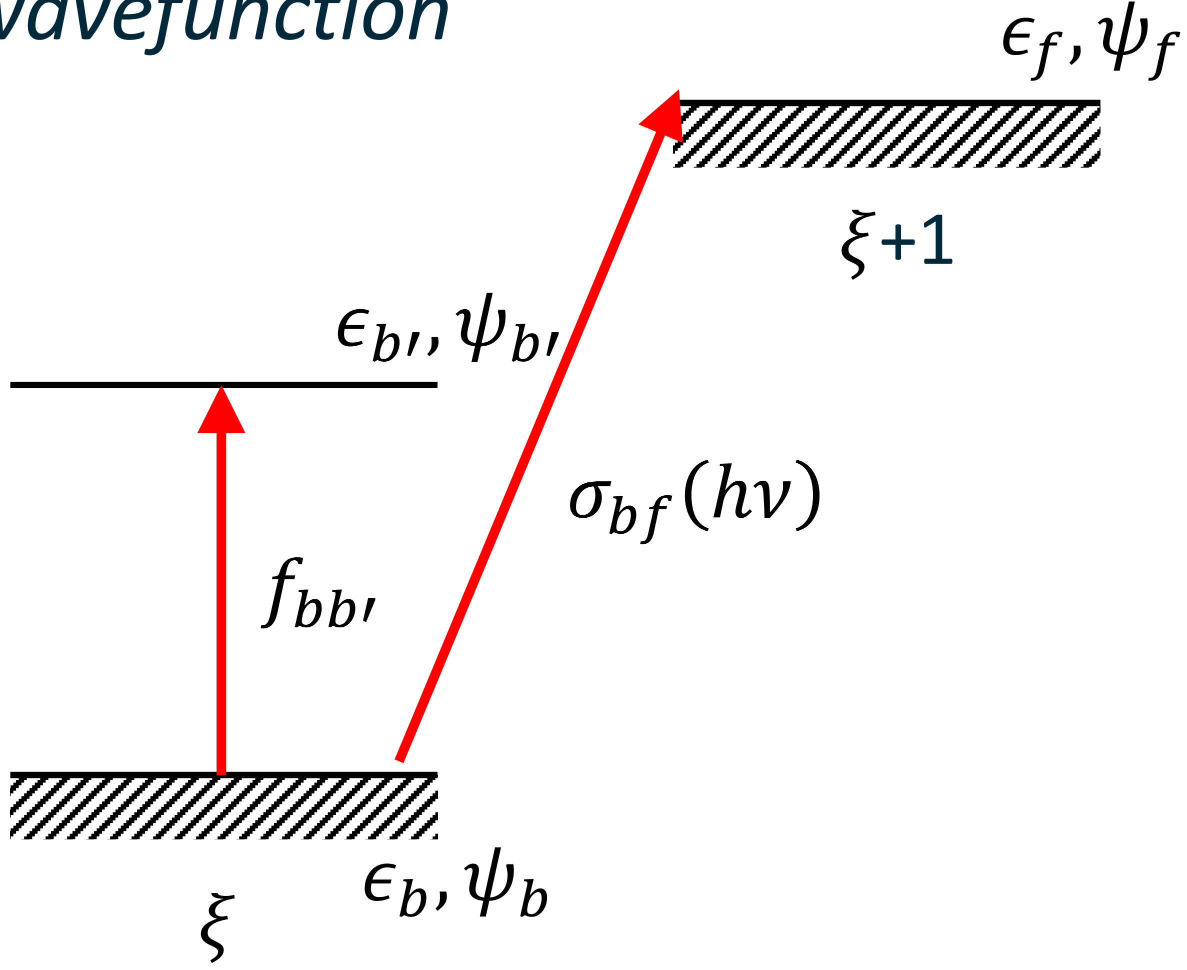
(2) Compute *oscillator strengths* for each *bound-bound* transition, f_{bb}

$$f_{bb'} \propto |\langle\psi_{b'}|r|\psi_b\rangle|^2$$

Collision code**

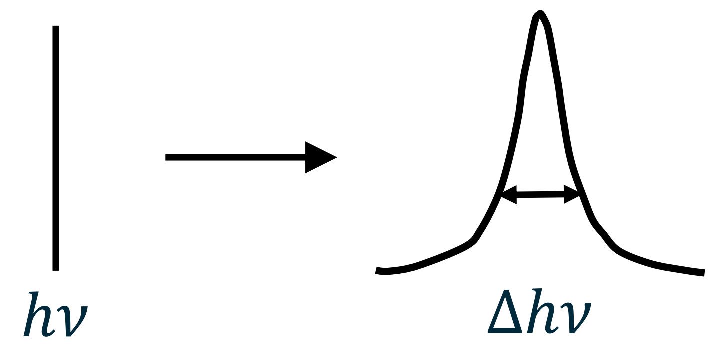
(3) Compute *bound-free cross-section*

$$\sigma_{bf}(h\nu) \propto \left|\langle\psi_f|r|\psi_b\rangle\right|^2$$



Ingredient 2: Incorporate spectral line shape to get bound-bound atomic absorption cross-section

$$\sigma_{bb'}(h\nu) \propto f_{bb'}\phi(h\nu)$$



Spectral line shape

- Pressure broadening
- Doppler broadening
- Natural broadening

- $\sigma_{bb'}(h\nu)$ and $\sigma_{bf}(h\nu)$ are atomic absorption cross-section in cm^2
- We need to know how many atoms are in such initial states ($\#/cm^3$)

Ingredient 3: Determine the population using the Saha equation and Boltzman distribution → Depends on T_e and n_e

1) Saha equation: across the charge states

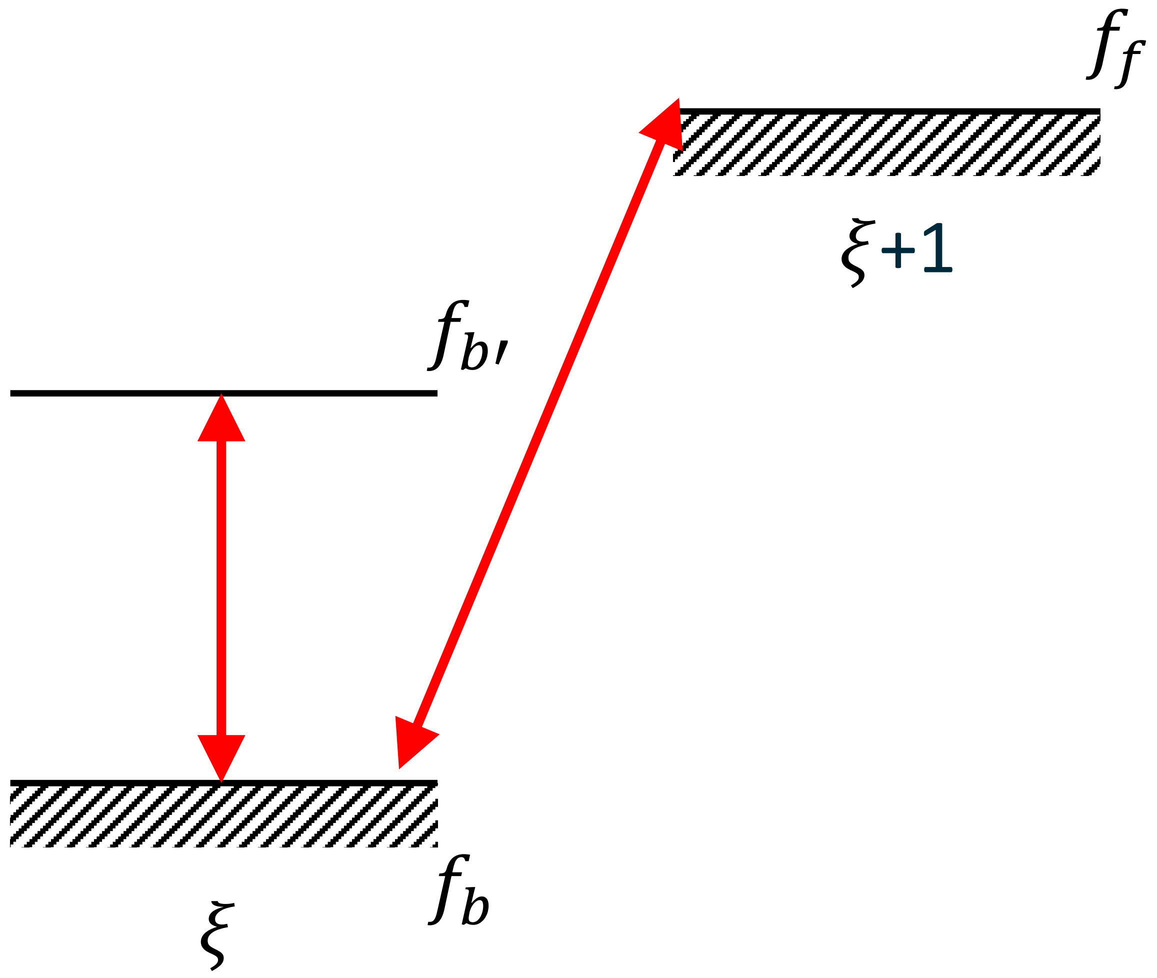
$$\frac{f_f}{f_b} \propto \frac{\exp(-\Delta E/T_e)}{n_e} \qquad \Delta E = \epsilon_f - \epsilon_b$$

2) Boltzmann distribution: within the charge states

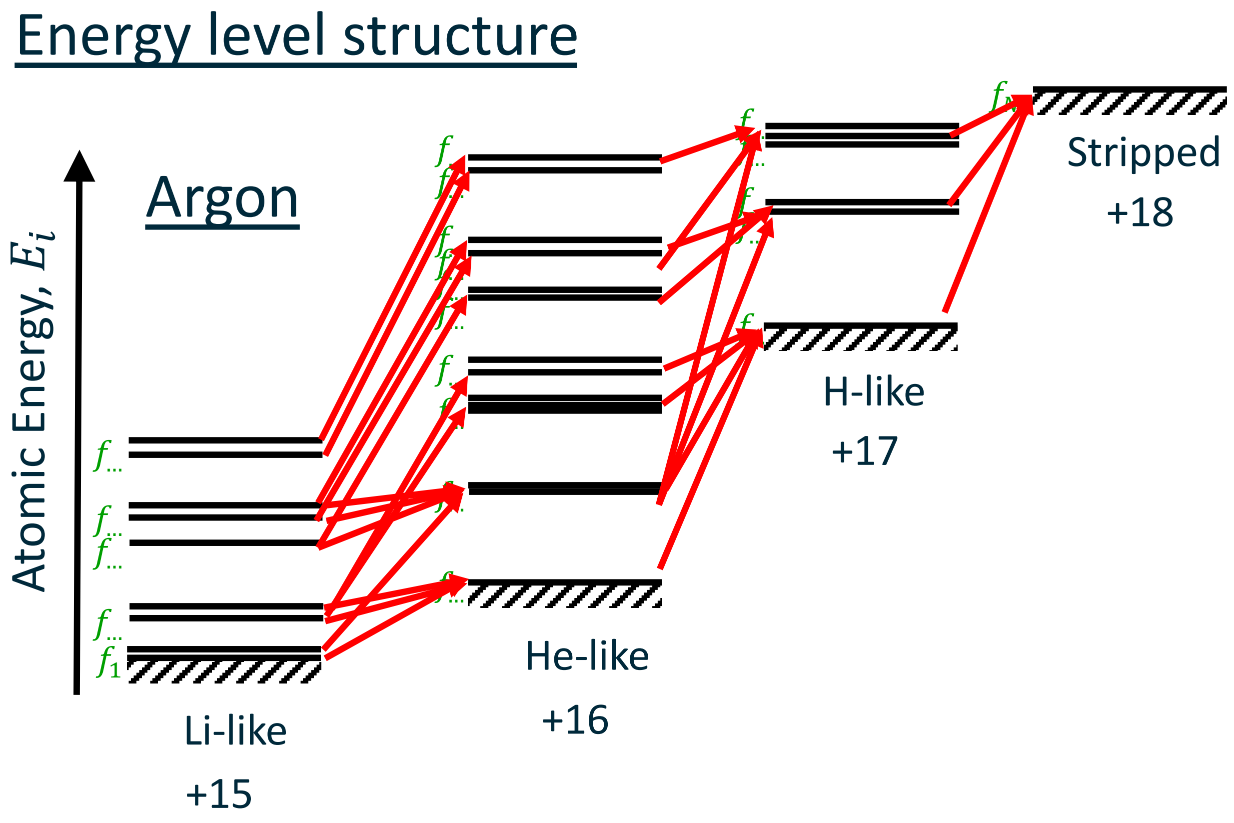
$$\frac{f_{b'}}{f_b} \propto \exp(-\Delta E/T_e) \qquad \Delta E = \epsilon_{b'} - \epsilon_b$$

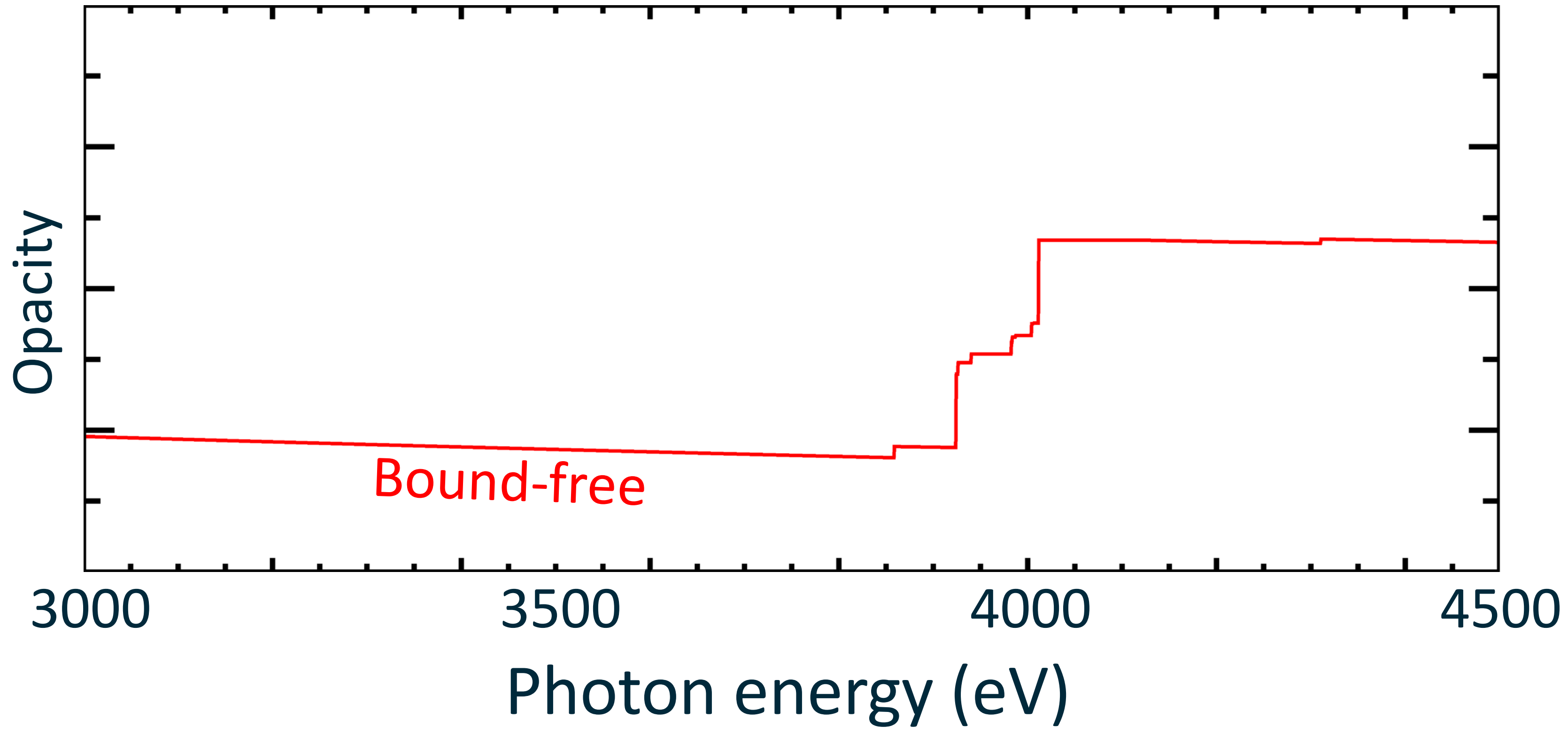
3) Normalize it:

$$\sum_i f_i = 1$$



Combine: Opacity spectrum is computed by (initial state population) x (cross-section)



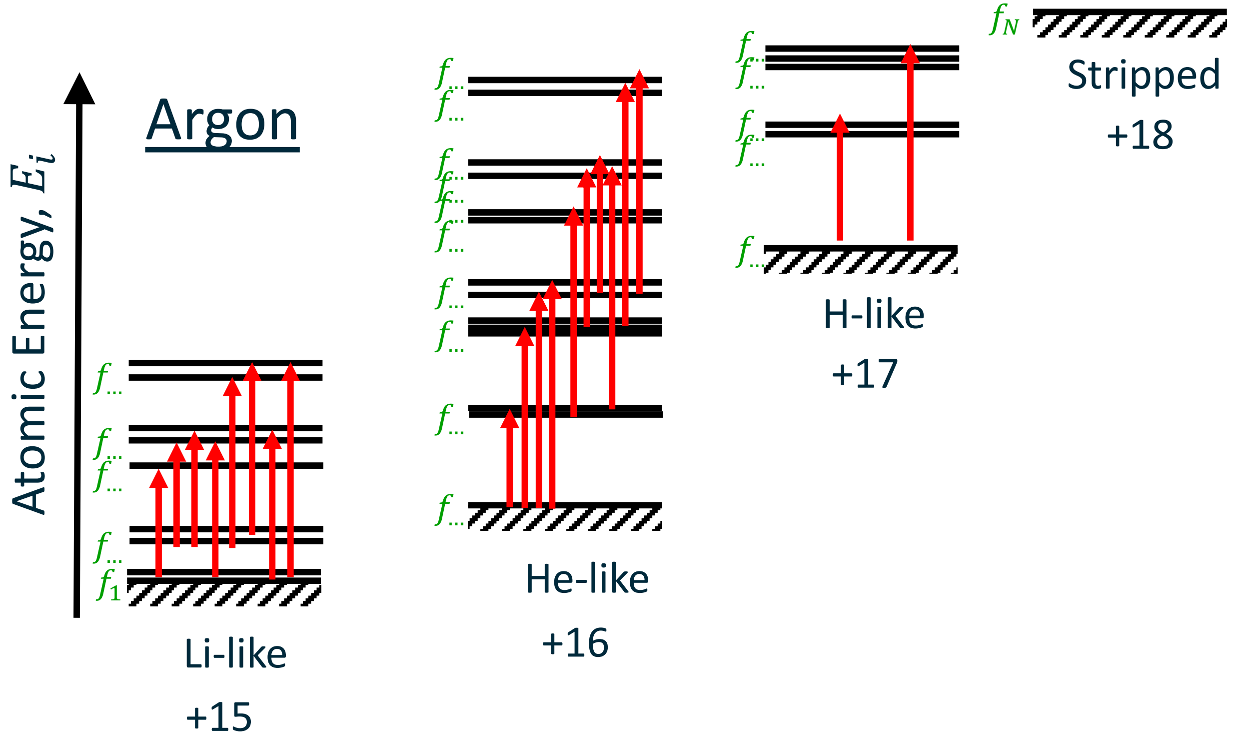


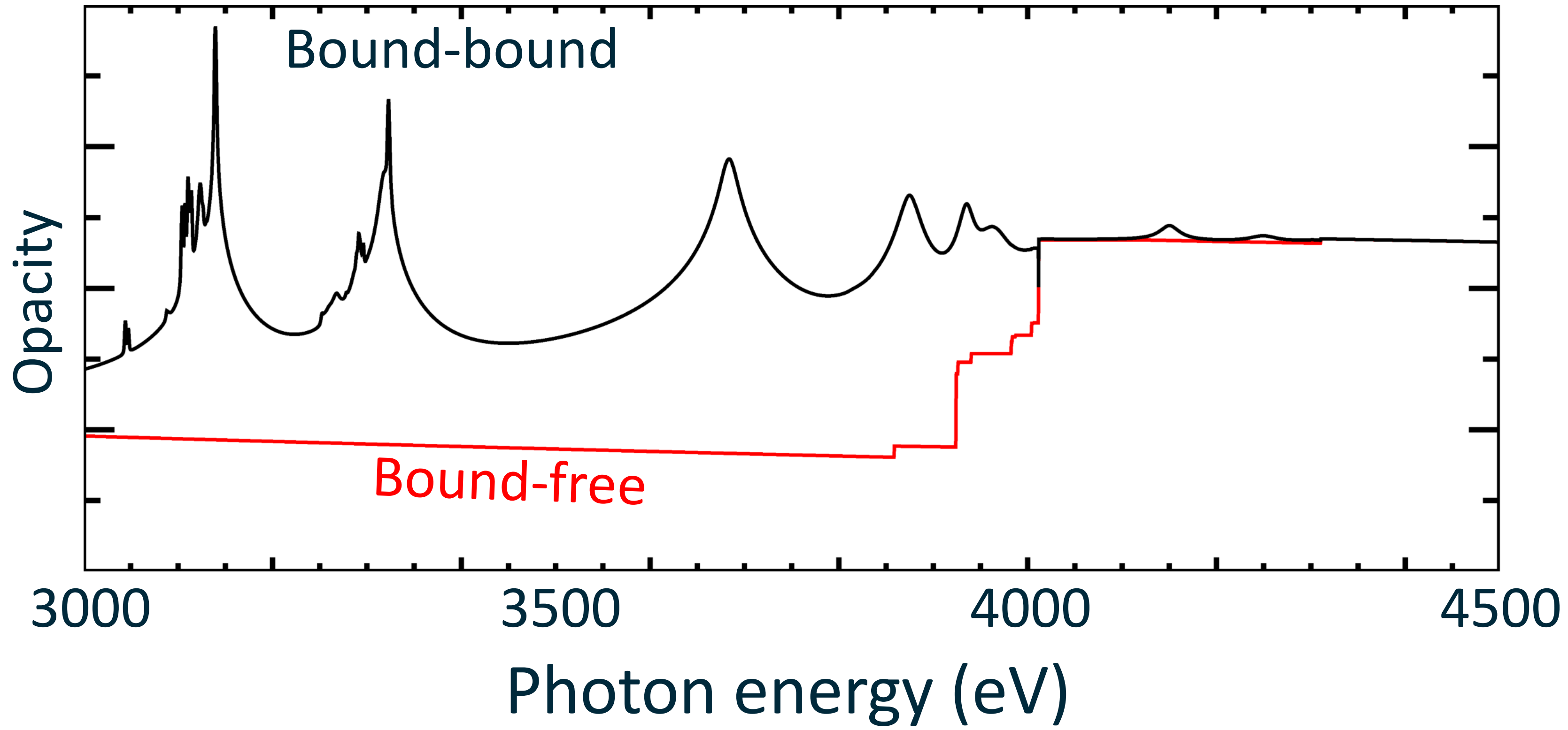
$$\kappa_\nu(h\nu) = \sum_{bf} n_{ion} f_b \sigma_{bf}(h\nu)$$

* Precisely speaking, this is attenuation (absorption, extinction) coefficient. Opacity is this divided by mass density.

Combine: Opacity spectrum is computed by (initial state population) x (cross-section)

Energy level structure





$$\kappa_\nu(h\nu) = \sum_{bf} n_{ion} f_b \sigma_{bf}(h\nu) + \sum_{bb'} n_{ion} f_b \sigma_{bb'}(h\nu)$$

* Precisely speaking, this is attenuation (absorption, extinction) coefficient. Opacity is this divided by mass density.

Opacity calculations become extremely difficult at high-energy density (HED).

High temperature, High density

HED theoretical challenge 1: It involves many excited states

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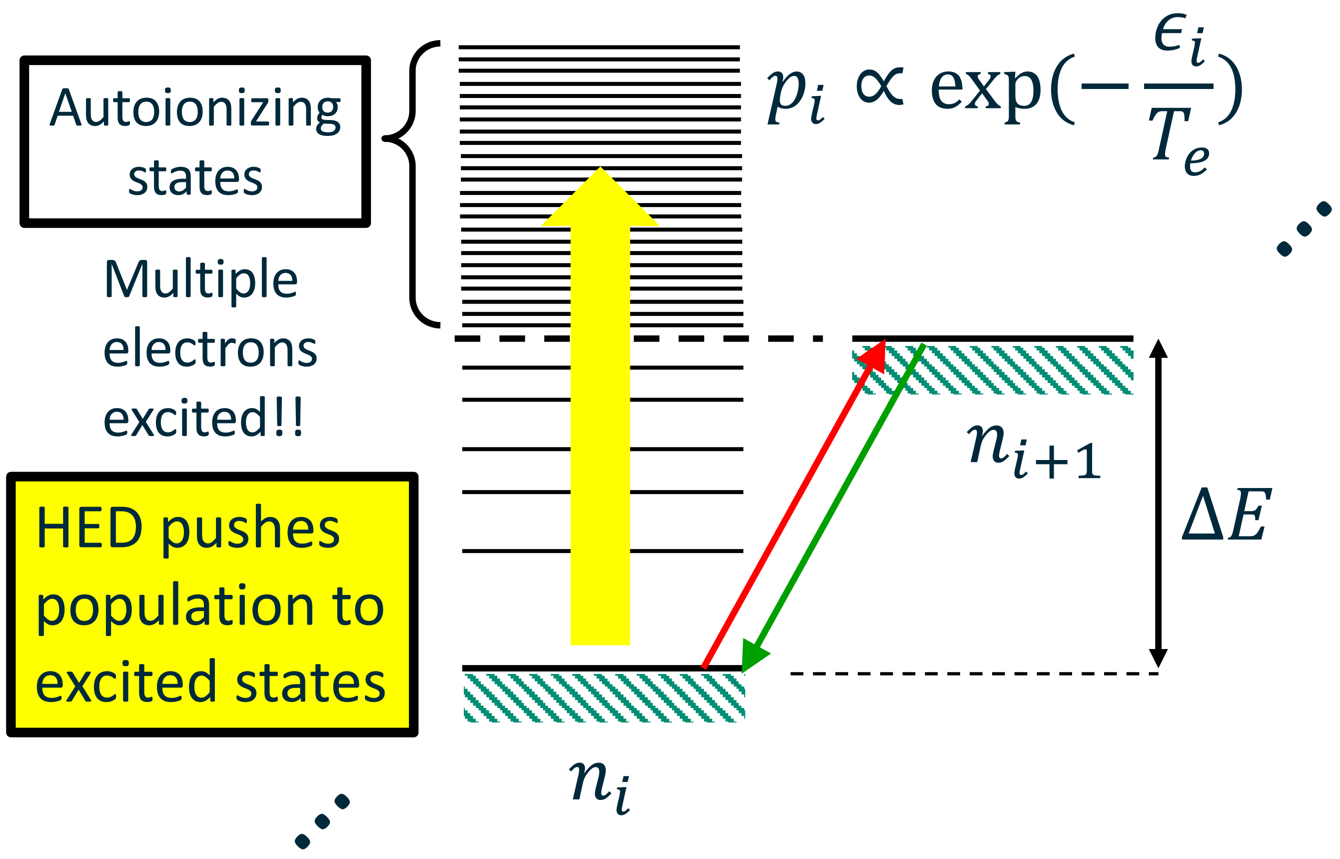

Ionization by the Saha equation

$$\frac{n_{i+1}}{n_i} \propto \frac{\exp(-\Delta E/T_e)}{n_e}$$

- Increasing temperature promotes ionization
- Increasing density promotes recombination

HED plasma can have similar ionization to low temperature, low density plasma, but …

- **Significant population in excited states!**
- **Complete inclusion of excited states is crucial**

Opacity contribution from ground states are relatively simple

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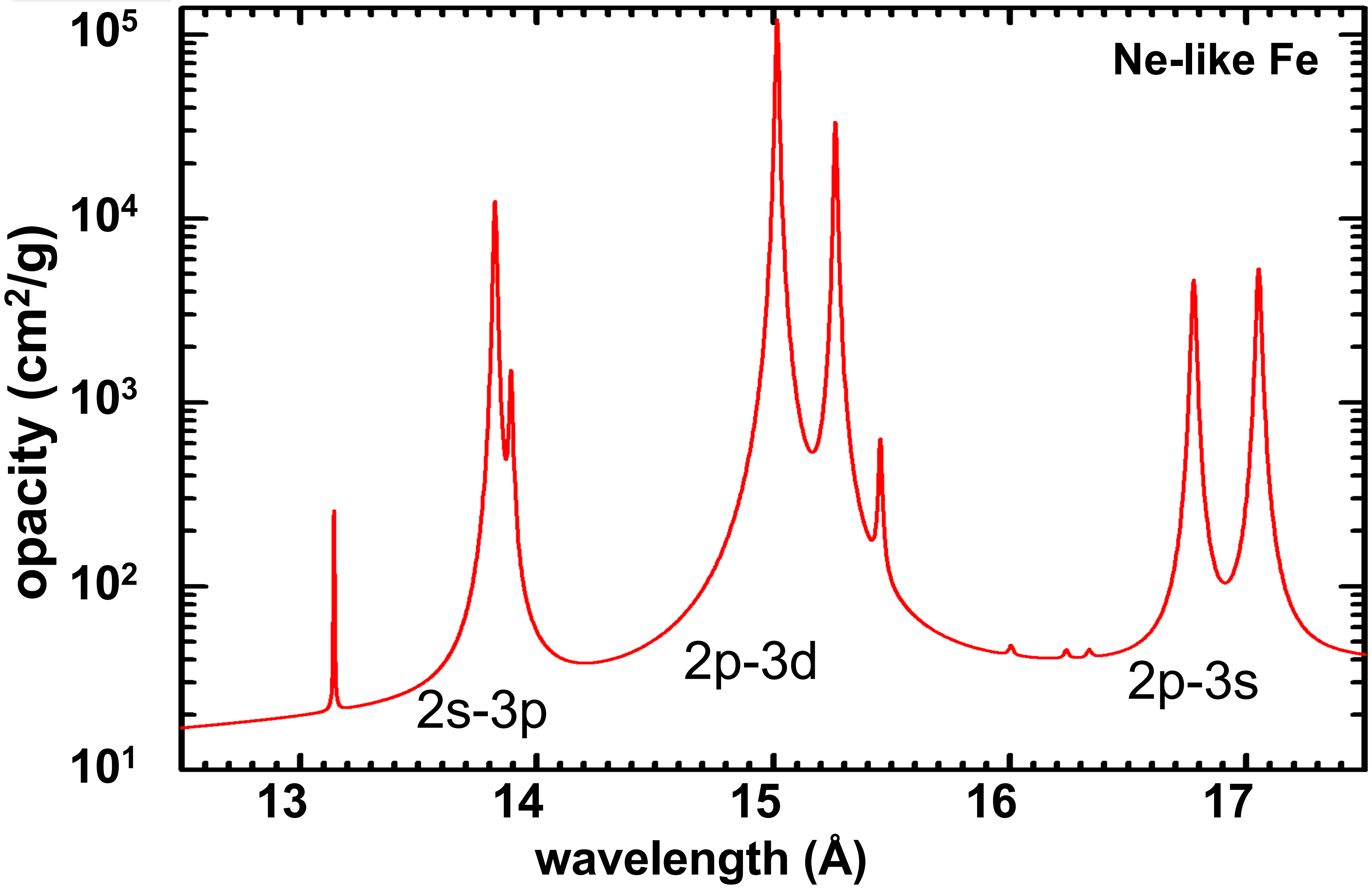

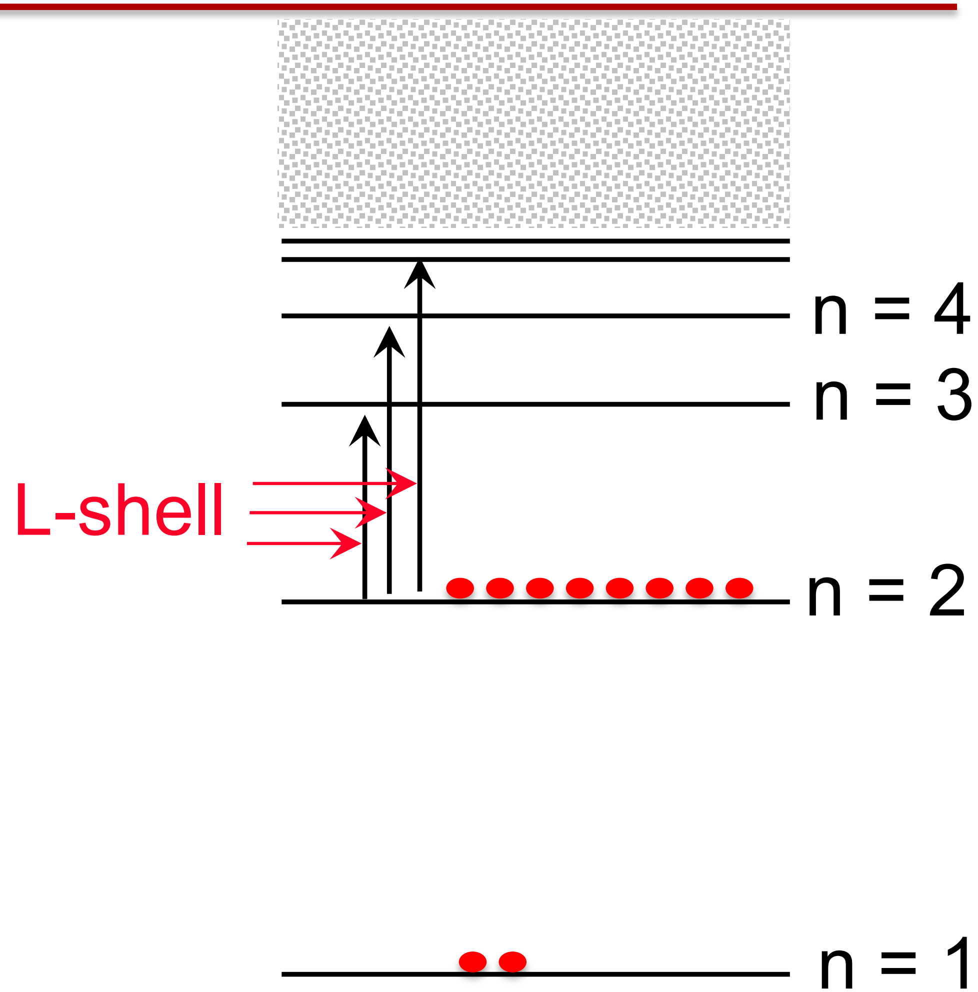

Fe^{+16} : $1s^2 2s^2 2p^6$
Ne-like

Contribution from excited states significantly adds complexity

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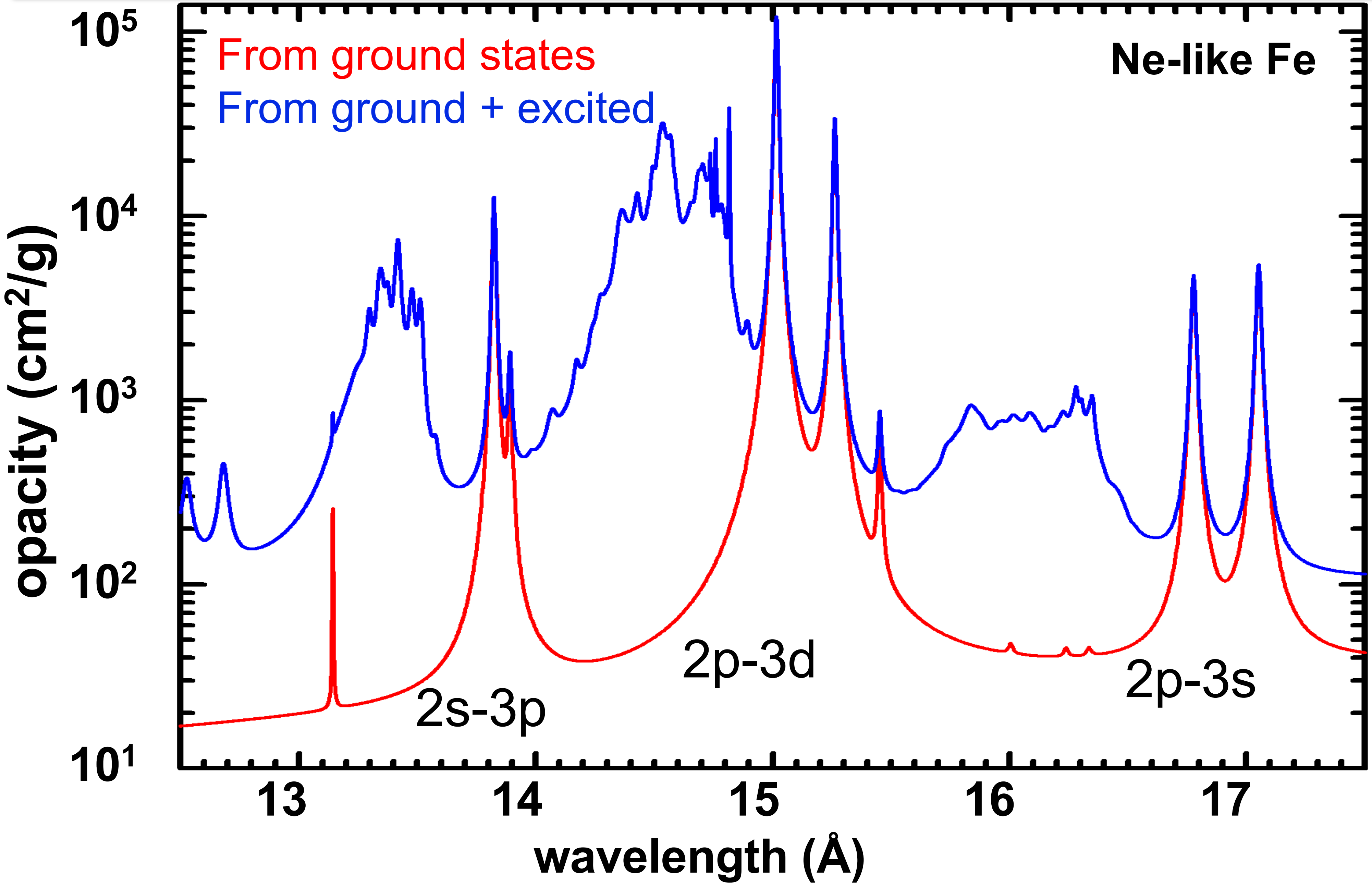
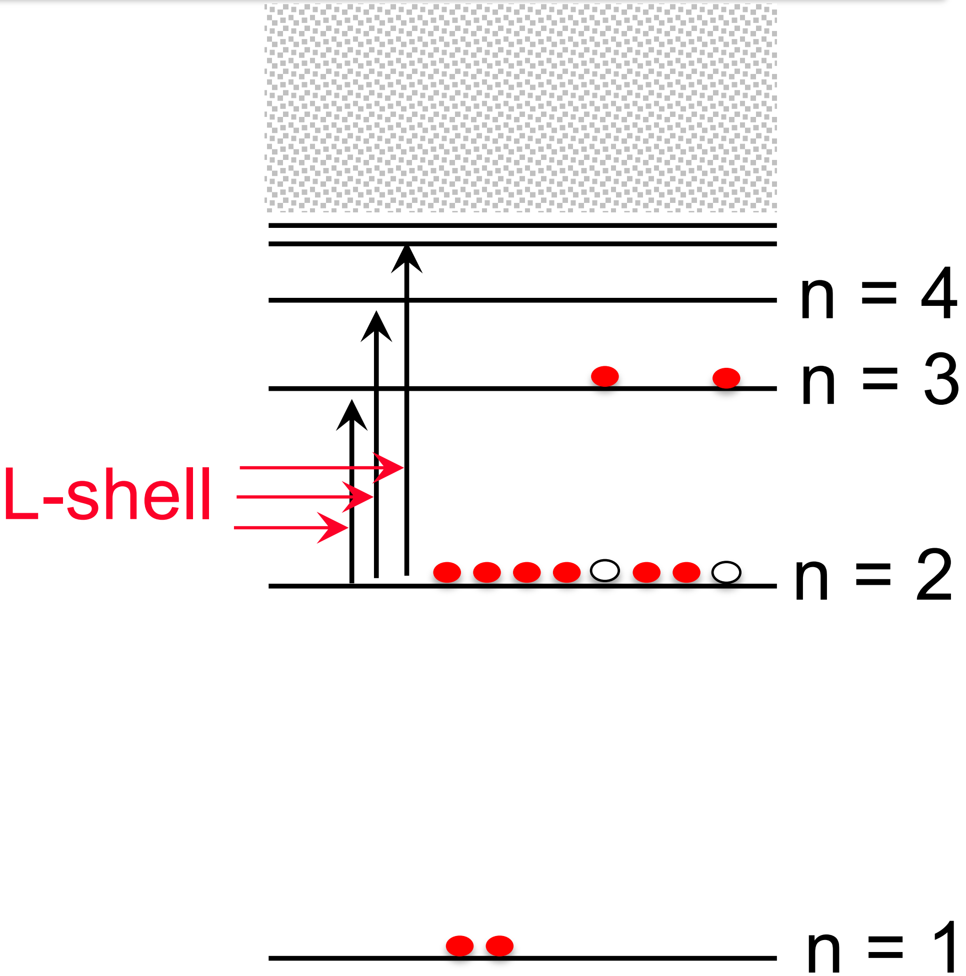




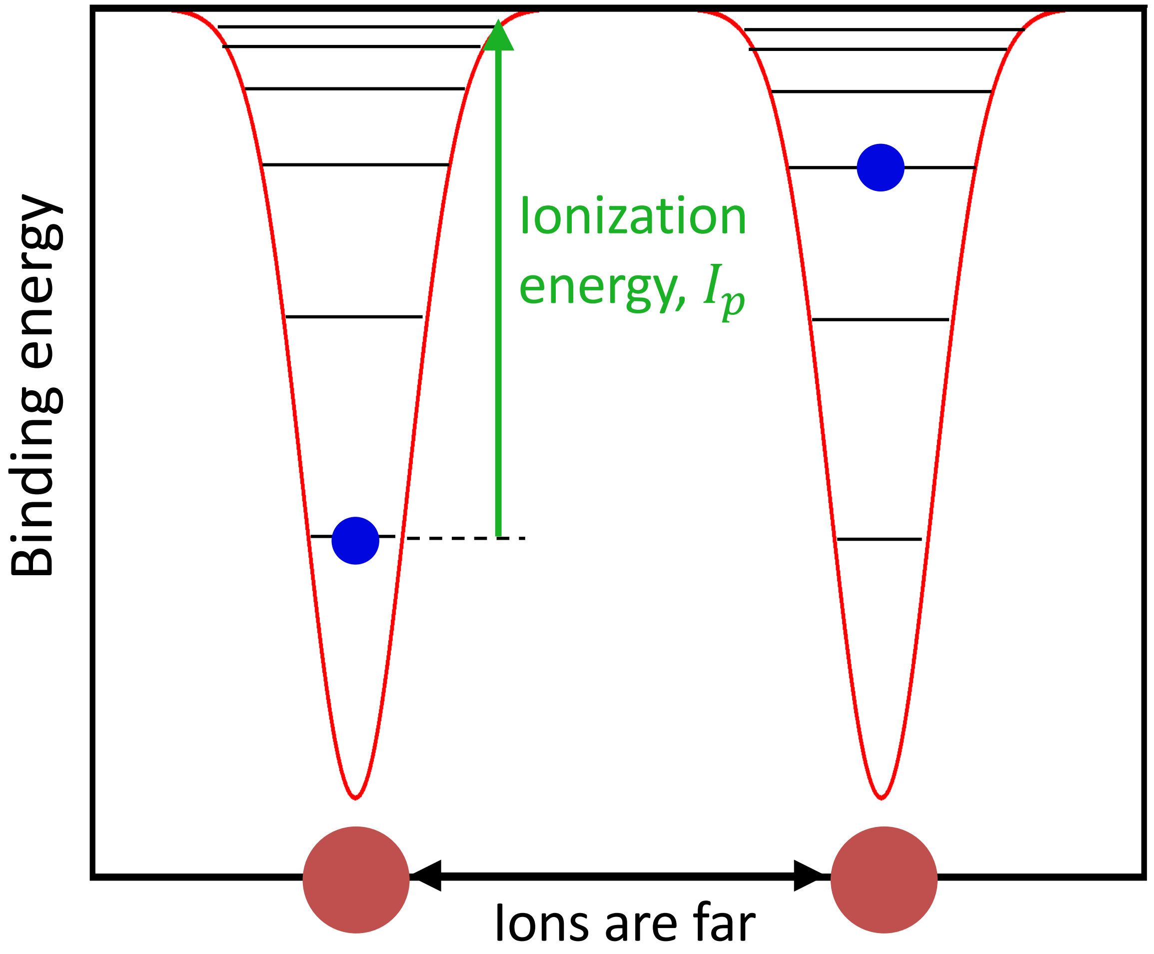
Fe^{+16} : $1s^2 2s^2 2p^6$

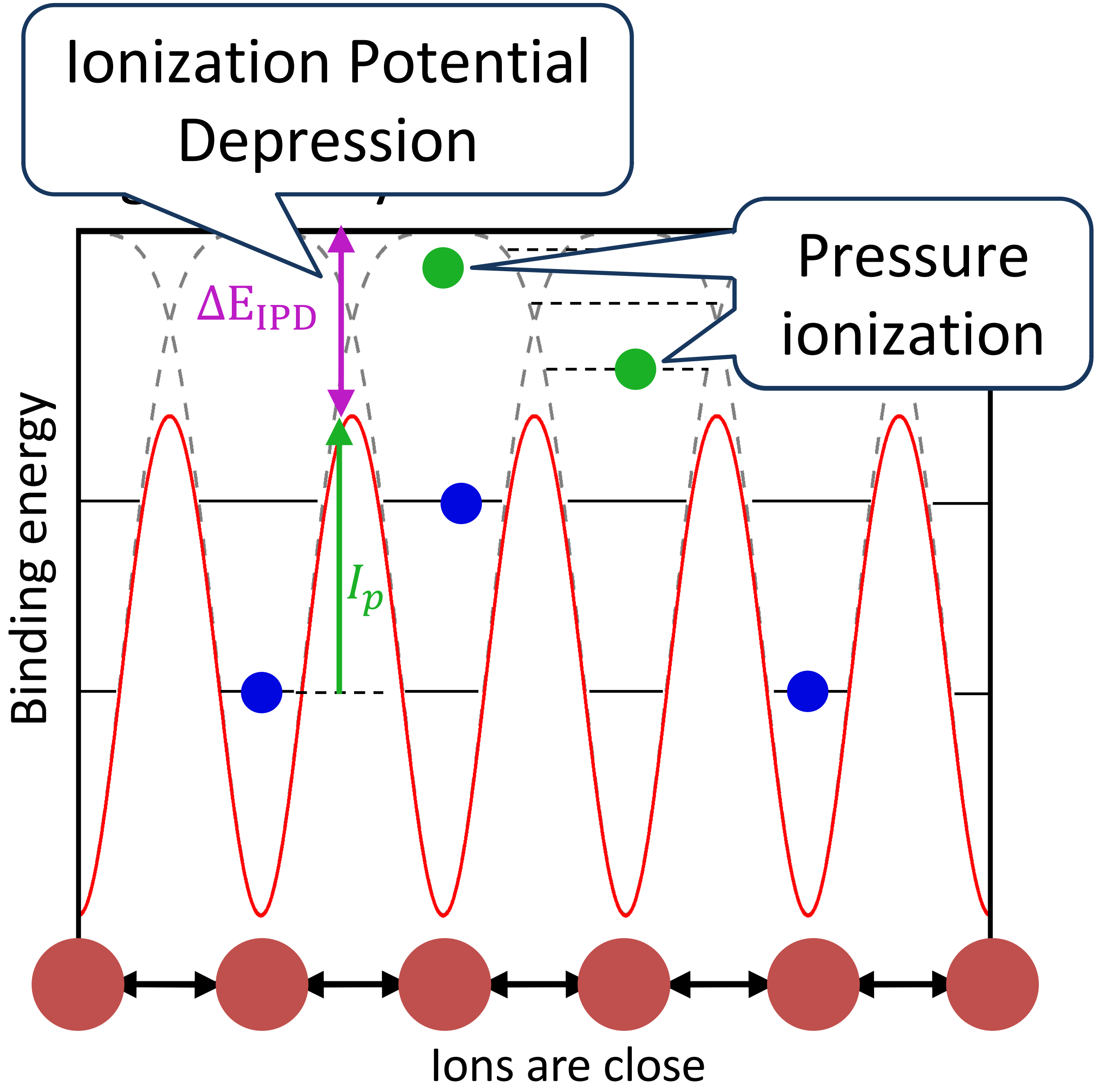
Ne-like

HED theoretical challenge 2: HED effects (density effects) complicate modeling

High density alters the atomic structure

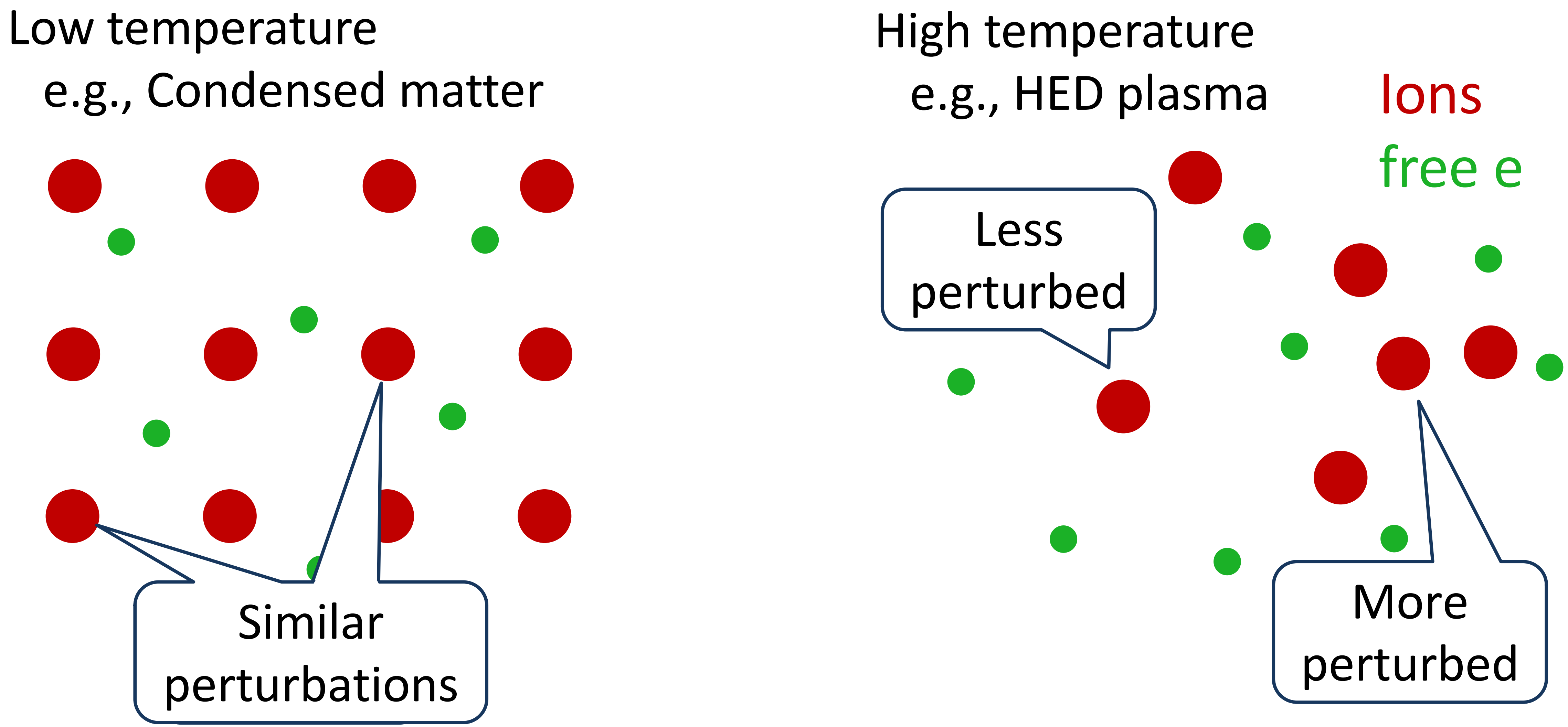
Low density





HED theoretical challenge 2: HED effects (density effects) complicate modeling

High temperature introduces randomness in perturbation



HED effects complicates ionization calculation and line-broadening calculation

Opacity is computed from first principles but has many approximations to be validated

Atomic structure code and collision code

- Is energy-level structure correct? ϵ_i, ψ_i
- Are oscillator strengths and cross-sections correct? $f_{bb'}, \sigma_{bf}$

Equation of state f_i

- Contain enough excited states?
- Correct ionization potential depression (IPD)?
- Correct treatment of partial level depression (or occupation probability)?

Spectral line shapes $\phi_{ij}(h\nu)$

- Correct line broadening?

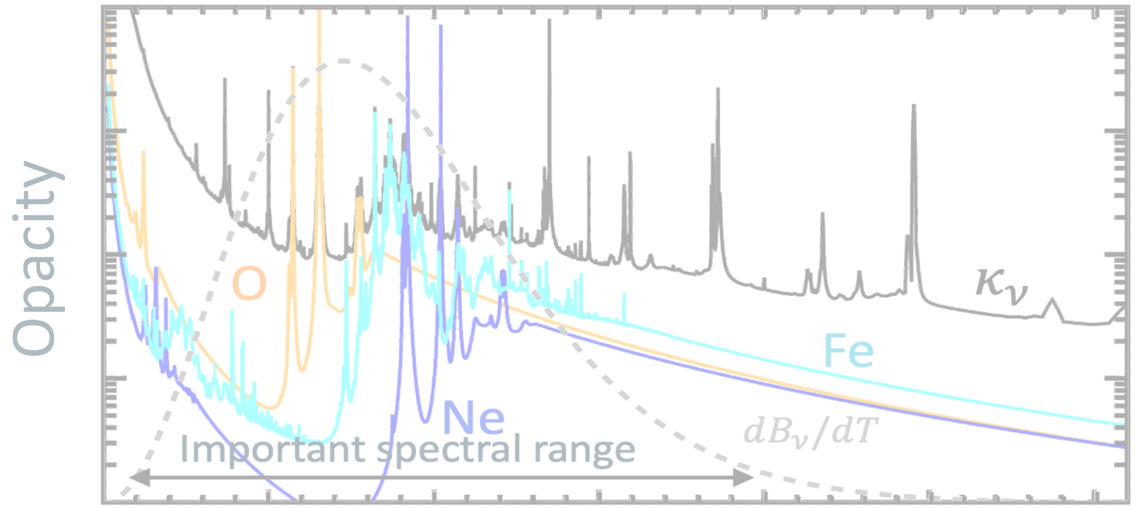
Any missing physics?

- Higher-order absorption
- etc

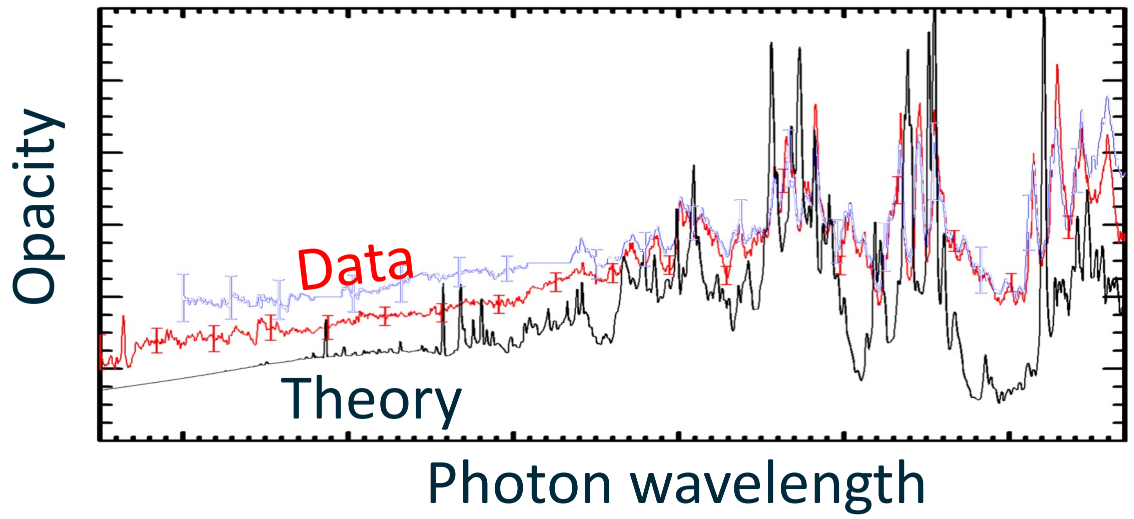
Best way to validate opacity models → Measure element spectral opacity

Understanding solar opacity is challenging due to complex nature of Rosseland mean opacity

1. **Basics:** Rosseland mean opacity
   - Derivations, assumptions, and complexity
   - If RMO is wrong:
     → (1) Abundance and/or
     → (2) Calculated element opacity.



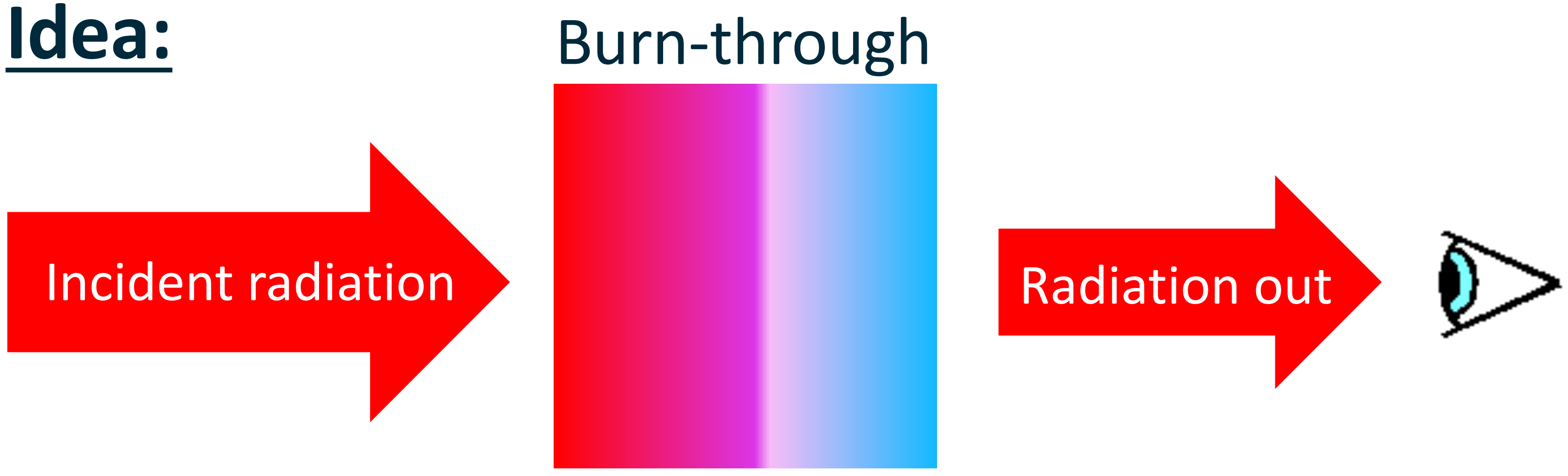
2. **Theory:** How element opacity is computed.
   - Opacity is computed by “first principle”
   - Models contain “untested” approximations
3. **Experiments:** experiments and future perspective
   - Experimental challenges
   - Z and NIF experiments



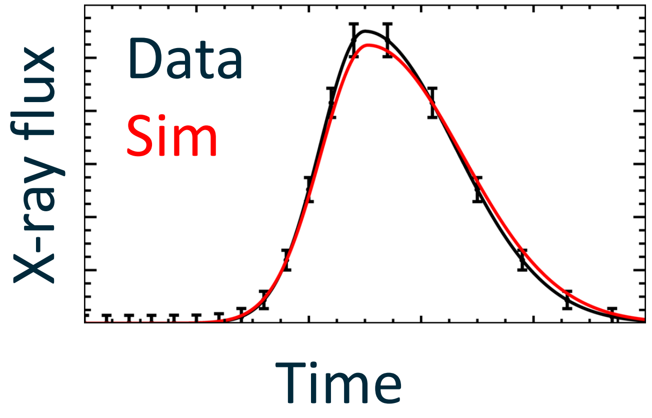
Worldwide opacity collaborations will soon help quantify the true accuracy of calculated element opacities

Burn-through experiments may help constrain Rosseland-mean opacity, but ***its usefulness is limited***.

Idea:



Assumption: If data and simulation agree, the calculated opacity is correct.



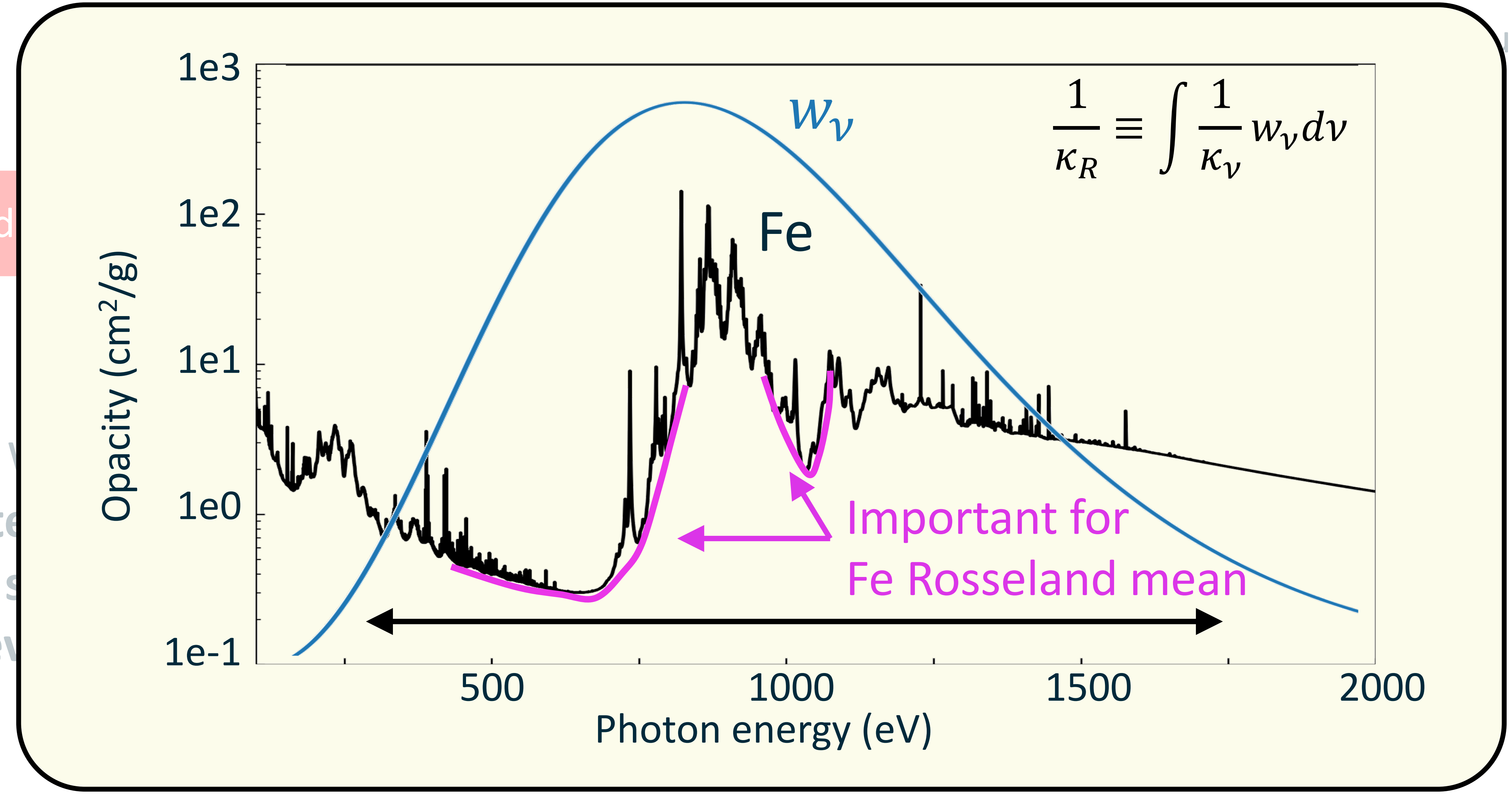
Limitations: We cannot conclude what the agreement/disagreement truly mean

- **Highly integrated:** Simulation depends on *opacity*, EOS, incident radiation, T_e, n_e as (z, t)
- **Checking sum:** This does not check spectral opacity in detail
- **Little relevance to the sun:** Fe Rosseland mean ≠ Solar Rosseland mean

Burn-through experiments may help constrain Rosseland-mean opacity, but ***its usefulness is limited***.

Idea: ulation is correct.

Incident rad



Limitations:

- Highly inte s (z, t)
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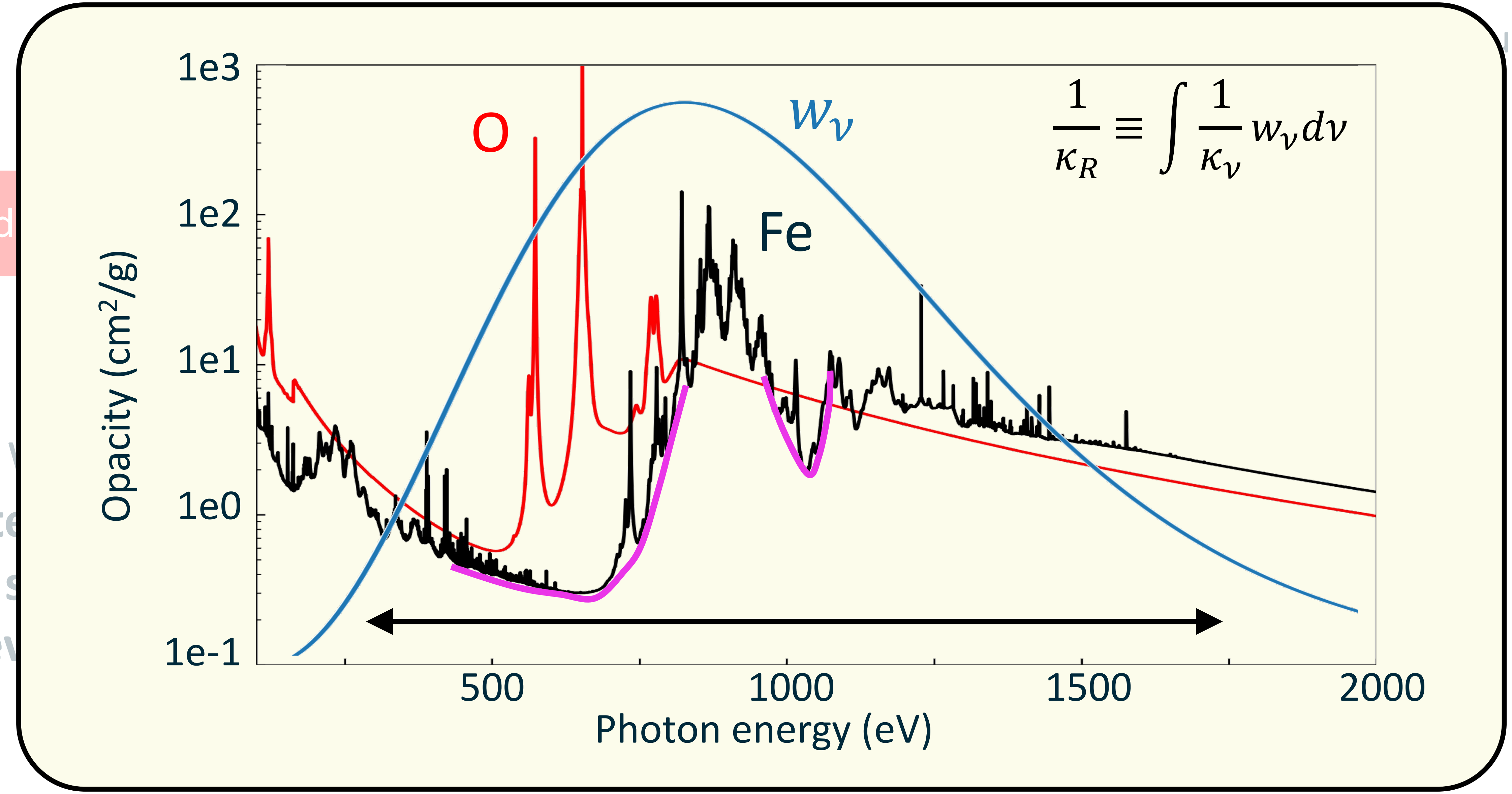

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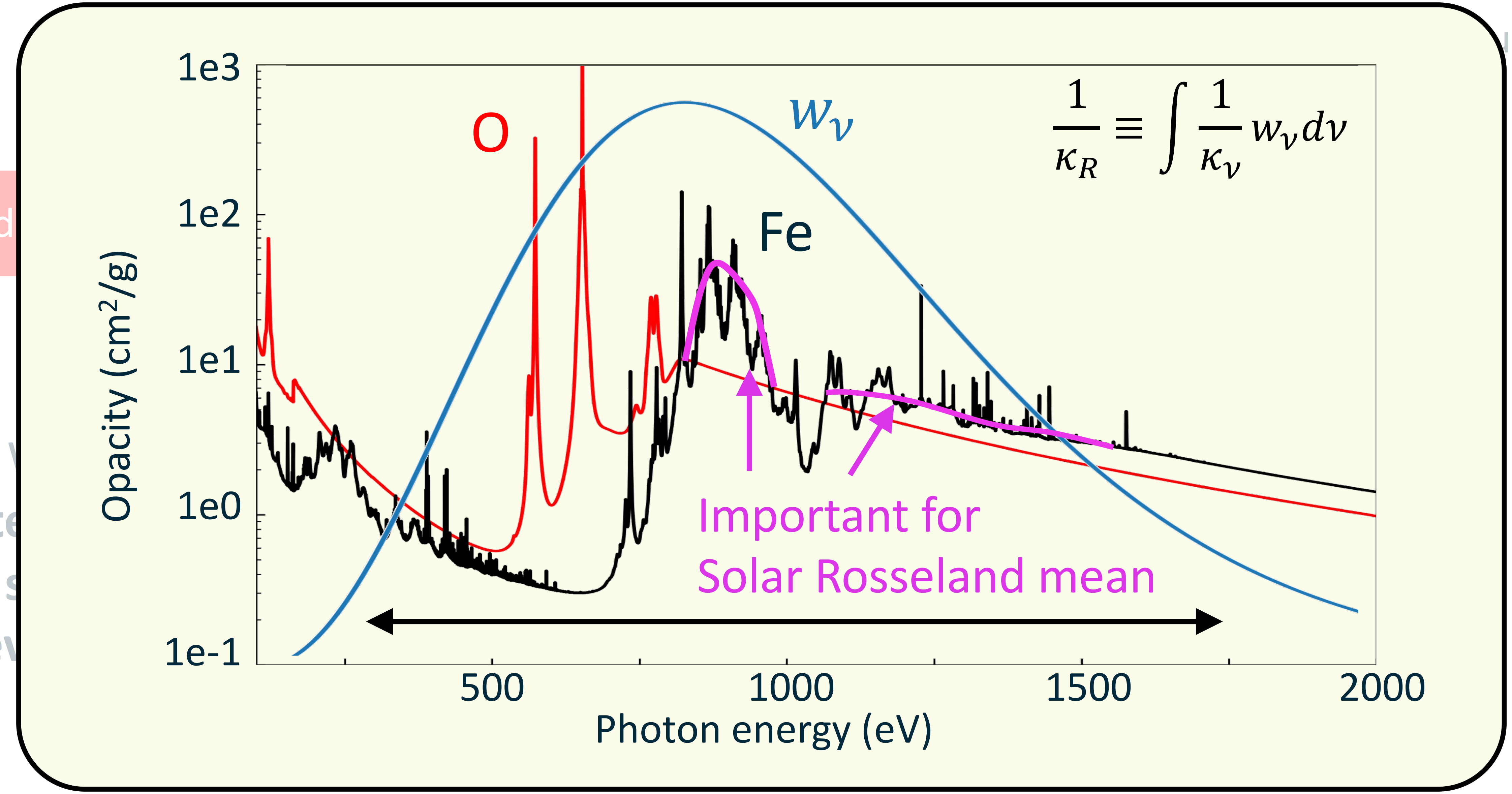

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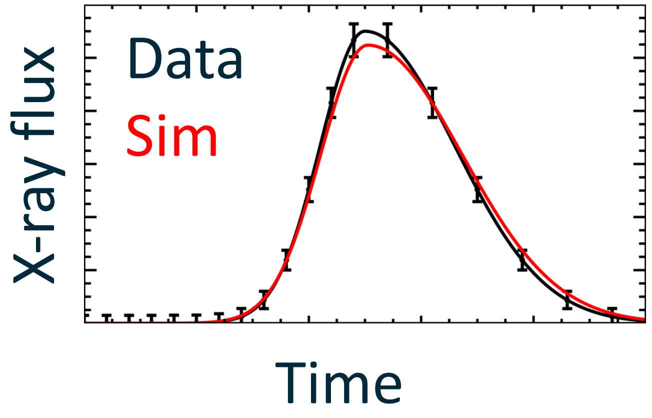

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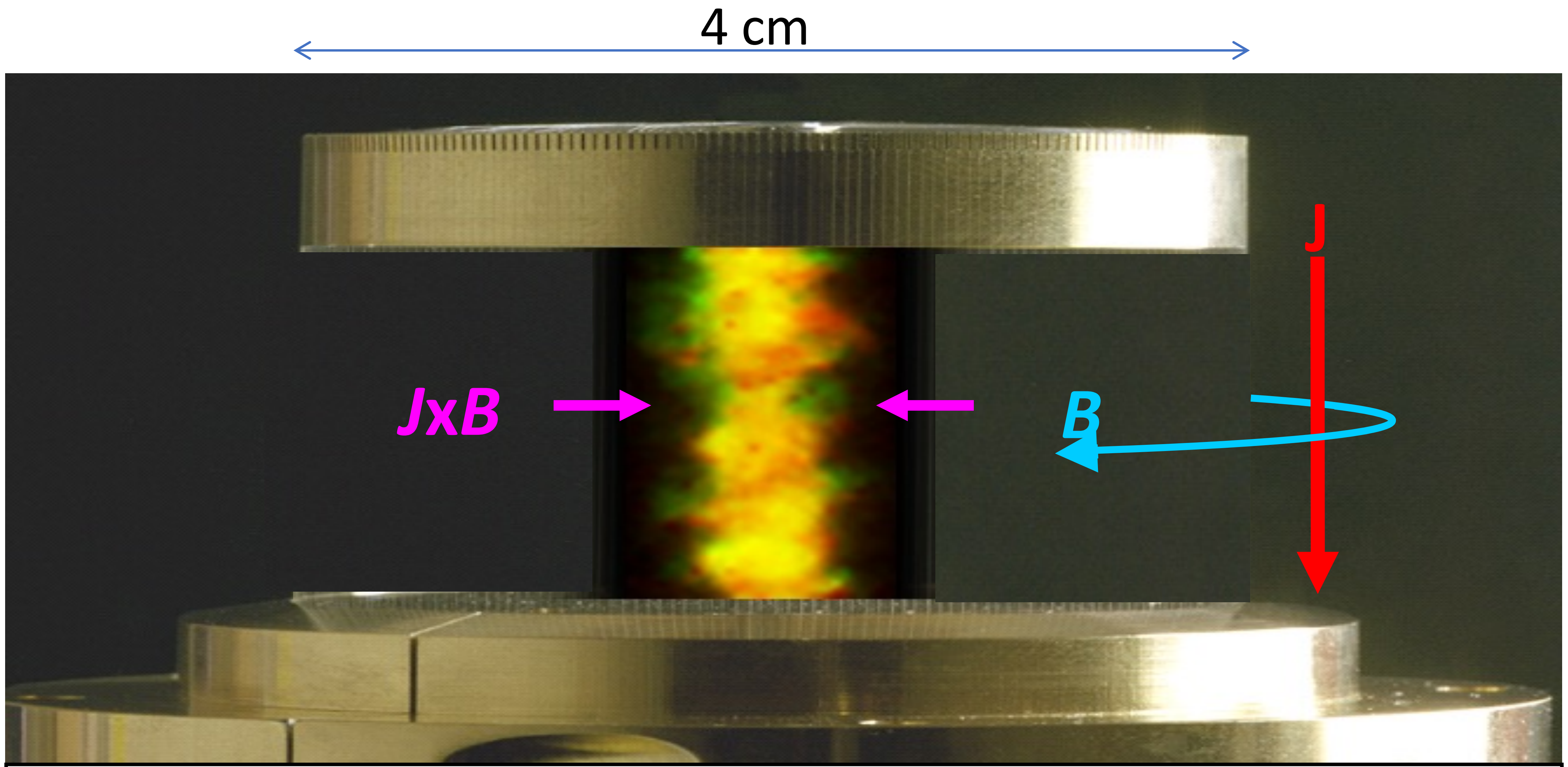
Element spectral opacity measurements are necessary to test opacity models

The Z machine uses 27 million Amperes to create x-rays



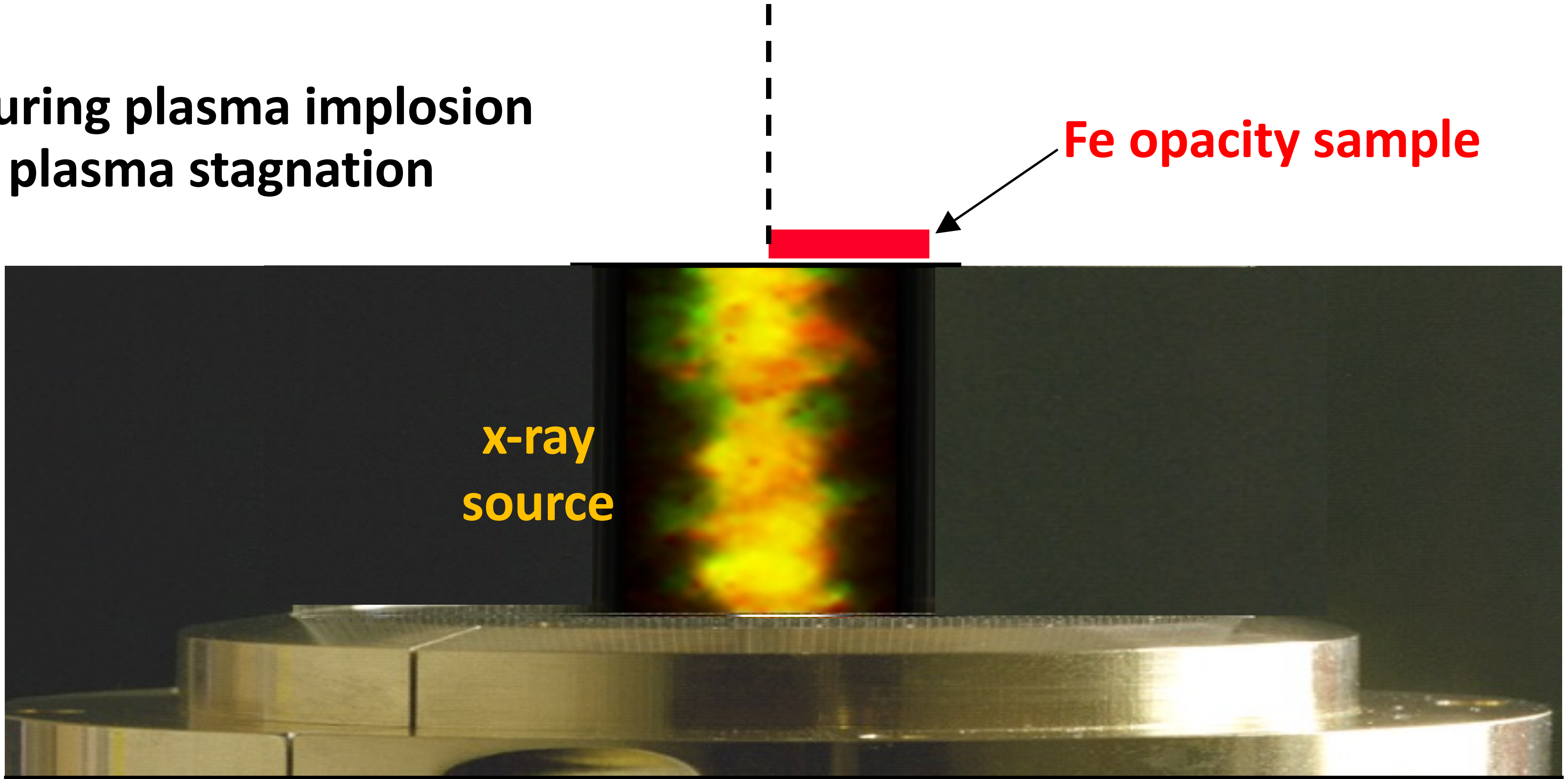
P_{rad} ~ 220TW (±10%), Y_{rad} ~ 1.6 MJ (±7%)

Sanford, *PoP* (2002); Bailey et al., *PoP* (2006); Slutz et al., *PoP* (2006); Rochau et al., *PPCF* (2007)

The Z x-ray source both heats and backlights samples to stellar interior conditions.

Sample is:

- **Heated during plasma implosion**
- **Backlit at plasma stagnation**



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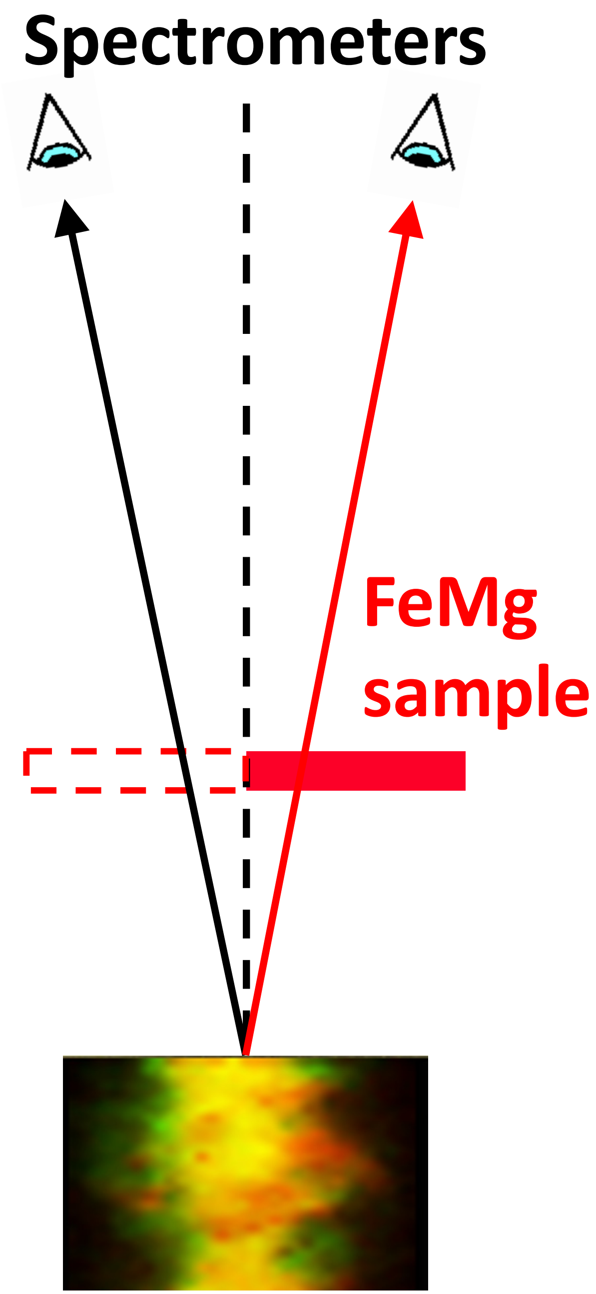
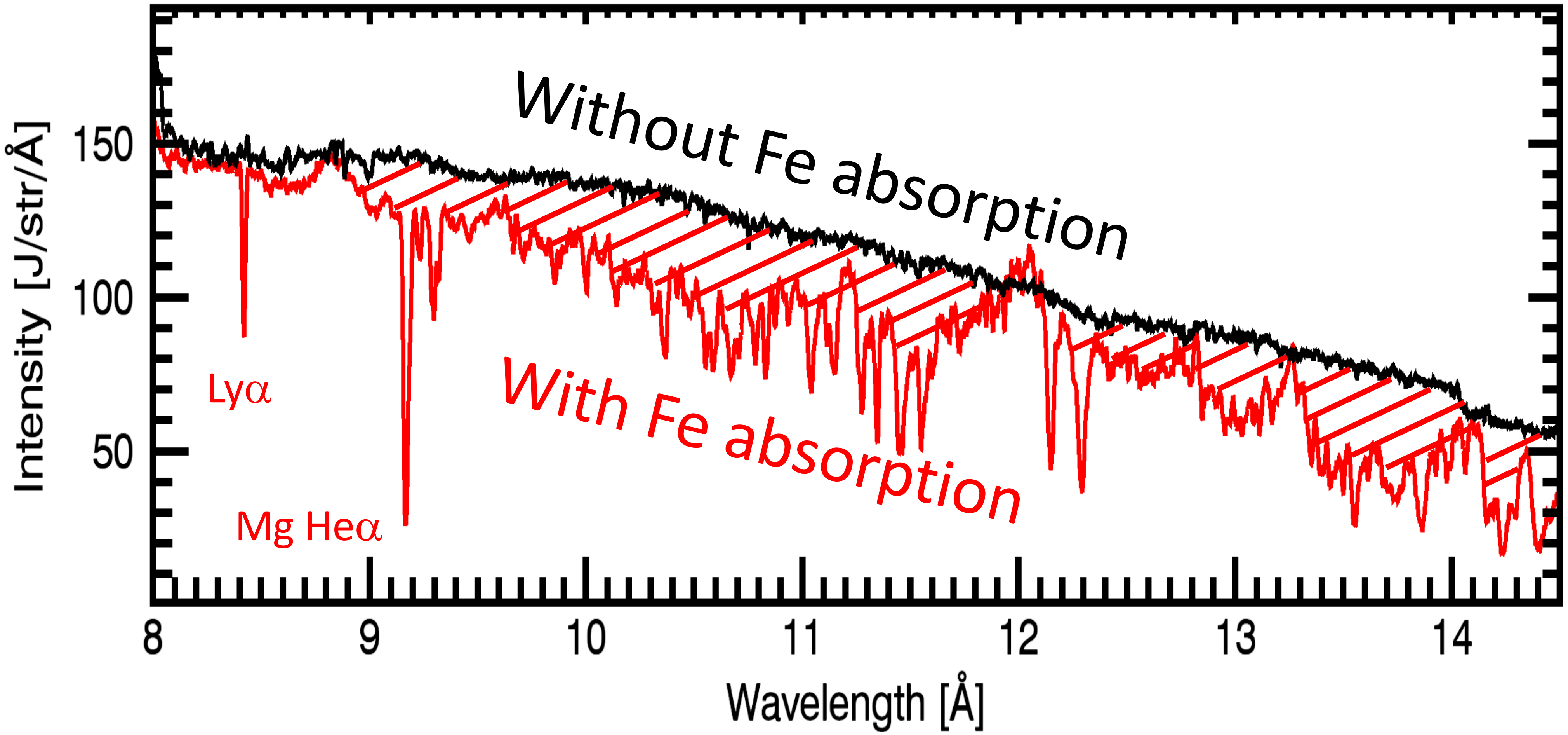
High-temperature Fe opacities are measured using the Z-Pinch opacity science platform





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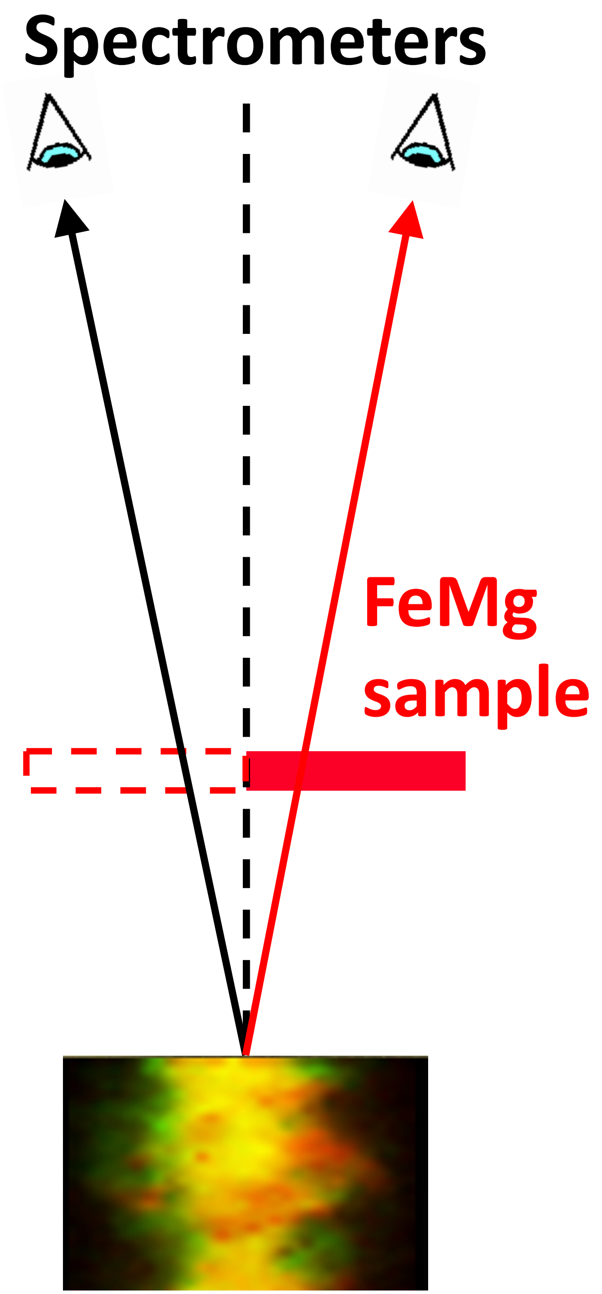
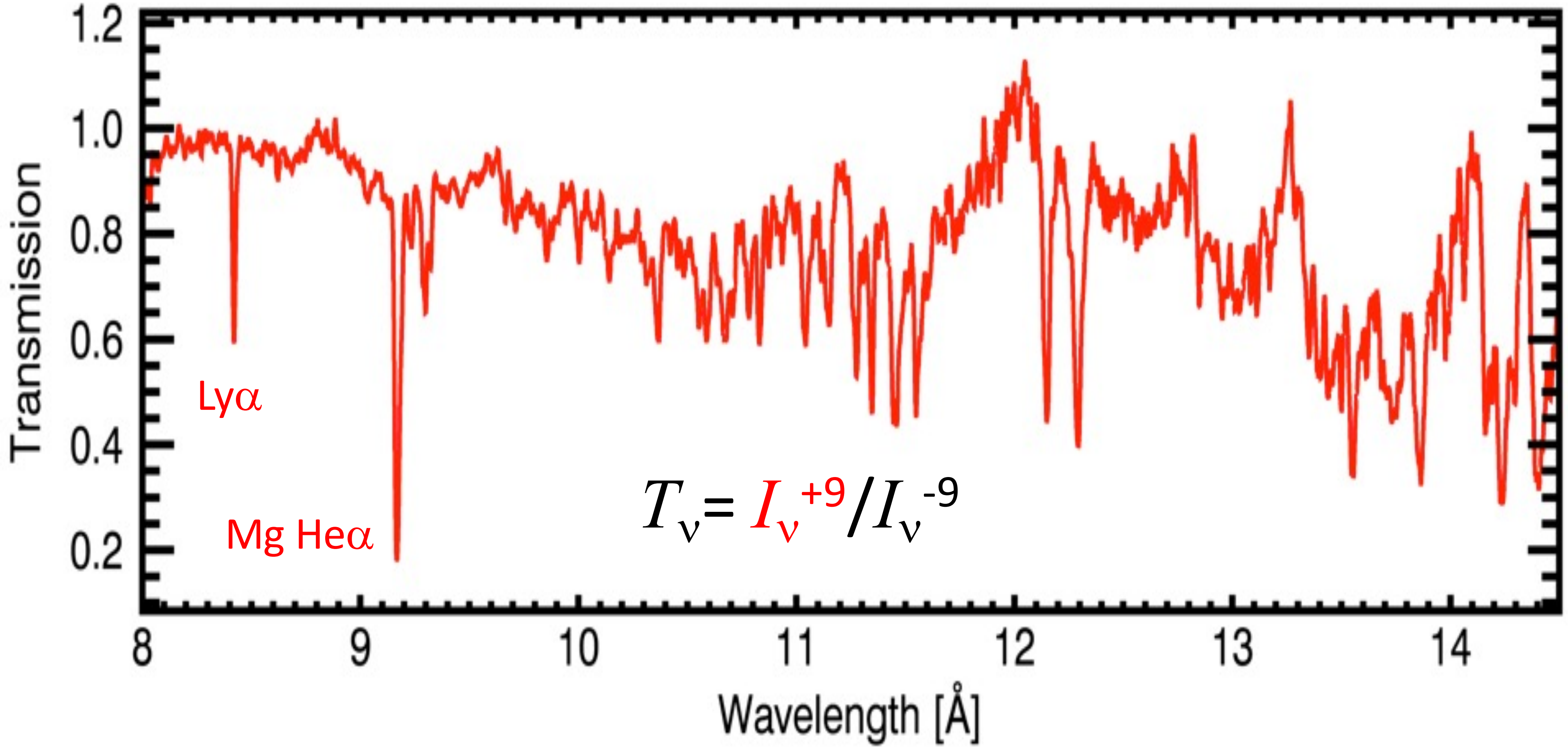
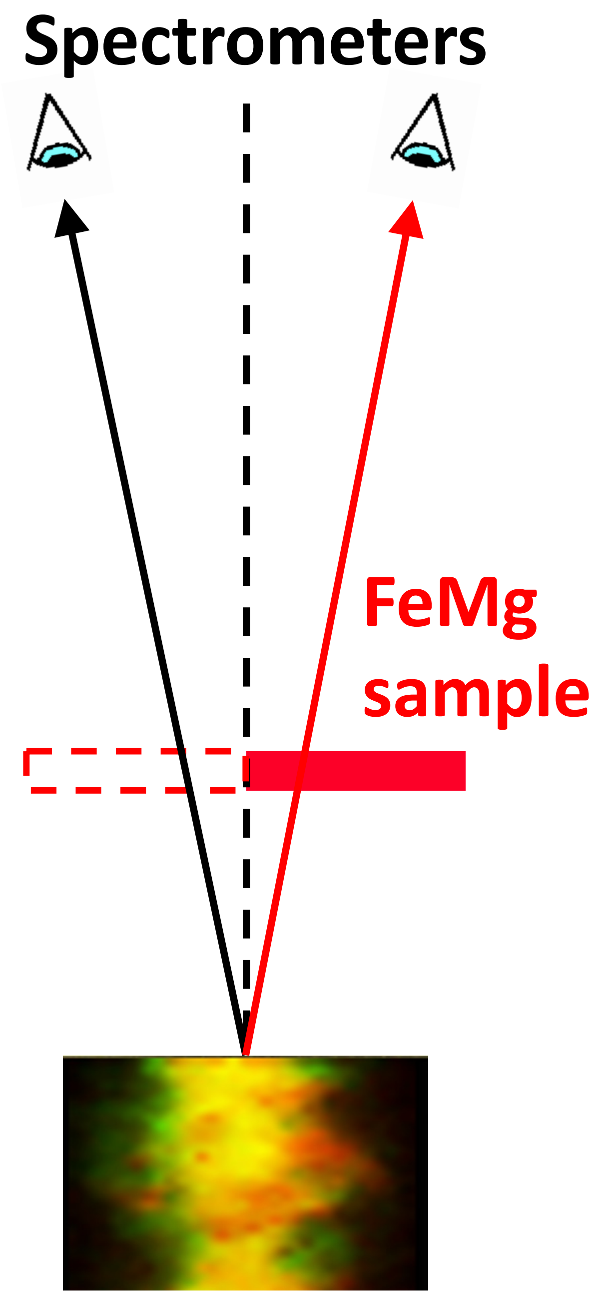
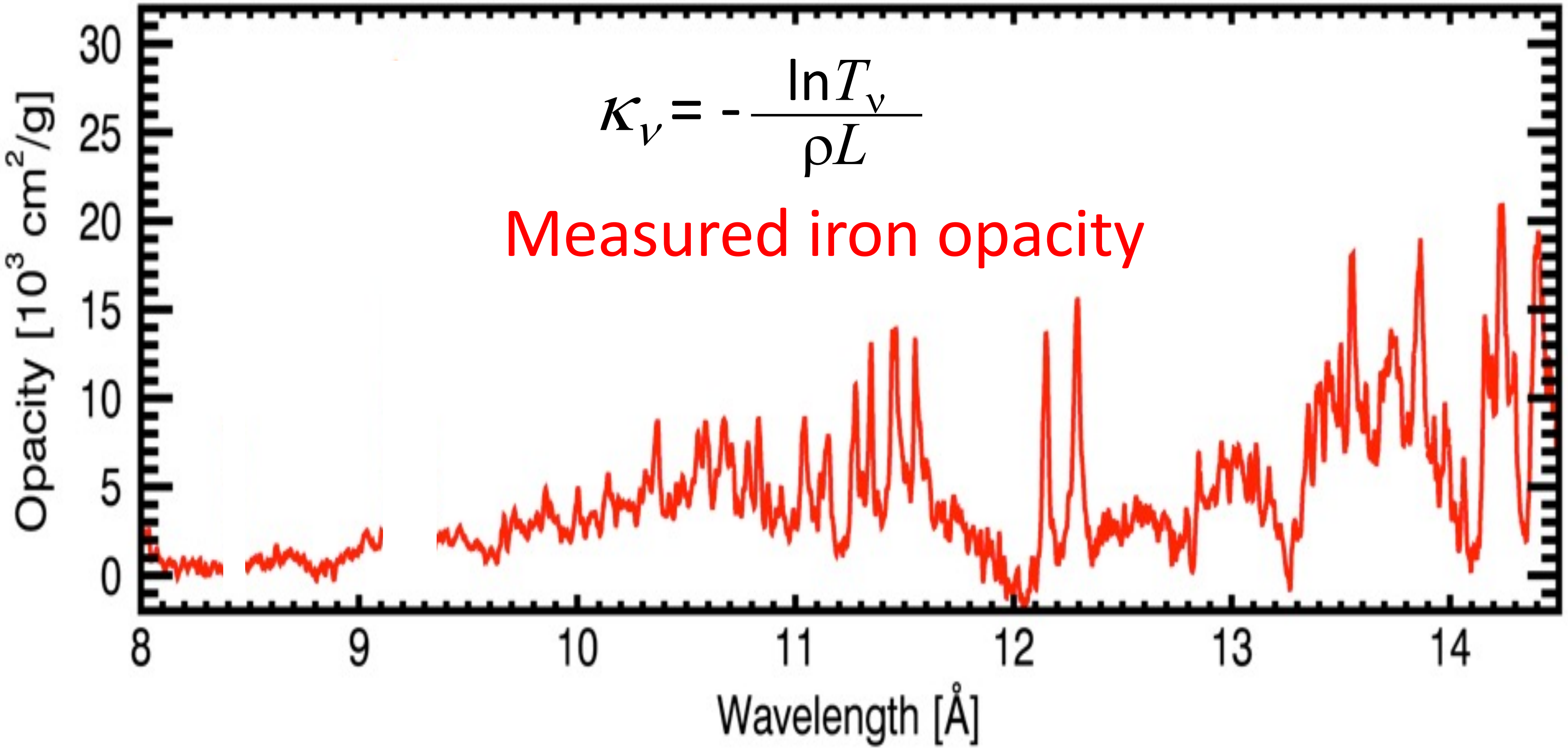




$$T_\nu = I_\nu^{+9} / I_\nu^{-9}$$

High-temperature Fe opacities are measured using the Z-Pinch opacity science platform





Opacity models disagree with the Z iron data as the condition approaches the solar CZB conditions

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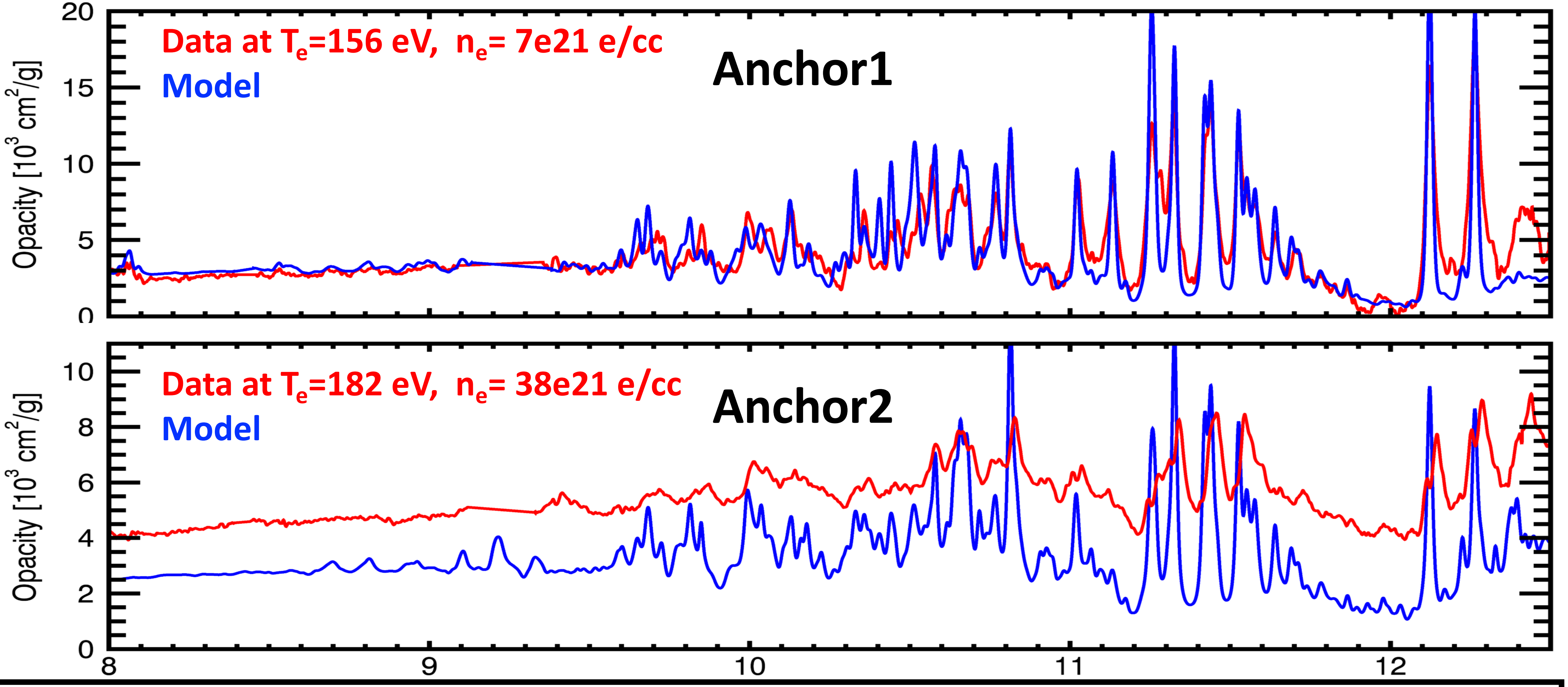
Convection Zone Base: T_e=185 eV, n_e = 90e21 e/cc



What's causing the discrepancy? Is theory flawed? Is experiment flawed?

[1] Bailey et al., Nature 517, 56 (2015)

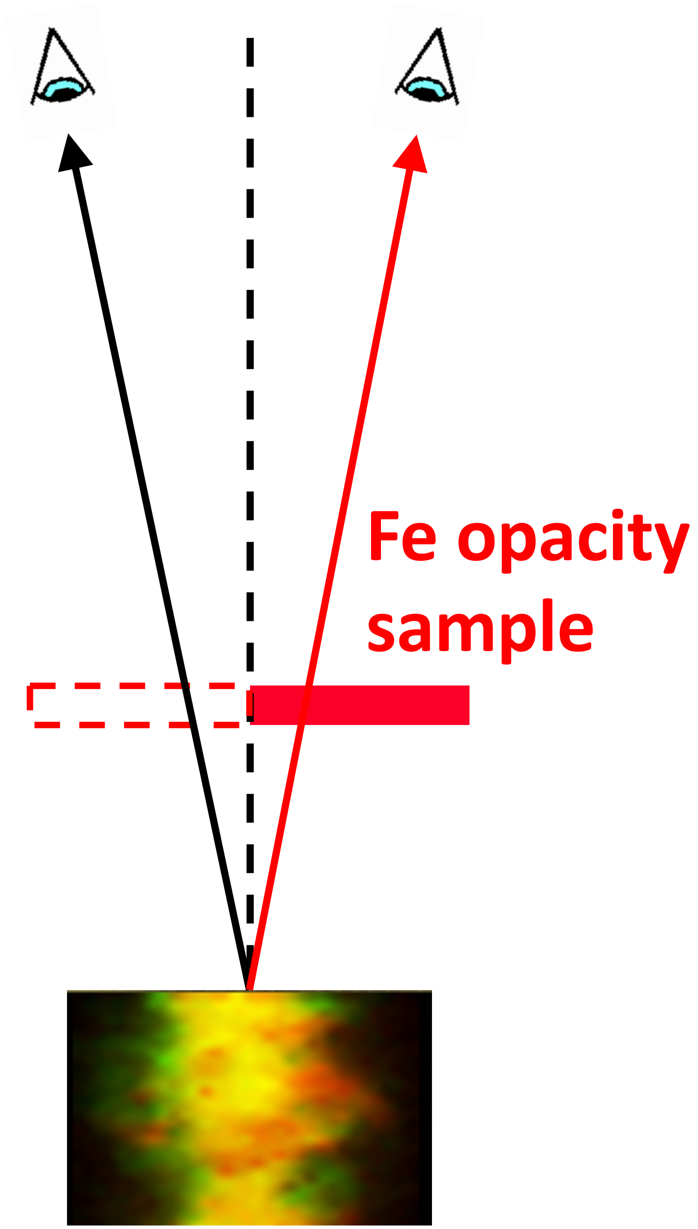
Model: PrismSpect [McFarLane et al IFSA (2004)]

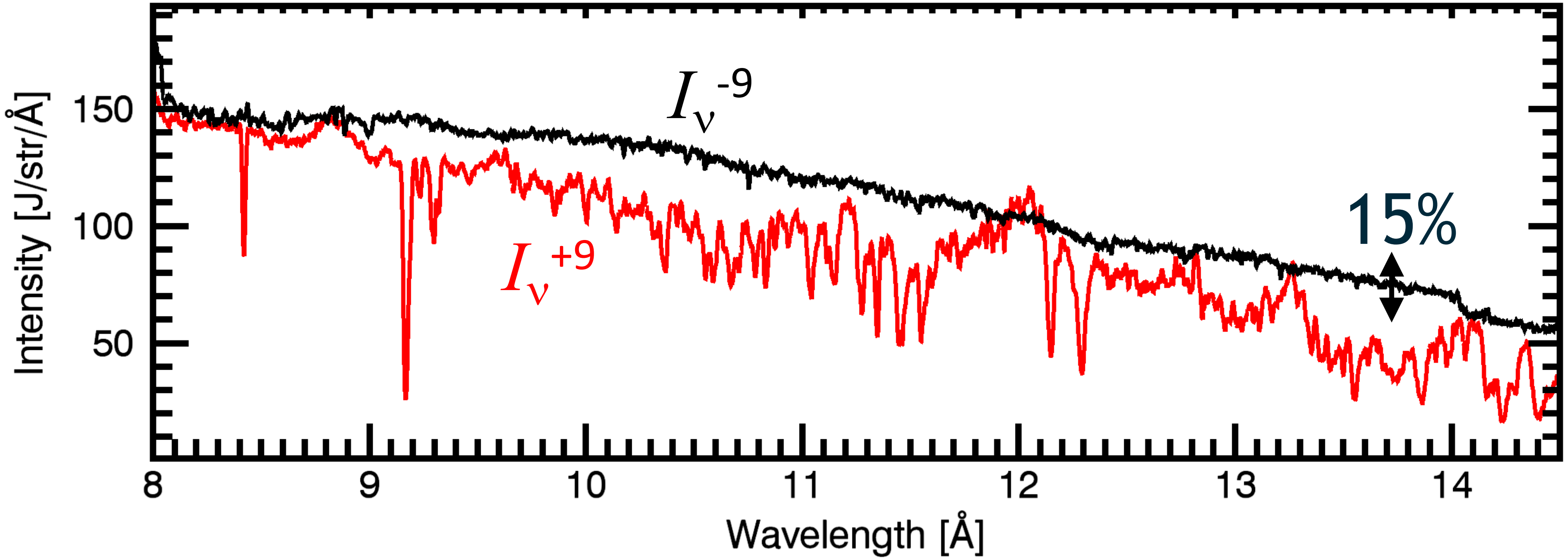
Experiments: We have investigated potential sources of systematic errors experimentally and/or numerically

Possible systematic errors in	Experimental	Numerical
• Opacity data analysis	✓ ✗	
• ~~Temperature and density diagnostics~~	✓✓	✓✓✓
• ~~Sample areal density~~	✓✓	
• ~~Non-uniformity~~		
• ~~Temporal gradients~~	✓	✓✓
• ~~Spatial gradients~~	✓	✓
• ~~Self-emission~~	✓	✓
• ~~Background~~	✓	
• ~~Impact of tamping material~~		✓

Data analysis was refined, which made notable changes to the model-data comparison

Challenge at Z: Backlight intensities measured along different lines of sight is off by ±15%



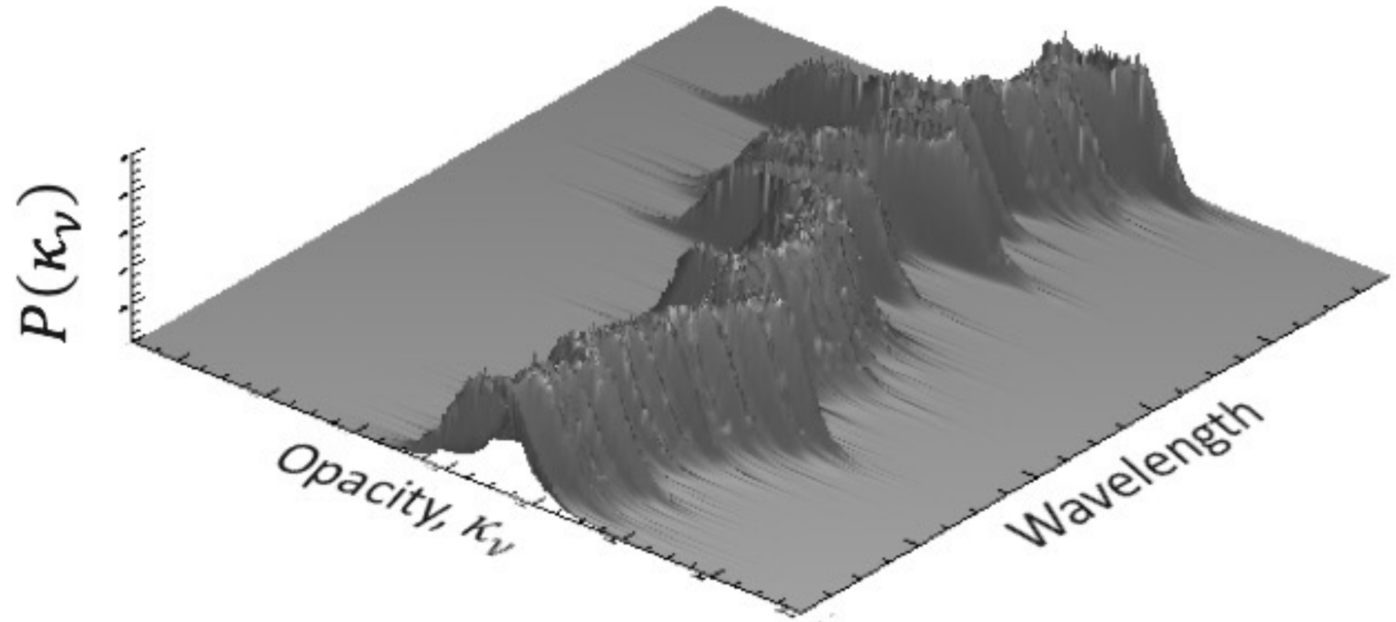


- This was a persistent concern.
- Better analysis method has been developed.

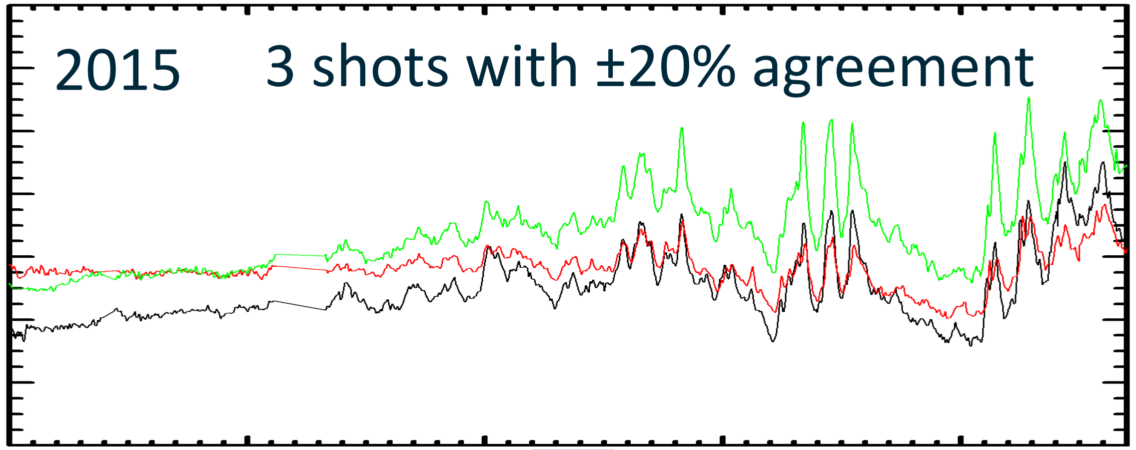
[1] Bailey et al., *Phys Plasmas* 16, 058101 (2009)
[2] Nagayama et al., *Phys Plasmas* 21, 056502 (2014)

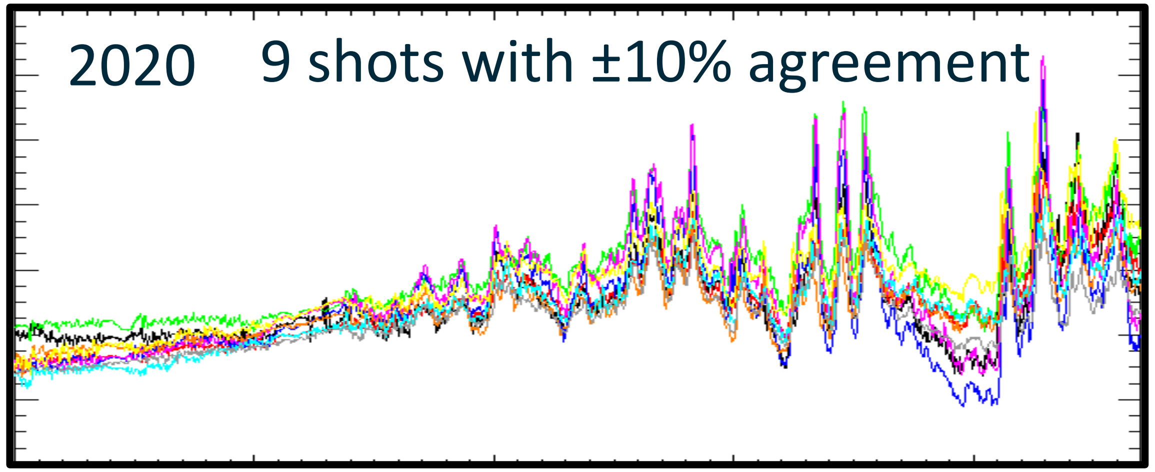
Z opacity measurements were refined by developing a statistical analysis method

Asymmetric non-Gaussian opacity PDF*



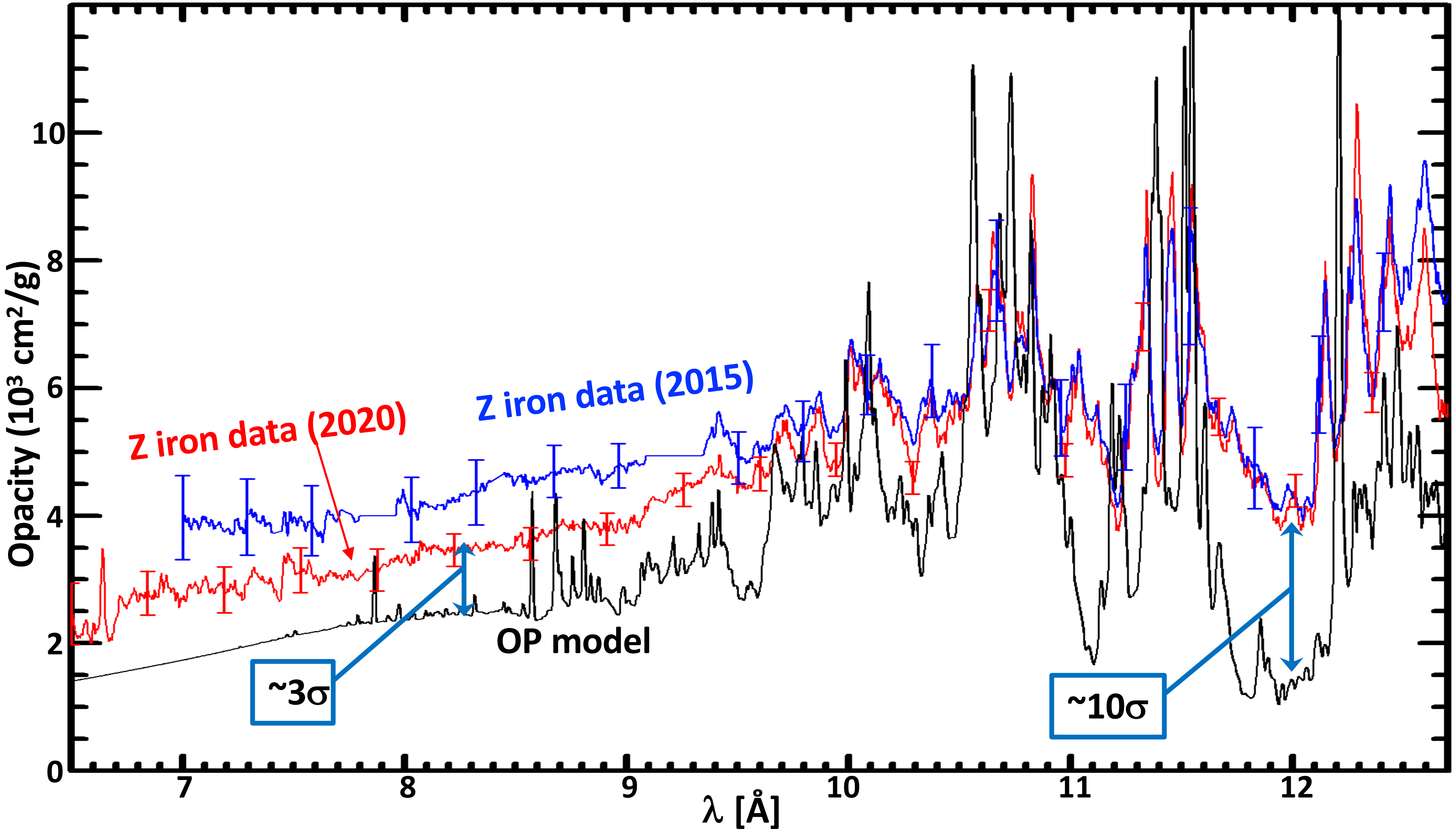
- Large volume of backlight-only data statistics
- Monte Carlo for robust errors propagations
  - Backlight intensity, B_ν
  - Background, ϵ_ν
  - Sample areal density, ρL





Reanalysis revealed that the half of the experimental variation was caused by insufficient accuracy of analysis method.

New experiments and analysis reduced the model-discrepancy for Anchor 2 iron, but ~ 3-10 σ differences remain



Quasi continuum discrepancy

2015: ~ 1800 cm2/g; ~4σ

2020: ~ 960 cm2/g; ~3σ

Window discrepancy

2015: ~ 2900 cm2/g; ~ 5σ

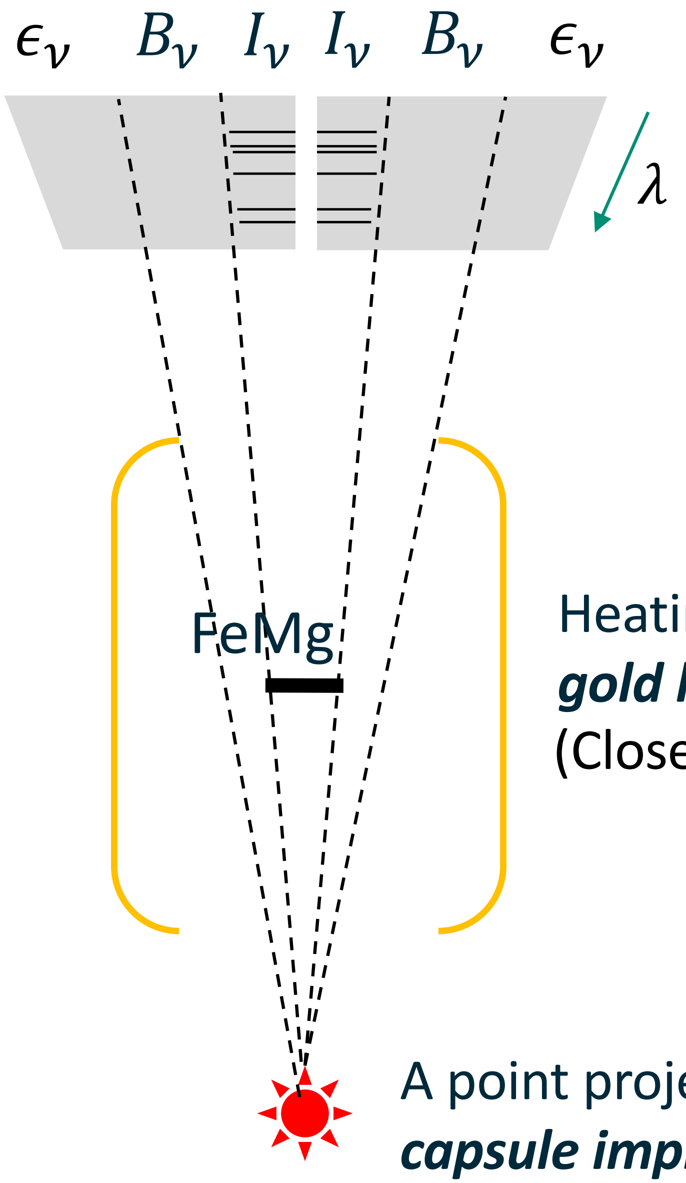
2020: ~ 2700 cm2/g; ~ 10σ

Theory: We have investigated many of possible limitations in the existing opacity theory

Possible limitations	Numerical
• Accuracy in atomic data?	✓
• Sufficient # of excited states?	✓
• Accuracy in spectral line shapes?	✓ ✗
• Missing physics	
• Two photon opacity	✓ ✗
• Transient space localization	✓
• More …	

- **Significant investigations done by both theory and experiment teams**
- **The scrutiny will continue until the model-data discrepancies are removed**

An independent experimental method is being developed at National Ignition Facility (NIF)



Heating by ***gold hohlraum*** (Close to LTE?)

A point projection by ***capsule implosion***

Advantages:

- Hohlraum sample heating
- Easier determination of I_ν, B_ν, and ϵ_ν
- Secondary T_e, n_e diagnostics

Challenges:

- **Large background and self-emission, ϵ_ν**
- Lower resolution (can be resolved with film, CMOS)

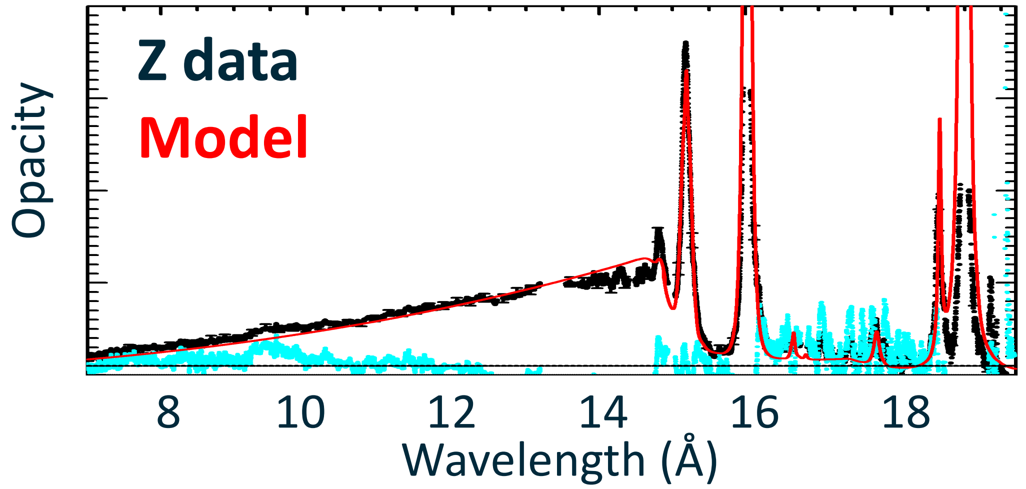
NIF and Z opacity experiments complement each other and speed up investigations

Perry et al PRL (1991); Perry et al HEDP (2017)

Other ongoing efforts from SNL and NIF opacity experiments

Oxygen opacity measurements

SNL: Te=148 eV, ne=8.6e21 e/cc*

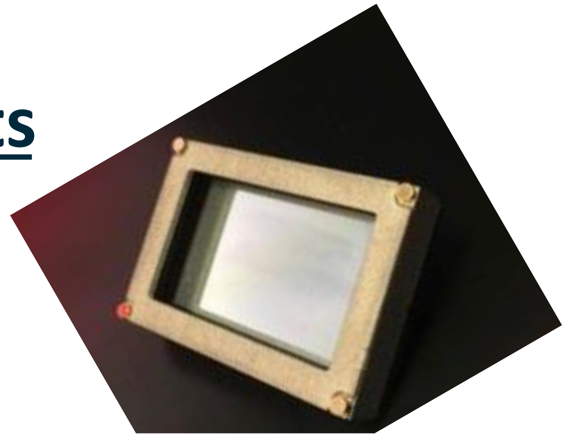


NIF:

- Oxygen opacity measured at multiple conditions
- The data are being analyzed

Time-resolved measurements

UXI detector**



SNL

- Investigate time-integration effects
- Achieve more extreme conditions
- Multiple opacity measurements from a single experiment

NIF

- Achieve higher spectral resolution
- Suppress background and self-emission

* Paper will be submitted soon

** Ultrafast X-ray Imager (UXI) developed at SNL

Understanding solar opacity is challenging due to complex nature of Rosseland mean opacity

1. **Basics:** Rosseland mean opacity
   - Derivations, assumptions, and complexity
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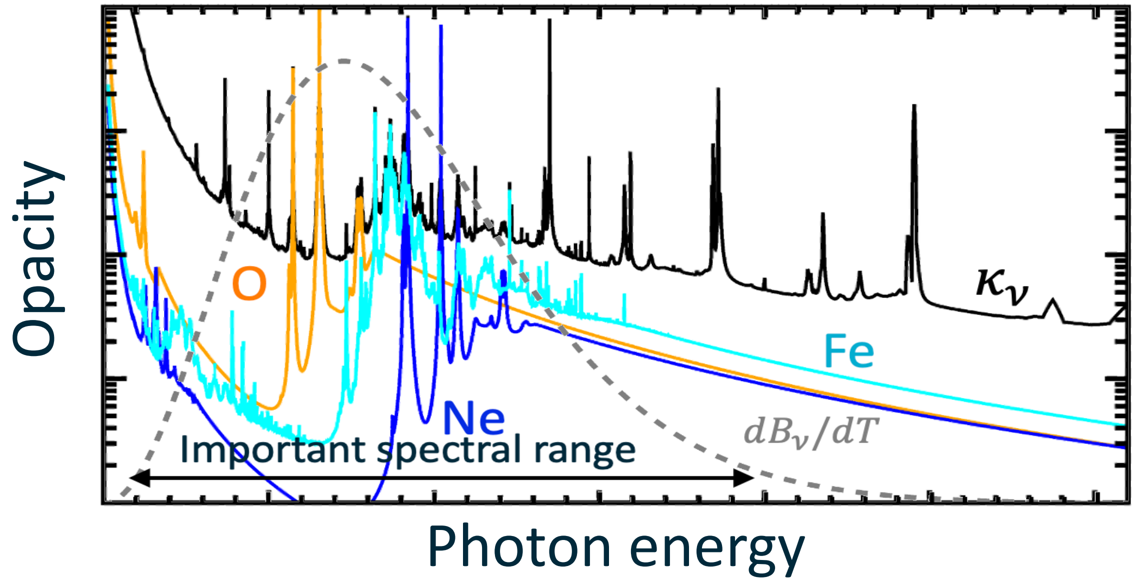

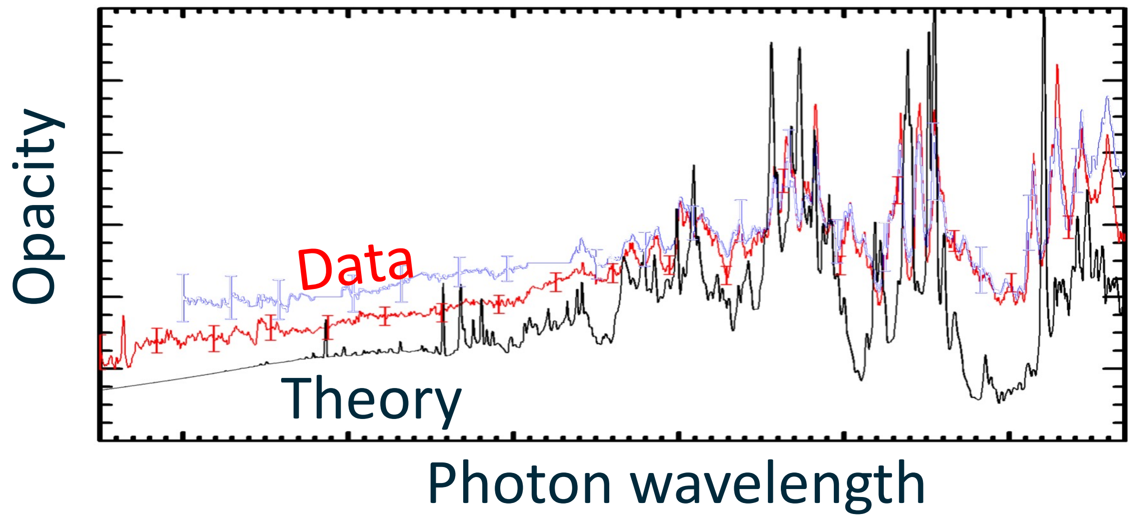

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