OPACITIES: MEANS & UNCERTAINTIES

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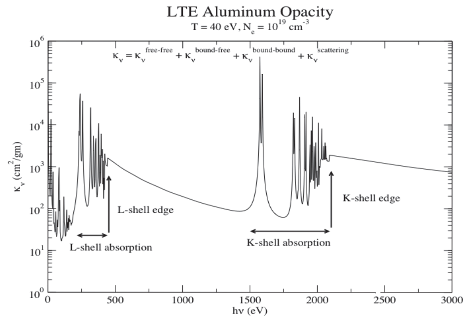
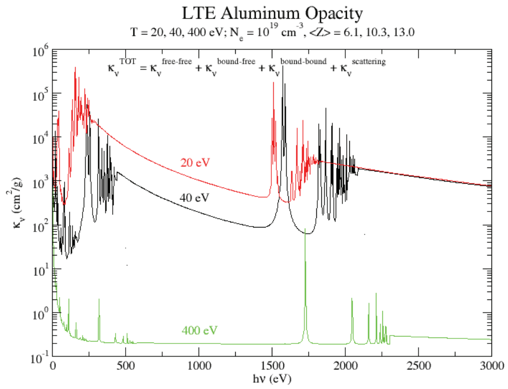
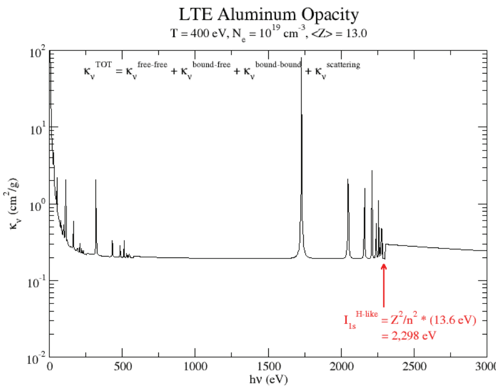
Previously...

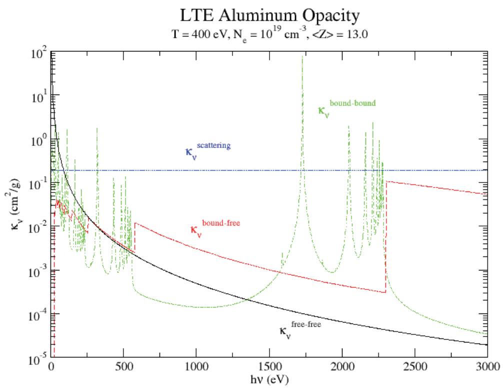


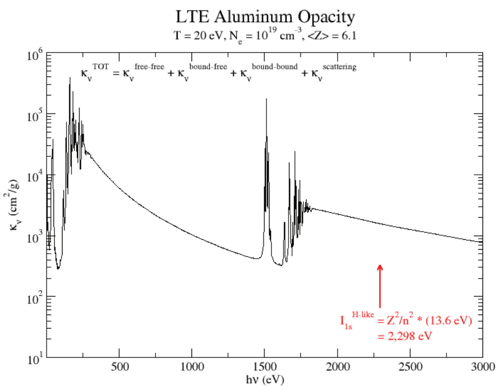
Before moving on to the topic of mean opacities, let's look at Al opacities at different temperatures

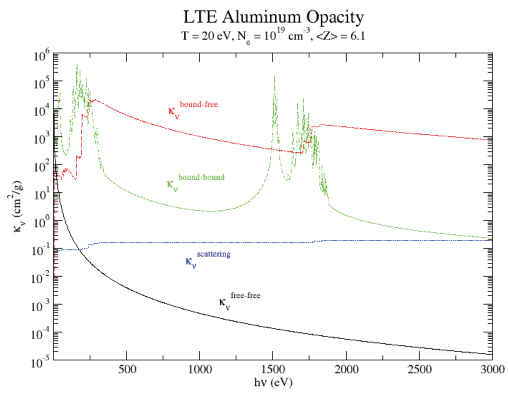
- Our main example is kT = 40 eV and $N_e = 10^{19}$ cm^{-3} with <Z> = 10.05 (Li-like ions are dominant)
- Consider raising and lowering the temperature:
  - kT = 400 eV (<Z> = 13.0; fully ionized)
  - kT = 20 eV (<Z> = 6.1; nitrogen-like stage is dominant)











Road map to mean opacities

In order of most to least refined
with respect to frequency resolution:

κ_ν (monochromatic)

↓

κ^{MG} (multigroup)

↓

$\bar{\kappa}$ (gray)

Mean (gray) opacities

- Under certain conditions, the need to transport a frequency-dependent radiation intensity, I_ν, can be relaxed in favor of an integrated intensity, I, given by

$$I = \int_0^\infty I_\nu \, d\nu$$

- Applying this notion of integrated quantities to each term of the radiation transport equation results in a new set of equations, similar to the original, frequency-dependent formulations
- Frequency-dependent absorption terms that formerly contained κ_ν will instead contain a suitably averaged "mean opacity" or "gray opacity" denoted by $\bar{\kappa}$

Mean opacities (continued)

- The mean opacity $\bar{\kappa}$ represents, in a single number, the tendency of a material (at a specific ρ and T) to absorb/scatter radiation of all frequencies
- Naturally, the transport of a frequency-integrated intensity is computationally much less expensive than the corresponding frequency-dependent case

Types of mean opacities

- Two most common types of gray opacities are the "Planck mean" (or "emission mean") and "Rosseland mean" opacities
- Other types of mean opacities include "flux-weighted" (or "radiation-pressure") and "absorption" means
- The various means arise if one wants to obtain correct values for a particular frequency-integrated physical quantity, such as radiation flux or energy
- The calculation of Planck and Rosseland mean opacities does not require a knowledge of the radiation field quantities (flux, energy, etc.) which makes them easier to calculate, but they do not necessarily lead to the correct answer

Rosseland mean opacity

- The Rosseland mean opacity, $\bar{\kappa}_R$, yields the correct value for the integrated energy flux *for an optically thick plasma*
- It is calculated from $\kappa_\nu^{\mathrm{TOT}}$ in the following manner:

$$\frac{1}{\bar{\kappa}_R(\rho,T)} = \frac{\int_0^\infty \frac{\partial B_\nu(T)}{\partial T} \frac{1}{\kappa_\nu^{\mathrm{TOT}}(\rho,T)} d\nu}{\int_0^\infty \frac{\partial B_\nu(T)}{\partial T} d\nu}$$

where $B_\nu(T)$ is the Planck function

- The weighting function peaks at hν ≈ 3.8 × kT, which indicates where the monochromatic opacity, $\kappa_\nu^{\mathrm{TOT}}$, will be most strongly sampled when taking the Rosseland mean

Rosseland mean opacity (continued)

- Note that the Rosseland mean opacity is obtained from $\kappa_\nu^{\mathrm{TOT}}$ using an *inverse*, or harmonic, average ⇒ $\bar{\kappa}_R$ will more heavily favor the regions of low absorption displayed by $\kappa_\nu^{\mathrm{TOT}}$
- Also, the use of a harmonic average implies that the individual contributions (bound-bound, bound-free, free-free, scattering) can not be averaged first and then added together to obtain the proper mean value
- As mentioned above, the Rosseland mean opacity is obtained by averaging over the *total* opacity

$$\kappa_\nu^{\mathrm{TOT}} = \kappa_\nu^{\mathrm{ABS}} + \kappa_\nu^{\mathrm{SCAT}}$$

Planck mean opacity

- The Planck mean opacity, $\bar{\kappa}_P$, yields the correct value for the integrated thermal emission *for an optically thin plasma*
- It is calculated from $\kappa_\nu^{\mathrm{ABS}}$ in the following manner:

$$\bar{\kappa}_P(\rho,T) = \frac{\int_0^\infty B_\nu(T)\kappa_\nu^{\mathrm{ABS}}(\rho,T) d\nu}{\int_0^\infty B_\nu(T) d\nu}$$

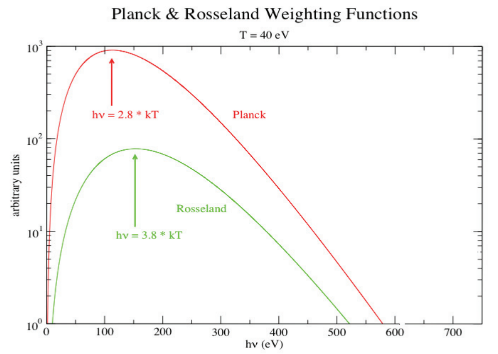
- The weighting function peaks at hν ≈ 2.8 × kT, which indicates where the monochromatic opacity, $\kappa_\nu^{\mathrm{ABS}}$, will be most strongly sampled when taking the Planck mean

Planck mean opacity (continued)

- Note that the Planck mean opacity is obtained from $\kappa_\nu^{\mathrm{ABS}}$ using the familiar arithmetic mean ⇒ $\bar{\kappa}_P$ will more heavily favor the regions of high absorption displayed by $\kappa_\nu^{\mathrm{ABS}}$
- Also, the various contributions to the opacity can be averaged separately and then added together to obtain the correct mean value
- As mentioned above, the Planck mean opacity is obtained by averaging over only the *absorption* opacity $\kappa_\nu^{\mathrm{ABS}}$

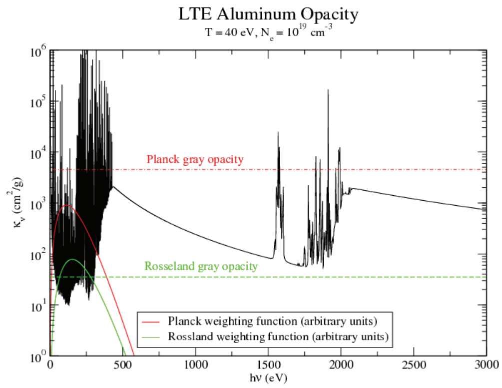
Rosseland vs. Planck (numerical example)

- Again consider the example of an aluminum plasma in LTE with kT = 40 eV, $N_e = 10^{19} cm^{-3}$ (If the plot of κ_ν looks a bit different, that is because a more complex atomic model has been used to generate the following plots. However, the basic physics remains the same.)
- First, we consider the two weighting functions at kT = 40 eV. Note how the Rosseland and Planck weighting functions peak at different values of the photon energy, $h\nu$.



Rosseland vs. Planck (numerical example)

- Next, we consider the two weighting functions superimposed on the frequency-dependent opacity, κ_ν, along with the corresponding gray opacities, $\bar{\kappa}_R$ and $\bar{\kappa}_P$
- Note that the two mean opacities differ by more than two orders of magnitude due to the inverse vs. arithmetic averaging prescriptions



Which mean opacity should you use?

- Consider the transport equation in the gray-diffusion approx.

$$\frac{\partial E_r}{\partial t} = \vec{\nabla}\cdot(D\vec{\nabla}E_r) + c(\rho\bar{\kappa}_P)(aT_e^4 - E_r)$$

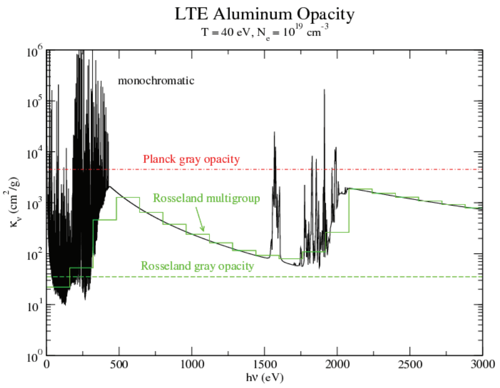
$$D = \frac{c/3}{(\rho\bar{\kappa}_R)}$$

- Note the presence of two physically meaningful mean free paths, $\lambda^{mfp} = 1/(\rho\kappa)$
- Rosseland mean is used in the diffusion coefficient, Planck mean is used in the radiation-electron coupling term
- These choices are not valid for all conditions: time-dependence issues, two-temperature opacities, etc…

Multigroup opacities

- When frequency-dependent transport is not feasible and frequency-integrated transport is inaccurate, there is a third option that can yield reasonable results without a huge investment of computing resources: multigroup opacities
- This approach requires that the photon frequency space be binned into a small number of frequency "groups". All frequencies within a group are suitably average (Rosseland, Planck, etc.) and then transported as if they were a single frequency.
- The expressions for multigroup opacities are extremely similar to their gray counterparts. For example, if a particular group has a width $\Delta\nu = \nu_2 - \nu_1$, then the "Planck multigroup opacity" can be written:

$$\kappa_P^{MG}(\rho,T,\nu_1,\nu_2) = \frac{\int_{\nu_1}^{\nu_2} B_\nu(T)\kappa_\nu^{ABS}(\rho,T)d\nu}{\int_{\nu_1}^{\nu_2} B_\nu(T)d\nu}$$



Multigroup opacities (continued)

- As the number of groups increases and the width of each group decreases ($\Delta\nu \rightarrow 0$) the value of each multigroup opacity approaches the monochromatic opacity. The term "monochromatic" arises from the notion that there is only a single frequency or "color" in each infinitely narrow group as the limit $\Delta\nu \rightarrow 0$ is obtained.
- The accompanying figure revisits the numerical example for aluminum, showing a 20-group Rosseland multigroup opacity, in addition to the monochromatic and gray opacities already discussed

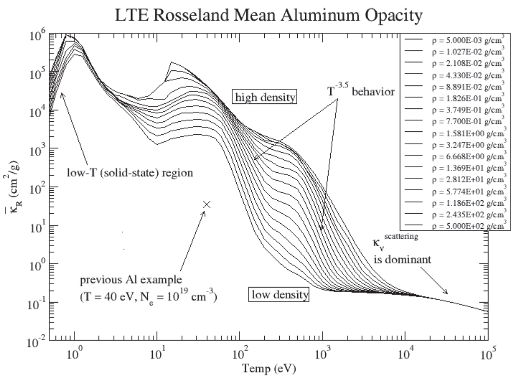
General trends for gray opacities as a function of ρ and T

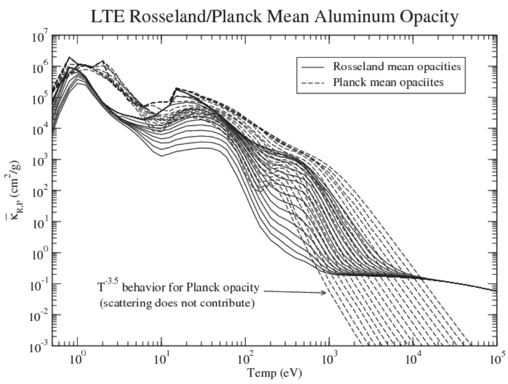
- If an LTE plasma is at a high enough temperature such that all of the ions are completely ionized, then there are only two possible sources of opacity (free-free and Compton scattering)
  - For low densities, Compton scattering dominates the Rosseland gray opacity (remember there is no scattering contribution to Planck mean opacities)
  - For high densities, free-free absorption dominates the gray opacity
- If the temperature is insufficient to completely ionize all bound electrons, then there can be strong contributions to the gray opacity from bound-bound and bound-free processes
- According to Kramers' Law of Opacity (derived from Kramers' fundamental cross sections), when bound-free or free-free proceses dominate, the mean opacity can be expressed as:

$$\bar{\kappa} = \kappa_0 \rho / T^{3.5}$$

General trends...(continued)

- For a numerical illustration of the trends listed on the previous slide, consider the following two figures
- The first figure plots the Rosseland mean opacity, $\bar{\kappa}_R(\rho,T)$, vs. temperature (0.5 - 10^5 eV) for 17 densities ranging from 0.005 - 500 g/cm^3
- The second figure overlays the Planck mean opacity on top of the Rosseland mean opacity for the same conditions
- Each of the trends listed above can be observed if you look carefully





LTE opacity availability for transport codes

- In practice, the monochromatic opacities are not used in radiation transport calculations (too expensive)
- For LTE applications, raw OPLIB data files of "numerical", monochromatic opacities. The files can be manipulated by code users to create numerical tables of gray and/or multigroup opacities. A user must choose appropriate values of (ρ,T) and group boundaries for their specific application.
- The TOPS code allows this sort of manipulation of the raw monochromatic data: http://aphysics2.lanl.gov/opacity/lanl
- A new set of OPLIB opacities (Z ≤ 30) is expected to be released in 2015 [Colgan et al, High Energy Density Phys. **9**, 369 (2013).]

NLTE opacity availability for transport codes

- For NLTE applications, a tabular approach is typically not feasible. Instead, the rate equations must be solved for each cell during every time step (very expensive).
- In this case, one must build a model that contains all of the relevant fundamental atomic physics data (energy levels, radiative rates, collisional rates, etc). For example, the LANL suite of atomic physics codes can be used to construct such models: http://aphysics2.lanl.gov/tempweb/lanl

Uncertainties in the opacity

- Uncertainties in opacity are caused by uncertainties in the calculation of the fundamental atomic cross sections, plasma effects caused by perturbing ion, computational limitations, etc.
- Measurements of fundamental cross sections are usually carried out on neutral atoms, rather than on charged ions, due to the difficulty in preparing a sample in a specific ion stage and because of the myriad possibilities of excited levels
- Cross sections of neutral atoms are more difficult to calculate accurately because of the many-body, electron-electron interaction. Thus, comparison of calculations with measured cross sections for neutral species should provide an upper bound on uncertainties, at least as far as cross sections are concerned.
- Most information about uncertainties comes from the astrophysics community (Z ≤ 30)

Uncertainties in gray opacities

- The following is taken largely from W. Huebner's chapter in "Physics of the Sun" (see references on final viewgraph). These statements refer to the Rosseland mean opacity only.
- When scattering dominates (high T, low ρ), the uncertainty in the opacity is ~5%
- As the density increases and free-free processes become more important, the uncertainty is less than ~10%
- As the temperature decreases and bound-free becomes important, the uncertainty increases to ~15-20% and as the temperature decreases still further (bound-bound can contribute), the uncertainty increases to ~30%

Uncertainties in monochromatic opacities

- Uncertainties in the monochromatic opacity, κ_ν, are much more difficult to determine for a variety of reasons
- In practice, one attempts to calculate a small portion of a measured κ_ν spectrum by considering a very large atomic model, confined to a very limited frequency range, depending on the application of interest
- For even moderately complex ions, the number of bound-bound transitions is too large to fit on a large-scale computer
- There is also the issue of line broadening (plasma effects) in order to predict the correct shape of the bound-bound features
- Recent opacity experiments have been performed by Bailey et al (SNL) for iron on the Sandia Z machine (see next viewgraph) that show good agreement between experiment and theory. However, more recent iron experiments display a large, puzzling disagreement with theory [Bailey et al, *Nature* **517**, 56 (2015)]

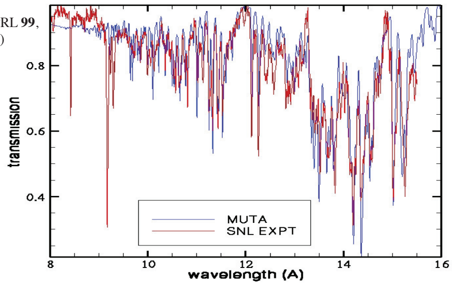
Comparison of LANL MUTA calculations with Sandia-Z iron opacity experiments; Impressive agreement!

Thanks to Jim Bailey, SNL

kT=160 eV, $N_e=1.5x10^{22}$ cm^{-3}

Calculations by Joe Abdallah, LANL

Bailey et al, PRL **99**, 265002 (2007)



Useful references

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- "The Los Alamos Suite of Relativistic Atomic Physics Codes", C.J. Fontes *et al*, *J. Phys. B*, in press (2015).
- GUI interface to TOPS:
  http://aphysics2.lanl.gov/opacity/lanl
- GUI interface to LANL Suite of Atomic Physics Codes:
  http://aphysics2.lanl.gov/tempweb/lanl