OPACITIES: LTE & NON-LTE

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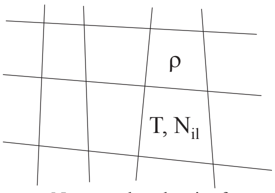
  Norm Magee
  Manolo Sherrill
  Honglin Zhang

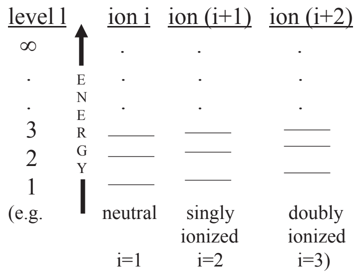
Some helpful illustrations

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



The main players

- Photons (radiation field)
- Bound electrons (orbiting around the nucleus)
- Free electrons (formerly bound electrons that have been ionized by free electrons or photons)

- The photons and electrons interact via fundamental atomic processes, which can be used to determine the atomic level populations, N_{il}
- These populations can then be used to compute an opacity, κ_ν, which is used in radiation transport calculations

Explanatory definitions/symbols

- ρ - ion (or material) mass density: $[\rho]$ = grams/cm^3
- $N_I = \sum_{il} N_{il}$ - ion number density: $[N_I] = 1/cm^3$; $\{N_I = \rho(A_0/A)\}$
- N_e - free electron number density: $[N_e] = 1/cm^3$
- T or kT = temperature (ion, electron, radiation): [T] = eV
- $\overline{Z}(\rho,T)$ ("Z bar") or $< Z >$ - average charge state ($N_e = \overline{Z}N_I$)

radiation quantities

- $h\nu$ - photon energy: $[h\nu]$ = eV
- $\kappa_\nu(\rho,T)$ - opacity: $[\kappa_\nu]$ = cm^2/gram
- $\varepsilon_\nu(\rho,T)$ - emissivity: $[\varepsilon_\nu]$ = ergs/(gram sec Hz)
- I_ν - (isotropic) radiation intensity: $[I_\nu]$ = ergs/(cm^2 sec Hz)

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 ($\sigma_{l\to l'}$)

↓

rate coefficients, rate equations

↓

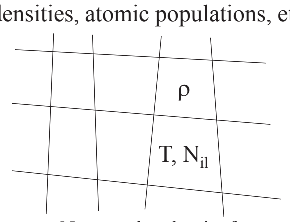
atomic level populations (N_{il})

↓

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

Excitation and de-excitation processes

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



N_{il} = number density for level l, ion stage i
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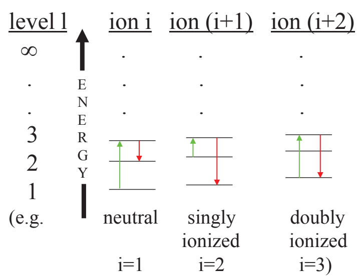
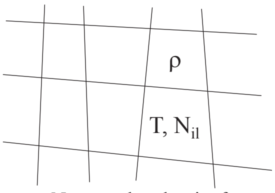
Our sample ions/atoms inhabiting each cell



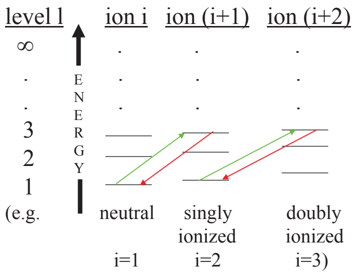
Ionization and recombination processes

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



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

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

A specific example: collisional excitation/de-excitation

- Each element of the rate matrix is computed from fundamental cross sections associated with each process
- Consider collisional excitation/de-excitation as a specific example:

$$\frac{dN_{il}}{dt} = (\text{"rate" of excitations into il}) - (\text{"rate" of de-excitations out of il}) + \ldots$$
$$= \sum_{im} [s(im,il;T)N_e N_{im} - t(im,il;T)N_e N_{il}] + \ldots$$

- s(im,il;T) is the "rate coefficient" for electron collisional excitation from level m to level l in ion stage i, symbolically written as

$$e^- + (\text{im}) \rightarrow (e^-)' + (\text{il})$$

- Similarly, t(im,il;T) represents the rate coefficient for all possible collisional de-excitations into level l of ion stage i

A specific example: collisional excitation/de-excitation (continued)

- The result looks like

$$s(\text{im,il};T_e) = \int_{E_0}^{\infty} F(E,T_e)\, v(E)\, \sigma_{\text{iml}}(E)\, dE$$

- $F(E,T_e)$ is the free-electron energy distribution function
- $v(E)$ is the velocity of a free electron $[v(E) = \sqrt{(2E)/m_e}]$
- $\sigma_{\text{iml}}(E)$ is the excitation cross section
- E_0 is the threshold energy, above which excitation can occur

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- The ***rate*** at which excitations occur from level m to level l is s(im,il;T)N_e and the ***rate per unit volume*** is s(im,il;T)$N_e N_{im}$

A specific example: collisional excitation/de-excitation (continued)

- The rate coefficients for collisional de-excitation are determined from the principle of detailed balance and can also be expressed in terms of the same excitation cross section
- The rate coefficients for the remaining collisional and photo processes are determined in a similar fashion
- Just as electron-collision processes require a knowledge of the free-electron energy distribution function, F(E,T_e), photo processes require that the photon energy distribution function also be specified
- These concepts lead naturally to a discussion of LTE vs. non-LTE (NLTE) atomic physics

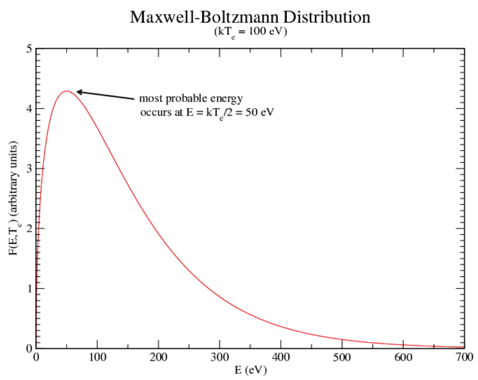
Free electrons in thermodynamic equilibrium

- 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



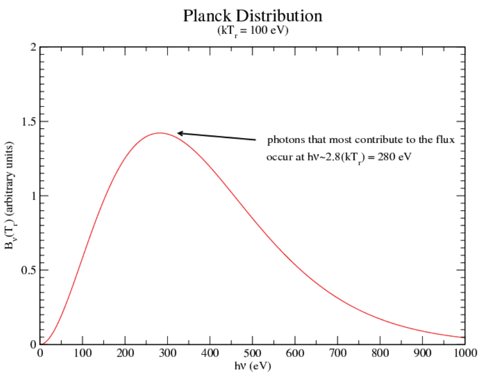
Photons in thermodynamic equilibrium

- 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 = Local Thermodynamic Equilibrium
- LTE is valid at a particular point in the plasma if the electron and photon distributions are in equilibrium ***with each other*** : $T_e=T_r=T_I=T$. This is one of the "textbook" definitions of LTE.
- There are other descriptions of LTE...

LTE applies if any of the following are true:

- At a given point in the plasma, the (atomic) conditions can be described by a single temperature ($T=T_e=T_r=T_I$)
- The rate at which any atomic process occurs is exactly balanced by the rate of its inverse process (this condition makes the physics much simpler to deal with than NLTE)
- The energy distribution of the free electrons in the plasma is described by a Maxwellian distribution and the radiation field is described by a Planck function (all at the same temperature)
- The FREE ELECTRON density is so high that electron collisions dominate the various atomic processes ("collision-dominated plasma"). In this case, there is not a true balance between all processes, but the following, and perhaps most important, bullet is still true:

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

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

- 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 $(dN_{\rm il}/dt = 0)$ which could have been found by solving the much simpler Botzmann relationship above

Non-LTE

- Non-LTE applies if:
  - LTE conditions are not satisfied (obviously!)
  - System is changing so rapidly that electron and/or photon energy distributions do not reach thermal equilibrium (i.e. Maxwellian or Planckian is not valid, lasers, $T_r \neq T_e$, etc.)
  - Optically thin plasma: radiation escapes and is not available to provide LTE balance among the fundamental atomic processes
- 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

Photon scattering

- One additional, fundamental process must be discussed before an opacity can be constructed: Compton scattering of photons

$$\gamma + e^- \rightarrow \gamma' + (e^-)'$$

- This process differs from free-free absorption in that the incident photon loses only a small portion of its energy when interacting with a free electron, then continues on with a slightly smaller energy

$$\sigma^{\rm THOMSON} = \frac{8\pi}{3}\left(\frac{{\rm e}^2}{m_e c^2}\right)^2 = 6.66\times10^{-25}({\rm cm}^2) \quad (h\nu << mc^2)$$

$$\sigma^{\rm COMPTON}(\nu) = G(\nu)\sigma^{\rm THOMSON}$$

- $G(\nu)$ is a relativistic correction factor that accounts for the case when the photon energy becomes comparable to the electron rest mass and the electron's kinetic energy is treated in a fully relativistic manner

What is an opacity?

- An opacity, κ_ν, describes the coupling between matter and radiation via electron-photon interactions
- Opacity gives a measure of how much radiation a certain material will absorb/scatter (i.e. how "opaque" is the material)
- An opacity can be thought of as a macroscopic quantity that is built up from fundamental atomic cross sections
- The amount of radiation that is absorbed/scattered (i.e. removed) from the ambient radiation field, I_ν, in each cell of our sample plasma is given by:

$$\kappa_\nu I_\nu$$

What is an emissivity?

- An emissivity, ε_ν, gives the amount of radiation that will be emitted by the material in a plasma via electron-photon interactions
- As with the opacity, an emissivity is calculated from fundamental atomic cross sections
- The amount of radiation that is emitted (i.e. added to) the ambient radiation field, I_ν, in each cell of our sample plasma is given by:

$$\varepsilon_\nu/(4\pi) \quad \text{(isotropic emitter)}$$

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:

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

emissivity

radiation intensity

material density

radiation frequency

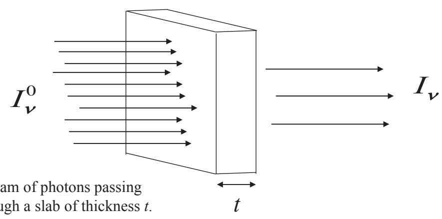
opacity

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 radiation transport equation:

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

- 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 $\lambda_\nu^{\text{mfp}} = (1/\rho\kappa_\nu)$ 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 << λ_ν^{mfp}.

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

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

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:

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

- 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, $\sigma_{\text{il}}^{\text{photo}}$
- 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}

The LANL Suite of Atomic Modeling Codes

Atomic Physics Codes → Atomic Models → ATOMIC

CATS: Cowan Code

RATS: relativistic

ACE: e^- excitation

GIPPER: ionization

http://aphysics2.lanl.gov/tempweb

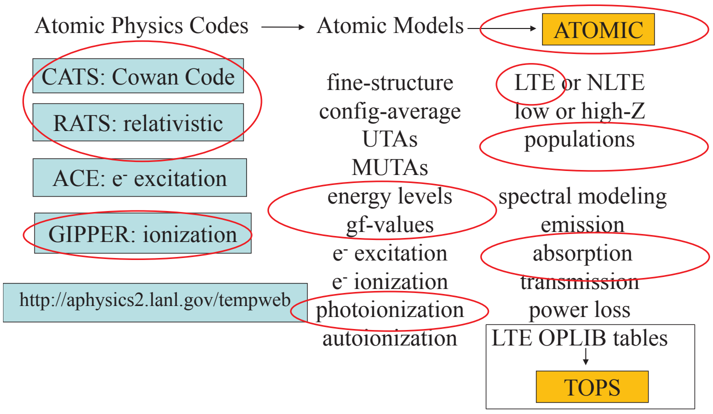
fine-structure
config-average
UTAs
MUTAs
energy levels
gf-values
e^- excitation
e^- ionization
photoionization
autoionization

LTE or NLTE
low or high-Z
populations

spectral modeling
emission
absorption
transmission
power loss

LTE OPLIB tables
↓
TOPS

To calculate LTE opacities, you need only:



What about emissivities?

- Simple relationship for LTE conditions:

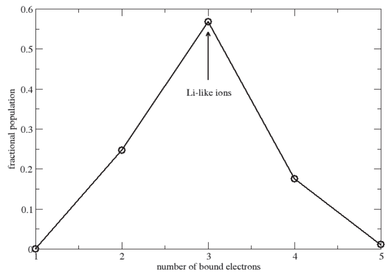
$$\varepsilon_\nu = (4\pi)\kappa_\nu^{ABS}(\rho,T)B_\nu(T)$$

emissivity — Planck function — 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

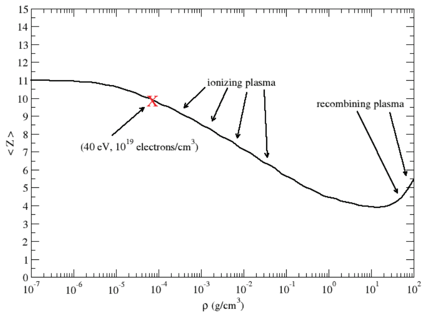
Numerical example of an LTE opacity: Aluminum plasma at kT = 40 eV, $N_e = 10^{19}$cm^{-3}

- 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:



Another useful plot to consider: <Z> vs. ρ

- Here is a plot of <Z> vs mass density for a fixed temperature of 40 eV:



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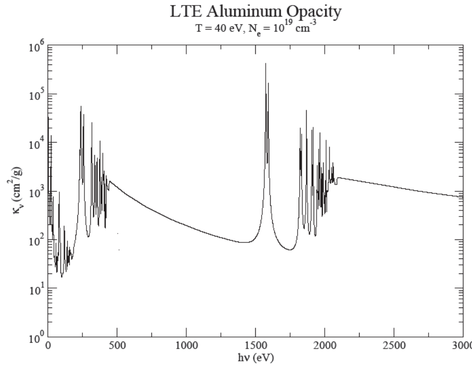
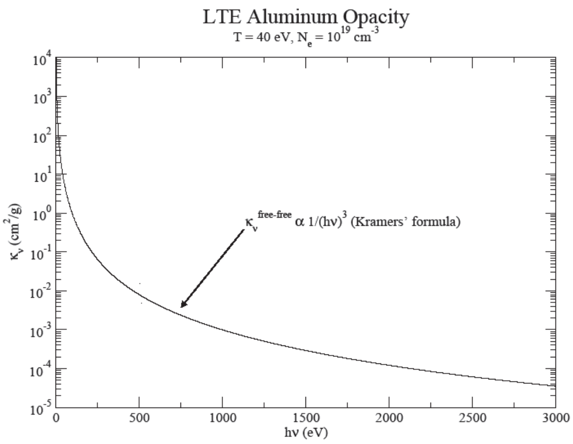
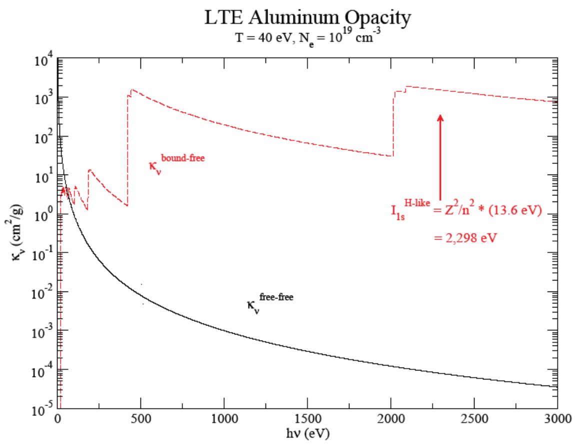
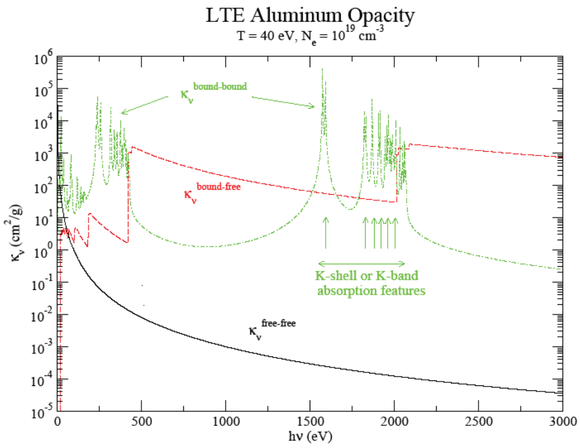
- The following plots show the contribution to the total opacity from each of the three photo-absorption processes as well as the contribution from Compton scattering
- You will see some arcane spectroscopic notation: bound electrons with the same principal quantum number n are said to inhabit the same "shell". Each shell is identified by a capital letter: n=1, K-shell n=2, L-shell n=3, M-shell ….
- Bound-bound absorption involving an active bound electron that initiates from the K-shell is referred to as "K-shell" absorption, etc. Bound-bound emission that terminates with a bound electron ending up in the K-shell is referred to as "K-band" emission, etc.

First, a snapshot of the total LTE opacity for this aluminum plasma









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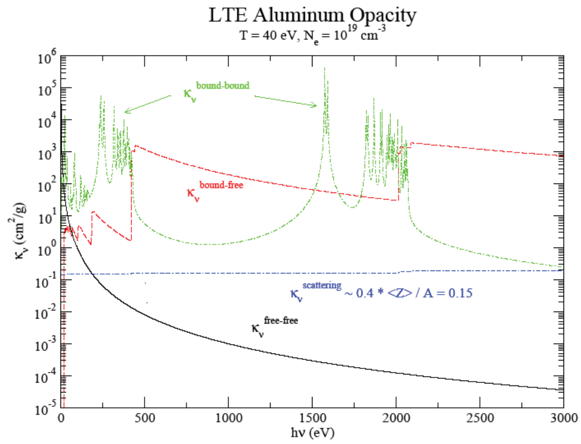

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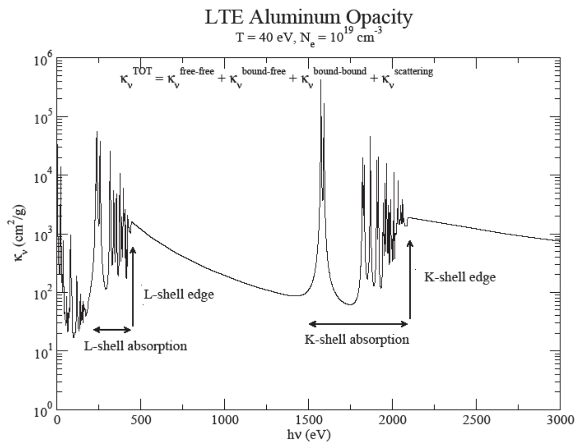

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