Photoionization Modelling

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1. Photoionization Physics

The general problem of calculating the reprocessing of ionizing continuum radiation from a star or compact object into longer wavelength lines and diffuse continuum has broad importance in astrophysics. The fundamental microphysical process involved is photoionization, the ionization of an atom or ion by a photon. History has led to the standard definition of the entire reprocessing problem as 'photoionization modelling', although calculations which include detailed treatments of the transport of radiation are generally referred to under the category of stellar atmospheres calculations.

This review is intended to be a basic and brief introduction to the subject. More detail, for those interested in constructing their own numerical models is found in the text by Osterbrock (1989); in the context of AGNs the subject has been discussed by Krolik (1999) and by Peterson (1997), and for galactic nebulae in reviews by Harrington (1989), Ferland et al. (1997a), Viegas (2000), and Osterbrock (1988).

2. Rates

Here and in what follows we will consider photoionization in a cloud of gas of fixed density illuminated by a point source of radiation which radiates isotropically. The rate of photoionization per ion can be written in terms of the spectrum and cross section as:

$$\gamma_i \equiv \int_{\varepsilon_{Th}}^{\infty} F_\varepsilon \sigma_i(\varepsilon) \frac{d\varepsilon}{\varepsilon}$$

where $F_\varepsilon = \frac{L}{4\pi R^2} f_\varepsilon$ is the local mean intensity of radiation, L is the luminosity of radiation source (I will use energy luminosity integrated from 1 Ry to 10000 Ry), R is distance from the source to the cloud, f_ε is the shape of the spectrum, defined such that $\int_{1Ry}^{1000Ry} f_\varepsilon d\varepsilon = 1$, and $\sigma_i(\varepsilon)$ is the photoionization cross section.

A very simple approximation for the photoionization cross section is:

$$\sigma(\varepsilon) = \sigma_0 \left(\frac{\varepsilon}{\varepsilon_{Th}}\right)^{-3}$$

$$(\varepsilon \geq \varepsilon_{Th})$$

where

$$\sigma_0 = \frac{2^8\pi}{3e^4}\alpha\pi a_0^2 = 6.3 \times 10^{-18}\mathrm{cm}^2 Z^{-2} n^2$$

$$\varepsilon_{Th} = 13.6\mathrm{eV} Z^2 n^{-2}$$

A more accurate expression:

$$\sigma(\varepsilon) = \sigma_0 \left(\frac{\varepsilon_{Th}}{\varepsilon}\right)^4 \frac{e^{4-4\tan^{-1}(\eta)/\eta}}{1 - e^{-2\pi/\eta}}$$

$\eta = \sqrt{\frac{\varepsilon}{\varepsilon_{Th}} - 1}$

for multi-electron atoms, a detailed numerical calculation is needed.

3. Scaling behavior

The photoionization equilibrium equation which describes the relative abundances of various ions n_i of a given element can be written:

$$n_e n_i C_i(T) + \frac{L}{4\pi R^2} n_i \int_{\varepsilon_{Th}}^{\infty} f_\varepsilon \sigma_i(\varepsilon) \frac{d\varepsilon}{\varepsilon} = n_e n_{i+1} \alpha_i(T)$$

where $\alpha_i(T)$ is the recombination rate coefficient, $C_i(T)$ is the collisional ionization rate coefficient, and n_e is the electron number density. Rewriting:

$$\frac{n_i}{n_{i+1}} = \frac{\alpha_i(T)}{C_i(T) + \frac{L}{n_e 4\pi R^2} \int_{\varepsilon_{Th}}^{\infty} f_\varepsilon \sigma_i(\varepsilon) \frac{d\varepsilon}{\varepsilon}}$$

The right hand side depends on atomic constants, temperature, f_ε (the spectrum shape), and $\frac{L}{n_e R^2} \equiv \xi$ known as the ionization parameter. This is the single most important parameter describing the ionization balance. Common definitions include:

- $\xi \equiv \frac{L}{n_e R^2}$ (Tarter, Tucker and Salpeter 1969)
- $U_1 \equiv \frac{N}{n 4\pi R^2 c}$ (Davidson 1974)
- $\Gamma \equiv \frac{L_\varepsilon|_{13.6eV}}{n 8\pi R^2 c}$ (Kwan and Krolik 1981)
- $\Xi \equiv \frac{L}{4\pi n_e ckTR^2}$ (Krolik, McKee and Tarter 1982)
- $U_x \equiv \frac{N_X}{n4\pi R^2 c}$ (Netzer 1994)

  where

  $N \equiv \int_{13.6eV}^{\infty} L_\varepsilon \frac{d\varepsilon}{\varepsilon}$

  $N_X \equiv \int_{100eV}^{\infty} L_\varepsilon \frac{d\varepsilon}{\varepsilon}$

  $L \equiv \int_{13.6eV}^{\infty} L_\varepsilon d\varepsilon$

4. Thermal Balance

Photoionzation has the feature that we observe (in principle) the photons responsible for ionization and the photons produced by the gas, so it can be self consistent in the sense that it does not necessarily rely on an unobserved source of heat or ionization. If so, heat input from the source of illumination balances cooling by emission of reprocessed radiation.

Heating is caused by:

- Photoionization produces an electron with kinetic energy $\varepsilon - \varepsilon_{Th}$:

$$H_{PI} = \frac{L}{4\pi R^2} n_i \int_{\varepsilon_{Th}}^{\infty} d\varepsilon f_\varepsilon \sigma(\varepsilon)$$

- Compton scattering produces electron with recoil:

$$\langle \frac{\Delta\varepsilon}{\varepsilon} \rangle = \left(\frac{4kT}{m_e c^2} - \frac{\varepsilon}{m_e c^2} \right)$$

$$H_{Comp} = \frac{L}{4\pi R^2} n_e \sigma_{Th} \int_{\varepsilon_{Th}}^{\infty} d\varepsilon \langle \frac{\Delta\varepsilon}{\varepsilon} \rangle f_\varepsilon$$

Cooling is caused by any process with removes energy from the electron bath:

- Recombination

$$C_{rec} = n_{i+1} n_e \alpha_i(T)(\varepsilon_{Th} + kT)$$

- Collisional excitation/ionization

$$C_{coll} = n_i n_e C_i(T) \Delta\varepsilon$$

- Compton scattering is included as a subtraction from the heating
- Free-free emission

$$C_{ff} = n_i n_e \kappa(T) kT$$

The thermal equilibrium equation can be written:

$$H_{PI} + H_{comp} = C_{rec} + C_{coll} + C_{ff}$$

where the terms on the left hand side are all proportional to L/R^2, and the terms on the right hand side are all proportional to n_e. So the temperature also depends on ξ.

5. Ionization and Thermal Balance Results

Figures 1 and 2 show ionization and thermal balance results for an optically thin gas illuminated by a power law radiation field with $f_\varepsilon \sim \varepsilon^{-1}$. The mean ion stage is a monotonically increasing function of ionization parameter. Higher Z elements are more difficult to ionize than lower Z elements, so they survive against ionization to higher ionization parameter. At the highest ionization parameter, the most abundant ions are those from the heaviest elements. At $\log(\xi) \geq 5$ the gas is almost fully ionized, while at $\log(\xi) \leq$ -3 the gas is almost fully neutral. Some ions are fragile, and essentially never occur as a pure charge state. Examples are ions with one electron outside a filled shell: Li-like, B-like, and Na-like.

The gas temperature increases monotonically with ξ. At high ξ the temperature is determined primarily by Compton scattering. The "Compton temperature" depends only on the mean photon energy (for non-relativistic photon energies and temperatures), $T_{IC} = \frac{\langle\varepsilon\rangle}{4k}$, where $\langle\varepsilon\rangle$ is the mean photon energy. For many plausible spectra, such as

$f_\varepsilon \sim \varepsilon^{-1}$, $T_{IC} \simeq 10^7 - 10^8$K. At low ξ the temperature is $\sim 10^4$K, determined by cooling by H I, He I, and other neutrals. T_{IC} depends on the steepness of the spectrum: Steeper spectra result in lower T_{IC}, and less ionization of ions with high ionization potentials at a given value of ξ. Compared with the coronal case, the temperature is much lower for a given ionization state, ie. $T \sim 0.1\langle\varepsilon_{Th}\rangle$, where $\langle\varepsilon_{Th}\rangle$ is the mean ionization potential of the most abundant ions in the gas.

6. Thermal Instability

Since photoionization allows for self-consistent temperature calculations, it is interesting to note that the temperature obtained by assuming a local balance between heating and cooling may not be stable. The net cooling function of gas at constaant density can be written $\Lambda(T)$. If $d\Lambda/dT < 0$ the gas is thermally unstable. Perturbations in temperature will lead to a thermal runaway, which will be terminated only when the temperature reaches a range where the cooling function is stable. In order to assess thermal instability it is necessary to specify which other state variables are held constant when $d\Lambda/dT$ is evaluated. Examples are isobaric (constant pressure) and isochoric (constant density) variations. Gas which is stable to isochoric perturbations may not be stable to isobaric perturbations.

$$\left(\frac{d\Lambda}{dT}\right)_P = \left(\frac{d\Lambda}{dT}\right)_n - \frac{\Lambda}{T}$$

$$\left(\frac{d\log\Lambda}{d\log T}\right)_P = \left(\frac{d\log\Lambda}{d\log T}\right)_n - 1$$

So gas with $\left(\frac{d\log\Lambda}{d\log T}\right)_n < 1$ will be unstable to isobaric perturbations.

In photoionized gas, $\left(\frac{d\log\Lambda}{d\log T}\right)_n < 1$ can occur when the cooling is due to bremmstrahlung ($\Lambda \sim T^{1/2}$). $\left(\frac{d\log\Lambda}{d\log T}\right)_n < 0$ can occur if the ionizing radiation field is deficient in soft photons. Thermal instability at constant pressure is a common feature if the Compton temperature is $\geq 10^7$K. If so, there are two stable solutions for temperature (near 10^4K and 10^7K) and a third intermediate solution which is thermally unstable. This has been proposed as a mechanism for allowing cool ($\sim 10^4$K) clouds to be confined by hot gas in the same region in eg. AGN (Krolik, McKee and Tarter, 1982). This is illustrated in figure 3.

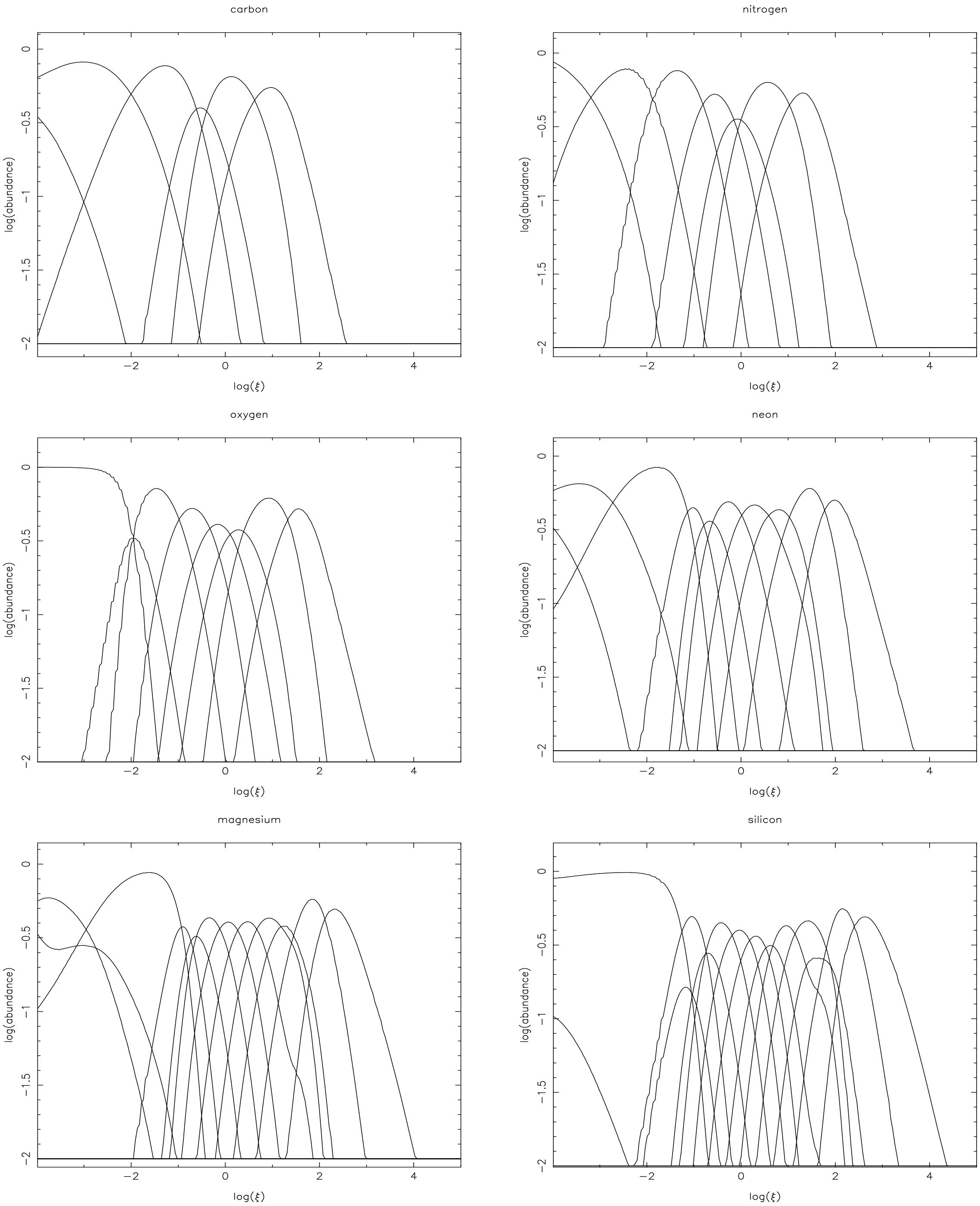

Fig. 1.— Ion fractions of an optically thin low density photoionized gas, as a function of ionization parameter for an ε^{-1} power law ionizing spectrum for elements C – Si

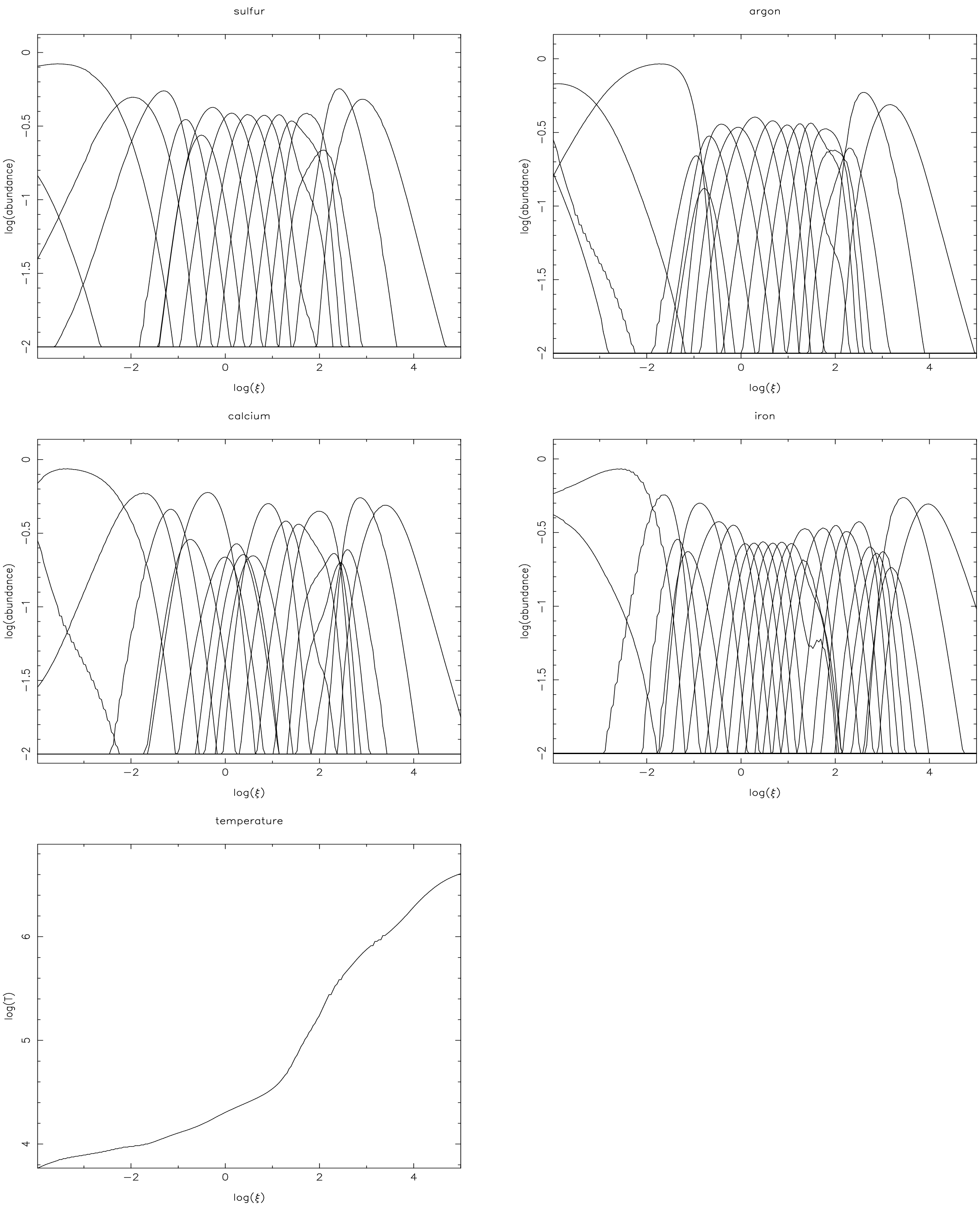

Fig. 2.— Ion fractions and temperature of an optically thin low density photoionized gas, as a function of ionization parameter for an ε^{-1} power law ionizing spectrum for elements S – Fe

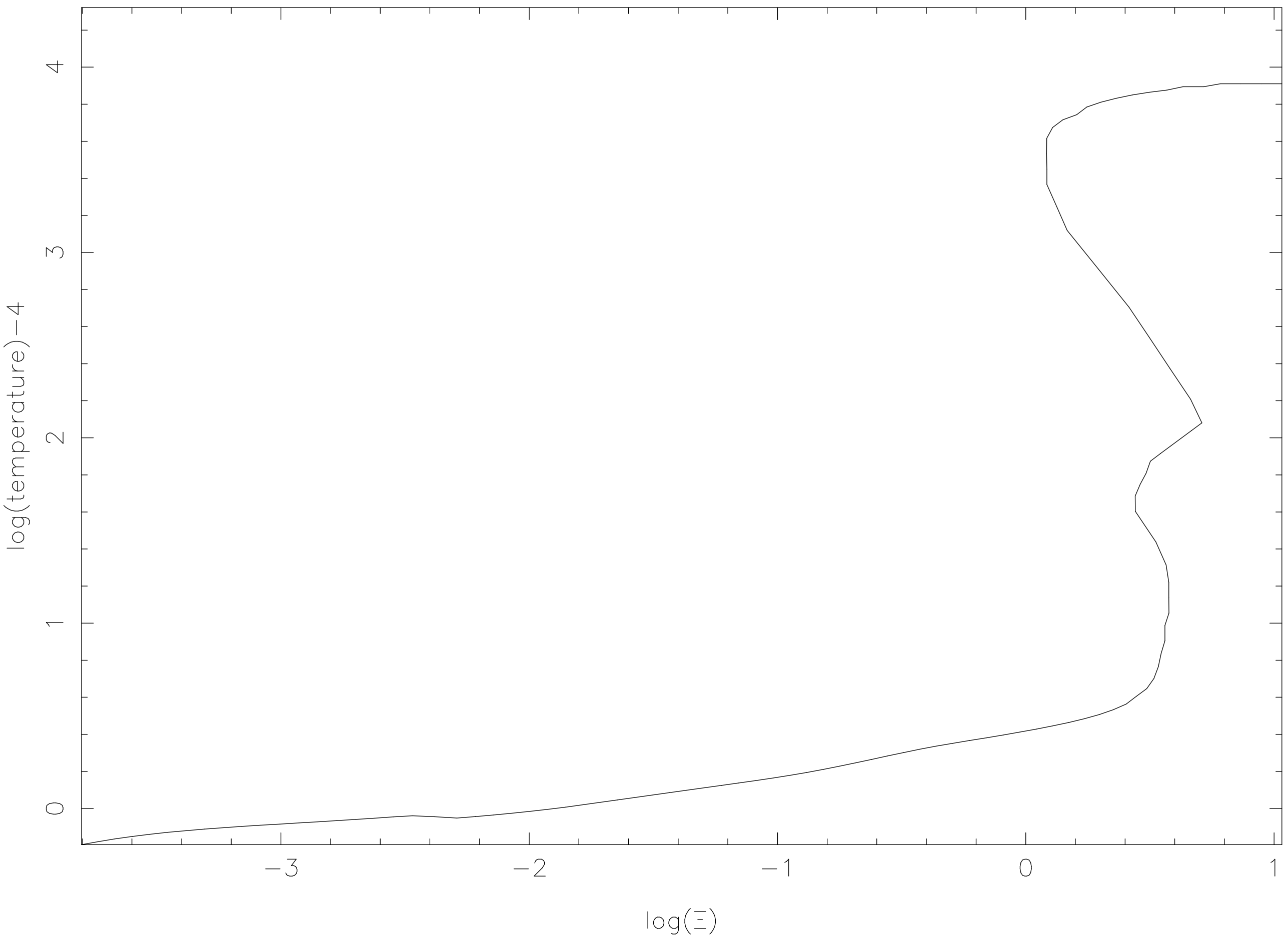

Fig. 3.— Temperature of an optically thin photoionized gas plotted as a function of Ξ, the constant pressure ionization parameter

7. Observable Effects I: Absorption

Photoelectric absorption is ubiqutous in astrophysics. Its spectrum can be estimated as follows: If we substitute for ε_0 in the crude approximation for $\sigma(\varepsilon)$:

$$\sigma(\varepsilon) = \sigma_0 Z^4 \left(\frac{\varepsilon}{1\mathrm{Ry}}\right)^{-3} \quad \varepsilon \geq \varepsilon_0$$

Now if we compare for various elements:

element	Z	abundance	$Z^4\times$abundance
H	1	1	1
He	2	0.1	1.6
C	6	10^{-4}	0.13
N	7	10^{-4}	0.24
O	8	10^{-4}	0.41
Ne	10	10^{-4}	1
Mg	12	10^{-5}	0.21
Si	14	10^{-5}	0.38
S	16	10^{-5}	0.66
Ar	18	10^{-5}	0.1
Fe	26	10^{-5}	4.6

This shows that the cross section at threshold are all comparable: There are no large jumps in the total cross section for absorption by neutral material with cosmic abundances. The total opacity of neutral gas with cosmic abundances is nearly a power law from 1-1000 Ry. Edges are expected, and observed from some objects, but they represent jumps in the opacity by factors ≤ 2. A crude approximation to the interstellar opacity is:

$$\sigma\varepsilon \simeq 1.5 \times 10^{-21} \left(\frac{\varepsilon}{1\mathrm{keV}}\right)^{-3}$$

A corollary, then, is that any large edges whigh are detected suggest the existence of departures from this picture, either partial ionzation, which can suppress the low Z elements (such as H and He) and thereby increase the prominence of the inner shell features of medium and high Z elements, or large departures from cosmic abundances.

8. Observable Effects Ib: Warm Absorbers

A crude approximation for the photoionization cross section:

$$\sigma(\varepsilon) = \frac{\sigma_0}{Z^2}\left(\frac{\varepsilon}{\varepsilon_0}\right)^{-3} \varepsilon \geq \varepsilon_0$$

$$\sigma(\varepsilon) = 0 \text{otherwise}$$

where $\sigma_0 = 6.3 \times 10^{-18}\text{cm}^{-2}$ is the threshold cross section for hydrogen, $\varepsilon_0 = 13.6Z^2\text{eV}$ is the energy at threshold and Z is the ion charge.

This shows that the cross section above threshold decreases as $\sim \varepsilon^{-3}$ and the threshold cross section decreases as $\sim Z^{-2} \sim \varepsilon_0^{-1}$. The net result is that higher charge cross sections dominate at high energies. An example is the inner shells of ions with more than ∼3 electrons. An example is shown in figures 4 and 5, which shows the cross sections for all ions of the 11 most abundant elements as a function of photon energy.

9. Observable Effects II: Emission

In photoionized plasmas collisional excitation is less important than for coronal plasmas since kT$\leq 0.1\varepsilon_{Th}$. It is important only for lines close to ground, for example the 2s – 2p transition in Li-like ions. Recombination cascades are generally the dominant line emission mechanism. Since the recombination rates for high n levels vary as $\alpha_n(T) \sim n^{-1}$ high n levels are important. The Lyman decrement is generally flatter than for coronal plasmas. Recombination favors high angular momentum states. This affects the strengths of lines such as, for example, the 2-1 transitions in He-like ions, by preferentially populating the S=1 (triplet) levels rather than the S=0 (singlet) levels. Fluorescence following inner shell ionization leads to formation of iron K lines.

Recombination continuum radiation accompanies lines formed by cascades. This is illustrated in figure 6, which shows the recombination spectrum of O VIII at 10^5K. Shape $\sim e^{-(\varepsilon-\varepsilon_{Th})/kT}$, so the width of the emission feature is a measure of T.

10. Observable Effects IIb: Emission from He-like Ions

He-like ions have 3 'lines':

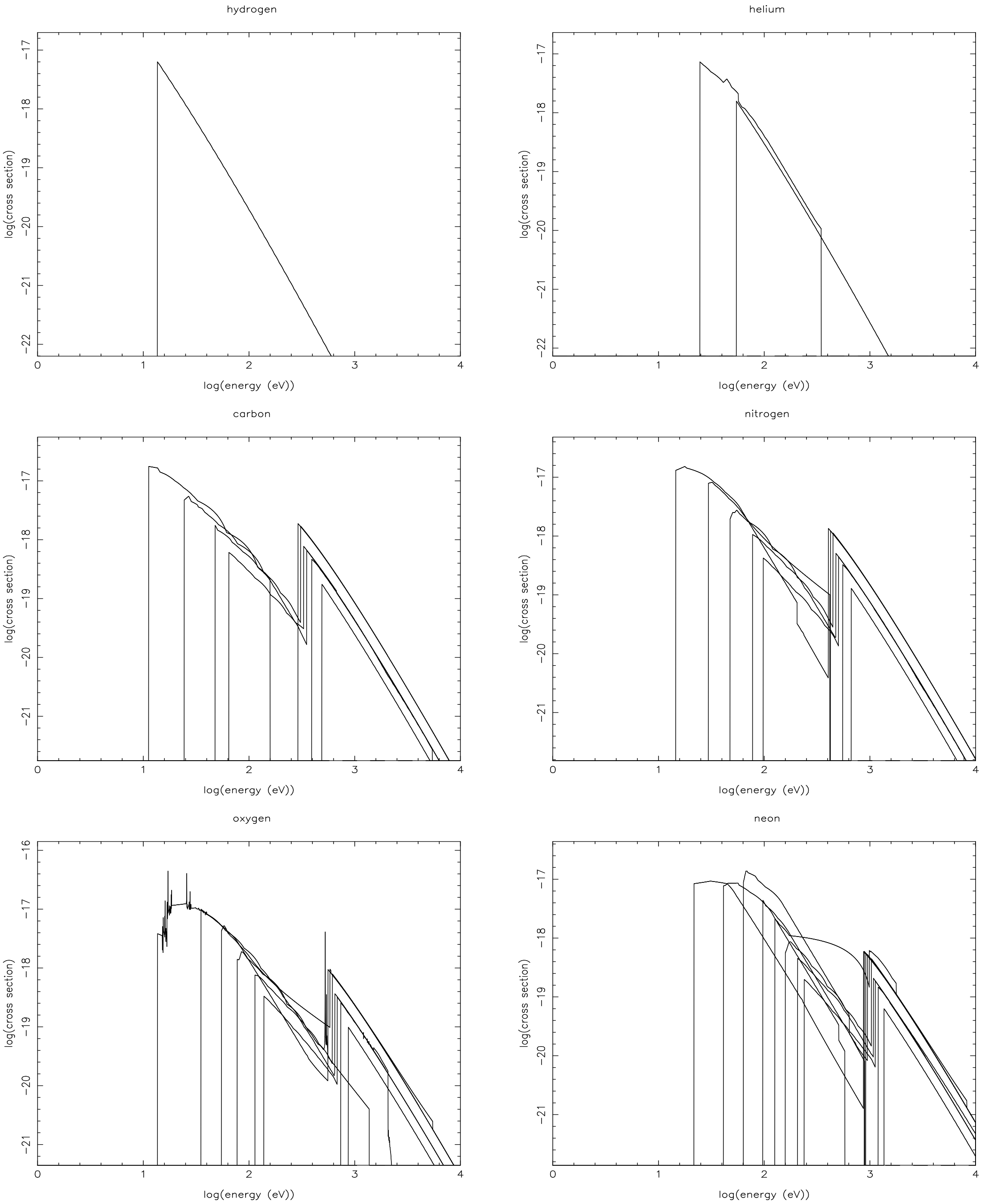

Fig. 4.— Ground state photoionization cross sections (cm^2) vs. photon energy plotted for elements H – Ne. Curves correspond to ions with increasing ionization potential.

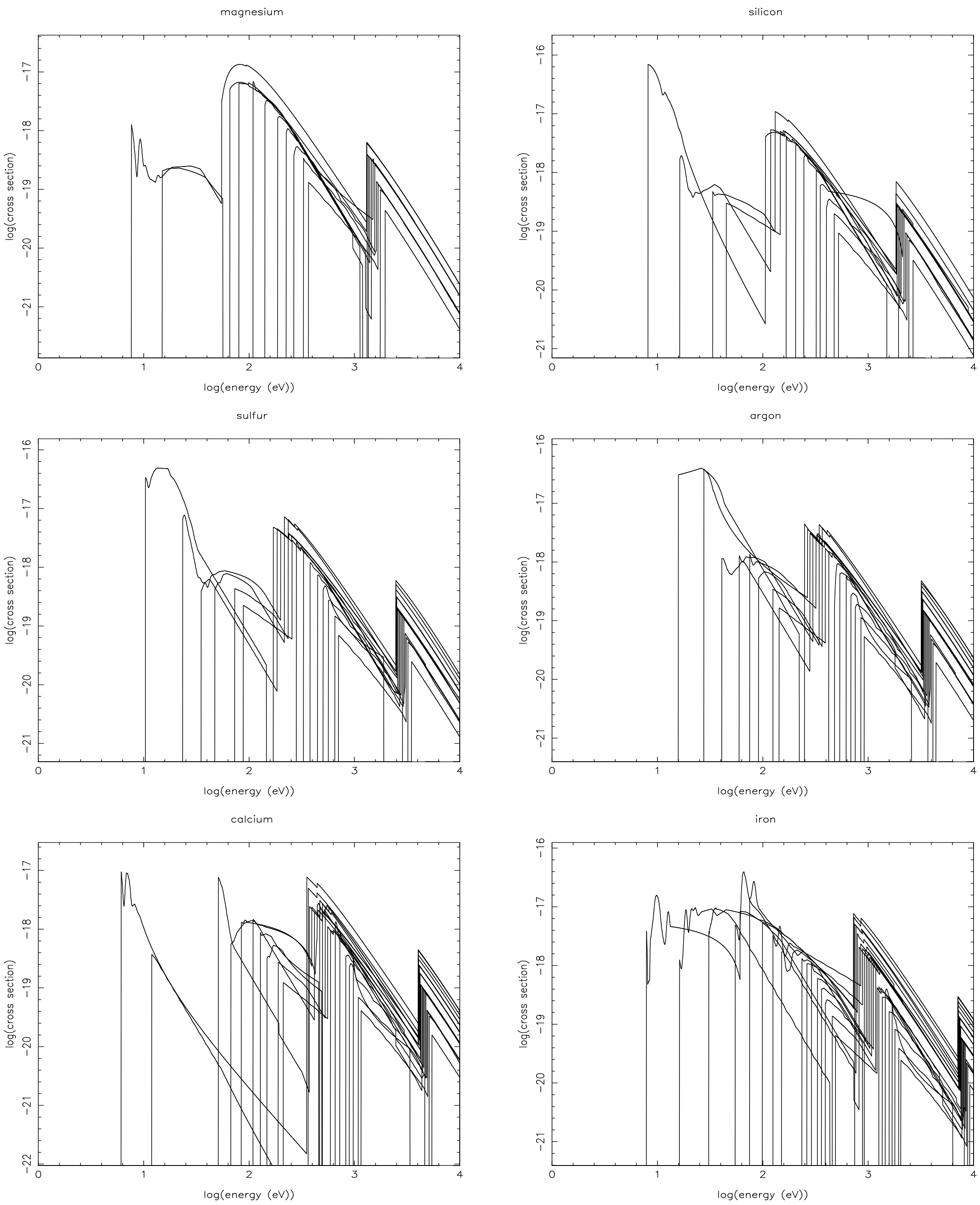

Fig. 5.— Ground state photoionization cross sections (cm^2) vs. photon energy plotted for elements Si – Fe. Curves correspond to ions with increasing ionization potential.

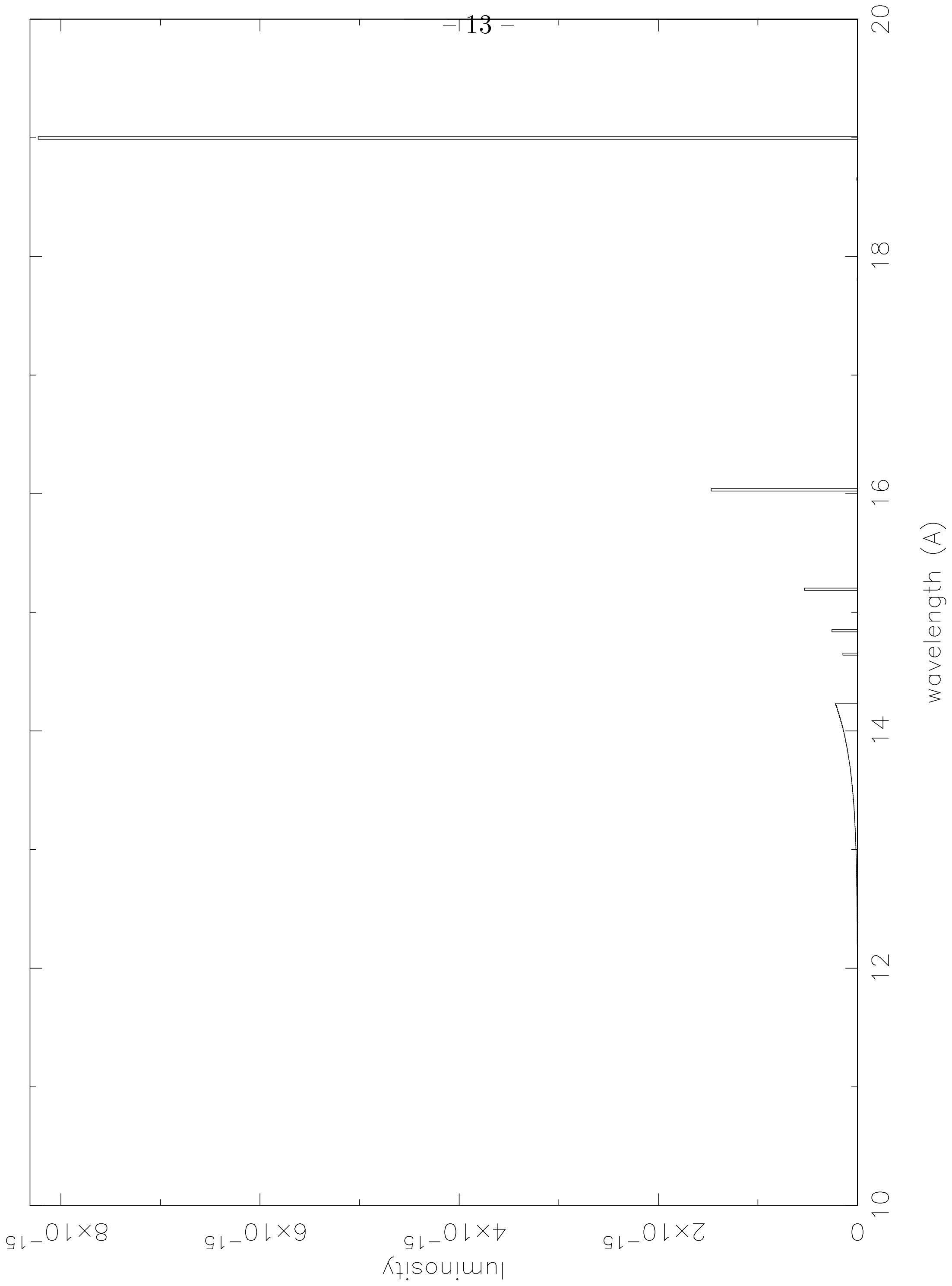

Fig. 6.— Emission spectrum due to oxygen in the 0.5-1 keV energy range at density of 10^4 cm^{-3}. The ionization parameter is $\log(\xi)$=2 and the temperature is 10^5K.

w= $1s^2(^1S)$ – $1s2p(^1P)$ ("Allowed" or "resonance")

x,y= $1s^2(^1S)$ – $1s2p(^3P_{1,2})$ ("intercombination")

z= $1s^2(^1S)$ – $1s2p(^3S)$ ("forbidden")

We can define 2 ratios:

$$R = \frac{z}{x+y}$$

and

$$G = \frac{x+y+z}{w}$$

The ratio R is sensitive to density since the z line has the lowest rate for radiative decay. At sufficiently high densities collisions can move electrons from the upper level of this line to the 2^3P level, thereby boosting the x and y lines at the expense of w. The lines are also sensitive to the mechanisms populating the upper levels. If this is done by electron collisions from the ground state, then the energy required is greatest for the upper level of the w line. Then G is primarily a function of temperature, and

$$R = \frac{R_0(T)}{1+n_e/n_c}$$

where $R_0(T)$ is a function only of T and n_e is the electron number density and $n_c = \frac{\mathrm{A}(^3\mathrm{S}-^1\mathrm{S})}{\mathrm{C}(^3\mathrm{S}-^3\mathrm{P})}$ is the critical density for the collisional transfer between the 2^3S and the 2^3P levels.

If the assumption of collisional population is correct, then using the 2 ratios it is possible to infer both T and n_e from measurements of the 3 lines w, $x+y$, and z.

Complications occur because: Recombination increases G and R at low n_e, K shell Ionization of Li-like ions can also lead to emission of these lines, and Resonance line scattering can affect the strength of the w line.

11. Observable Effects IIc: Iron K Lines

Iron K lines are unique in that they can be emitted efficiently from gas ranging from neutral to highly ionized. The intrinsic line energy is a measure of ionization state. Absence of confusing lines from other species facilitates this measurement. Iron is more likely to survive against photoionization than other abundant elements in environments with high fluxes of ionizing radiation, but the apparent detection of near-neutral iron within $\sim$a few gravitational radii of a black hole in AGN is somewhat surprising. For ions with $\leq$10 electrons, measurements of the line energy and structure are likely to yield sensitive constraints on the gas ionization state, and possibly also gas motions, relativistic effects, and Compton scattering.

12. Practical Issues

Free parameters which may be important in specifying a model include: ξ, f_ε, column density, 'geometry' (i.e. covering fraction, departures from spherical symmetry). Signatures of photoionization include recobmination continua, He-like line ratios (i.e. R, G ¿ 1), low temperature (as inferred from recombination continua, for example), and other line ratios such as a flat Lyman decrement.

Available photoionization modelling codes include:

- xstar

  `http://heasarc.gsfc.nasa.gov/docs/software/xstar/xstar.html`

  cf. Kallman and Bautista (2001)

- cloudy

  `http://www.pa.uky.edu/~gary/cloudy/`

- ion (Netzer)
- apec

  `http://hea-www.harvard.edu/APEC/`

- HULLAC (LLNL/Columbia)

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