

Typical spectra of AGN (and planetary nebulae) are dominated by Hydrogen lines, plus emission from O III at $5007 \AA$ ("nebulium").
Physics: gas is in photoionization equilibrium with radiation of the vicinity of the central black hole.

Ionization Equilibrium


(Francis et al., 1991, Tab. 1

Strength of emission lines
characterized by their equivalent width, defined by
$\mathrm{EW}=\int_{0}^{\infty} \frac{f_{\text {obs }}(\lambda)-f_{\text {cont }}(\lambda)}{f_{\text {cont }}(\lambda)} d \lambda$
units of EW: Å.
Similar definitions also also exist for $E$ - or $\nu$-space!

Ionization structure of gas in AGN determined from the rate equations:
Atoms can be ionized and can recombine
$\Longrightarrow$ number density of ions can change with time.
Define
$n_{Z}(z)$ : number density of species $Z$ in ionization stage $z$ (units: $\mathrm{cm}^{-3}$ ). $\lambda(z, z+1)$ : transition rate from stage $z$ to $z+1$ (units: $\mathbf{s}^{-1}$ ).
then

$$
\frac{\mathrm{d} n_{Z}(z)}{\mathrm{d} t}=n_{Z}(z-1) \lambda(z-1, z)
$$

$$
-n_{Z}(z)(\lambda(z, z+1)+\lambda(z, z-1))
$$

$$
+n_{Z}(z+1) \lambda(z+1, z)
$$

In equilibrium: $\mathrm{d} n_{Z} / \mathrm{d} t=0$ and thus

$$
\frac{n_{Z}(z+1)}{n_{Z}(z)}=\frac{\lambda(z, z+1)}{\lambda(z+1, z)}
$$

In Eq. (7.2) only adjacent ionization stages are connected, calculation gets (much) more complicated if also $z, z+2$, etc. are connected.

## Rate Equations, II

The rate equations are determined from all physical processes with result in ionization or recombination.

- Most important processes for ionization:
- Photoionization
- Collisional Ionization
- Most important processes for recombination:
- Radiative Recombination
- Dielectronic Recombination

We will now look at the physics of these processes in greater detail.

Photoionization, I


Photoionization: Ionization of an ion by a photon.

Reaction equation:

$$
(Z, z)+\gamma \longrightarrow(Z, z+1)+\mathrm{e}^{-}
$$

Photon needs energy $h \nu>$ ionization energy $I=: h \nu_{\text {thresh }}$, remaining energy, $h \nu-I$, goes into kinetic energy of electron and is thermalized
Photoionization rate:

$$
\gamma_{\gamma}(z, z+1)=\Gamma_{Z, z}=\int_{\nu_{\text {Utresh }}}^{\infty} \frac{F_{\nu}}{h \nu} \sigma_{\mathrm{bf}}(\nu) \mathrm{d} \nu
$$

where $\sigma_{\mathrm{bf}}$ : photoionization cross-section ("bf": bound-free).

Ionization Equilibrium

## Photoionization, II

$\sigma_{\text {bf }}$ is determined by quantum mechanics.
For Hydrogen, for absorption from the $n$th level (Menzel \& Pekeris, 1935):

$$
\begin{equation*}
\sigma_{\mathrm{bf}}=\left(\frac{64 \pi^{4} m_{\mathrm{e}} e^{10}}{3 \sqrt{3} c h^{6}}\right) \frac{1}{n^{5} \nu^{3}} g_{\mathrm{bf}}(n, \nu) \propto \frac{1}{\nu^{3}} \tag{7.5}
\end{equation*}
$$

where the Gaunt-factor, $g_{\mathrm{bf}}$, is tabulated, e.g., by Karzas \& Latter (1961) and is $\propto \nu^{-1 / 2}$ away from threshold.
For the ground state of hydrogen:

$$
\begin{equation*}
g_{\mathrm{bf} ; 1, \nu}=8 \pi \sqrt{3} \frac{\nu_{1}}{\nu} \frac{e^{-4 z \cot ^{-1} z}}{1-e^{-2 \pi z}} \tag{7.6}
\end{equation*}
$$

where $z^{2}=\nu_{1} /\left(\nu-\nu_{1}\right)$ and where $h \nu_{1}$ is the binding energy of Hydrogen.
Useful fitting formulae for all elements and ions with $Z \leq 30$ have been published by Verner \& Yakovlev 1995 and Verner et al. 1996, detailed calculations have been performed by the opacity project (TOP, Seaton et al.).

Photoionization, III



Photoionization cross sections for several subshells of Fe (cross sections from sections from 1996). 1996). 1 barn $=$
$10^{-24} \mathrm{~cm}^{2}$.

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$\sigma_{\text {bf }}$ per H -atom for material of solar composition from the optical to the X -ray regime.

$\sigma_{\mathrm{bf}} E^{3}$ in the EUV and X-rays (dashed: influence of dust), Wilms, Allen \& McCray (2000).

Note strong $E^{-3}$ dependency above the absorption edges!
In the X-rays, most of the absorption is not from hydrogen, although absorbing columns are still given in terms of an equivalent hydrogen column, $N_{\mathrm{H}}$.


Reaction equation:
$(Z, z)+\mathrm{e}^{-} \longrightarrow(Z, z+1)+\mathrm{e}^{-}+\mathrm{e}^{-}$

Collisional Ionization rate depends on the electron velocity distribution:

$$
\begin{equation*}
\gamma_{\mathrm{coll} .}(z, z+1)=n_{\mathrm{e}} C_{Z}\left(z, T_{\mathrm{e}}\right)=n_{\mathrm{e}} \int_{v_{\text {thresh }}}^{\infty} \sigma_{i}(v) v f(v) \mathrm{d}^{3} v=: n_{\mathrm{e}}\left\langle v \sigma_{i}\right\rangle \tag{7.7}
\end{equation*}
$$

where $\sigma_{\mathrm{i}}$ is the collisional ionization cross-section, and $C_{Z}$ is the collisional ionization rate coefficient (units $\mathrm{cm}^{3} \mathrm{~s}$ ).

In AGN one typically assumes $f(v)$ to be a Maxwell distribution.

$\sigma_{i}(v)$ for $\operatorname{Ar}$ IV (Arnaud \& Rothenflug, 1985, Fig. 8)
$C_{Z}$ is normally presented in tabulated form, a typical fitting formula is:

$$
C_{Z}(z, T)=A_{z} T^{1 / 2} \frac{\exp (-I / k T)}{1+a_{z}\left(T / T_{Z}\right)}
$$

where $T_{Z}=I / k T$.
See, e.g., Arnaud \& Rothenflug (1985) or Shull \& Van Steenburg (1982).

Radiative Recombination, II

(Nahar, Pradhan \& Zhang, 2001, Fig. 3)

The recombination cross-section, $\sigma_{\mathrm{fb}}$, can be obtained from the photoabsorption cross-section, $\sigma_{\mathrm{bf}}$ using the Milne relation (see handout),

$$
\sigma_{\mathrm{fb}}(v)=\frac{g_{z, n}}{g_{z+1,1}} \frac{h^{2} \nu^{2}}{m_{\mathrm{e}}^{2} c^{2} v^{2}} \sigma_{\mathrm{bf}}(\nu)
$$

The cross-section for recombination, $\sigma_{\mathrm{t}}$, can be easily derived using the princiiple of detailed balance. The derivation given here follows Osterbrock (1989).
The microphysial processes that are balanced are photoionization by photons in the energy range from $h \nu$ to $h(\nu+\mathrm{d} \nu)$ on the one hand, and (spontaneous or induced)
recombinations trom electrons in the velocity range from to to $v+$ dv on the other hand. Thus, $v$ and $\nu$ are related by recombinations from electrons in the velocity range from $v$ to $v+$ d $v$ on the other hand. Thus, $v$ and $\nu$ are related by

$$
\frac{1}{2} m_{0} \nu^{2}+h \nu \nu_{\text {miresh }}=h \nu
$$

In thermodynamical equilibrium, the rate of induced recombinations is $\exp \left(-h \nu / k T_{e}\right)$ times the rate of induced ionizations this is the "detailed balance", such that

$$
n_{\mathrm{e}} n_{Z, z+1}+v \sigma_{\mathrm{b}}(v) f(v) \mathrm{d} v=\left(1-\exp \left(-h \nu / k T_{\mathrm{e}}\right)\right) n_{Z, z} \frac{4 \pi B_{h}\left(T_{\mathrm{e}}\right)}{h \nu} \sigma_{\mathrm{b}}(\nu) \mathrm{d} \nu
$$

Because we are in thermodynamical equilibrium, the radiation field is a Planckian, $B_{\nu}$, and the elecctron distribution, $f(v)$, is given by the Maxwell-Boltzmann distribution,

$$
f(v)=\frac{4}{\sqrt{\pi}}\left(\frac{m_{e}}{2 k T_{\mathrm{e}}}\right)^{3 / 2} v^{2} e^{-m_{0} v^{2} / 2 k T_{\mathrm{e}}}
$$

As is shown in many introductory books to astrophysics, in thermodynamical equilibrium the ionization structure is given by the Saha equation

$$
\frac{n_{Z, z+1} n_{\mathrm{e}}}{n_{Z, z}}=\frac{2 g_{z+1}}{z_{i}}\left(\frac{2 \pi m_{e} k T_{\mathrm{e}}}{h^{2}}\right)^{2} e^{-h_{u_{\text {memem }} / k T_{\mathrm{e}}}}
$$

Where the $g_{i}$ are the statistical weights of the two ionization stages.
Inserting everything gives the Mine relation

$$
\sigma_{w_{0}}(\nu)=\frac{g_{z, n}}{g_{z+1,1,1}} \frac{h_{e}^{2} \nu^{2} c^{2} v^{2} v_{b 1}(\nu)}{}
$$

(7.10)
tor the recombination cross section $\sigma_{\text {sin }}$ into the $n$th level of the ion $(Z, z)$. Here, we've explicitly written down the statistical weight of this level as $g_{z, n}$ and assumed that
the recombining ion, $(Z, z+1)$ is in its ground state $(n=1)$.
An alternative derivation using quantum mechanics uses symmetry arguments for the relevant matrix elements $\langle z| H|z+1\rangle$.

## Assume: cloud irradiated by photons

Simplification: only source for ionization: photoionization
Equilibrium: number ionizations $=$ number of recombinations $\Longrightarrow$

$$
\begin{equation*}
\int_{\nu_{\text {ion }}}^{\infty} n\left(Z^{z}\right) \sigma_{\mathrm{bf}}(\nu) \frac{F_{\nu}}{h \nu} \mathrm{~d} \nu=\alpha(T) n_{\mathrm{e}} n\left(Z^{z+1}\right) \tag{7.16}
\end{equation*}
$$

where
$\sigma_{\mathrm{bf}}(\nu)$ : photoionization cross section $\left(\mathrm{cm}^{2} ; \propto E^{-3}\right)$
$\alpha\left(T_{\mathrm{e}}\right)$ : total recombination coefficent $\left(\mathrm{cm}^{3} \mathrm{~s}^{-1}\right)$
$n_{i}$ : particle density $\left(\mathrm{cm}^{-3}\right)$
$F_{\nu}$ : local photon flux ( $\mathrm{erg} \mathrm{cm}^{-2} \mathrm{~s}^{-1} \mathrm{keV}^{-1}$ )
where $F_{\nu}$ is related to the source luminosity via

$$
\begin{equation*}
F_{\nu}=\frac{L_{\nu}}{4 \pi D^{2}} \tag{7.17}
\end{equation*}
$$

Photoionization Equilibrium

## Photoionization

Since $\sigma_{\mathrm{bf}}(\nu)$ is a strongly peaked function, we can write Eq. (7.16) as

$$
\begin{equation*}
n\left(Z^{z}\right) \sigma_{\mathrm{bf}}\left(\nu_{\mathrm{ion}}\right) \frac{F_{\nu_{\mathrm{ion}}}}{h \nu_{\mathrm{ion}}} \sim \alpha(T) n_{\mathrm{e}} n\left(Z^{z+1}\right) \tag{7.18}
\end{equation*}
$$

and therefore

$$
\begin{equation*}
\frac{n\left(Z^{z+1}\right)}{n\left(Z^{z}\right)} \sim \frac{\sigma_{\mathrm{bf}}\left(\nu_{\mathrm{ion}}\right)}{\alpha(T)} \frac{L}{4 \pi D^{2} n_{\mathrm{e}}} \frac{1}{h \nu_{\mathrm{ion}}} \tag{7.19}
\end{equation*}
$$

i.e., ionization equilibrium mainly depends on

$$
\begin{equation*}
U=\frac{L / 4 \pi D^{2} h \nu_{\mathrm{ion}}}{n_{\mathrm{e}}} \frac{1}{c}=\frac{\text { \# ionizing photons } / \mathrm{cm}^{3}}{\# \text { electrons } / \mathrm{cm}^{3}} \tag{7.20}
\end{equation*}
$$

where $U$ is called the ionization parameter
many other definitions available!
Example: For the BLR: $D \sim 10$ light days, $L / h \nu \sim 10^{51}$ photons, and $n=$ $10^{11} \mathrm{~cm}^{-3}$ gives $U \sim 0.1$.

Photoionization
many radiative processes need to be considered:
In reality, as shown before many radiative processes need to be considered:

## Ionization:

- Photoionization
- collisional Ionization
- Auger-lonization


## Recombination:

- radiative recombination
- dielectric recombination


## Continuum Processes:

- Bremsstrahlung
- Compton-Scattering

Real life: Solution using advanced radiation codes such as Cloudy or XSTAR (it is not worthwhile to develop your own code...).


Photoionization

"Strömgren sphere" like structure of a cloud irradiated with a typical AGN spectrum (Mathews \& Ferland, 1987) with $U=0.1$, and $n_{\mathrm{H}}=10^{10} \mathrm{~cm}^{-3}$ (typical for BLR) Distance is "into" cloud.
(Hamann et al., 2002, Fig. 1)

Photoionization Equilibrium


Dependence of line ratios and cloud equilibrium temperature onto the slope of the irradiating power law.

Photoionization Equilibrium

## Line Diagnostics,

Before performing detailed spectral analysis of AGN spectra we need to understand how the physical properties of the emitting gas are determined.

- Density
- Temperature
- Mass

To get a first estimate for these parameters, full blown photoionization computations are not necessary
$\Longrightarrow$ Line diagnostics.

Line Diagnostics, II


Line diagnostics makes use of (de)excitation mechanisms for line emission:

- Collisional Excitation, $C_{12}$
- Radiative Deexcitation, $A_{21}$
- Collisional Deexcitation, $C_{21}$

Coefficients for stimulated emission, $B_{21}$, and for radiative excitation (=absorption), $B_{21}$, can generally be ig nored

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Collisional (De)Excitation,

## Computation of $C_{i j}$ :

For excitation, overall upwards rate is given by

$$
\begin{equation*}
R_{12}=n_{\mathrm{e}} n_{1} C_{12}=n_{\mathrm{e}} n_{1} \int_{E_{12}}^{\infty} \sigma_{12}(E) E f(E) \mathrm{d} E \tag{7.21}
\end{equation*}
$$

where

- $\sigma_{12}$ : collisional cross section
- $f(E)$ : electron velocity distribution
$\sigma_{12}$ varies roughly $\propto E^{-1}$. It can be parameterized as

$$
\begin{equation*}
\sigma_{12}(E)=\left(\frac{h^{2}}{8 \pi m_{\mathrm{e}} E}\right)\left(\frac{\Omega_{12}}{g_{1}}\right) \tag{7.22}
\end{equation*}
$$

where $\Omega_{12}$ is called the collision strength and obtained from quantum mechanics (Seaton, 1958)

$$
\begin{equation*}
\Omega_{i j}=\left(\frac{8 \pi}{\sqrt{3}}\right) \frac{g f_{i j}}{E_{i j}} \cdot G(T) \tag{7.23}
\end{equation*}
$$

where $G(T)$ is a Gaunt factor.
from the previous slide and assuming a Maxwell-
Using the information from the previous
Boltzmann distribution for $f$, the upwards rate is

$$
\begin{equation*}
R_{12}=n_{\mathrm{e}} n_{1}\left(\frac{2 \pi \hbar^{4}}{k_{\mathrm{B}} m_{\mathrm{e}}^{3}}\right)^{1 / 2} T^{-1 / 2}\left(\frac{\Omega_{12}}{g_{1}}\right) \exp \left(-\frac{E_{12}}{k T}\right) \tag{7.24}
\end{equation*}
$$

Analoguously, the rate for collisional de-excitation is

$$
\begin{align*}
R_{21} & =n_{\mathrm{e}} n_{1} \int_{0}^{\infty} \sigma_{12}(E) E f(E) \mathrm{d} E  \tag{7.25}\\
& =n_{\mathrm{e}} n_{2}\left(\frac{2 \pi \hbar^{4}}{k_{\mathrm{B}} m_{\mathrm{e}}^{3}}\right)^{1 / 2} T^{-1 / 2}\left(\frac{\Omega_{21}}{g_{2}}\right) \tag{7.26}
\end{align*}
$$

as for de-excitation the energy threshold is zero.

## Line Diagnostics: Density, II

Rate equations in equilibrium:

$$
\begin{align*}
& n_{1} n_{\mathrm{e}} C_{12}=n_{2} A_{21}+n_{2} n_{\mathrm{e}} C_{21}  \tag{7.31}\\
& n_{1} n_{\mathrm{e}} C_{13}=n_{3} A_{31}+n_{3} n_{\mathrm{e}} C_{31} \tag{7.32}
\end{align*}
$$

such that

$$
\begin{align*}
& \frac{n_{2}}{n_{1}}=\frac{n_{\mathrm{e}} C_{12}}{A_{21}+n_{\mathrm{e}} C_{21}}=\frac{n_{\mathrm{e}}}{A_{21}+n_{\mathrm{e}} C_{21}} \frac{g_{2}}{g_{1}} C_{21} \exp \left(-E_{12} / k T\right)  \tag{7.33}\\
& \frac{n_{3}}{n_{1}}=\frac{n_{\mathrm{e}} C_{13}}{A_{31}+n_{\mathrm{e}} C_{31}}=\frac{n_{\mathrm{e}}}{A_{31}+n_{\mathrm{e}} C_{31}} \frac{g_{3}}{g_{1}} C_{31} \exp \left(-E_{13} / k T\right) \tag{7.34}
\end{align*}
$$

Assuming the cloud is optically thin (i.e., absorption is negligable), the intensity of an emitted line is

$$
\begin{equation*}
4 \pi I_{21}=A_{21} n_{2} h \nu_{21} \tag{7.35}
\end{equation*}
$$

Line Diagnostics: Density, III
$h \nu_{21}$, the line ratio is

$$
\begin{equation*}
\frac{I_{21}}{I_{31}}=\frac{A_{21} n_{2} h \nu_{21} / 4 \pi}{A_{31} n_{3} h \nu_{31} / 4 \pi} \tag{7.36}
\end{equation*}
$$

since $\nu_{21} \sim \nu_{31} \ldots$

$$
\begin{equation*}
=\frac{A_{21} n_{2}}{A_{31} n_{3}} \tag{7.37}
\end{equation*}
$$

insert $n_{2} / n_{3}$ from Eqs. (7.33) and (7.34)

$$
\begin{align*}
& =\frac{C_{21}}{C_{31}} \frac{g_{2}}{g_{3}} \frac{A_{21}}{A_{31}} \frac{A_{31}+n_{\mathrm{e}} C_{31}}{A_{21}+n_{\mathrm{e}} C_{21}} \exp \left(-E_{32} / k T\right)  \tag{7.38}\\
& =\frac{g_{2} C_{21}}{g_{3} C_{31}} \frac{1+n_{\mathrm{e}} / n_{\mathrm{Cr}, 3}}{1+n_{\mathrm{e}} / n_{\mathrm{Cr}, 2}} \exp \left(-E_{32} / k T\right) \tag{7.39}
\end{align*}
$$

where the critical densities are defined by

$$
\begin{equation*}
n_{\mathrm{Cr}, i}=A_{i 1} / C_{i 1} \tag{7.40}
\end{equation*}
$$

Line Diagnostics: Temperature


Line Diagnostics

