Astro 501: Radiative Processes
Lecture 30
April 5, 2013

Announcements:
- **Problem Set 9** due 5pm next Monday
- ICES to be available online – please!

Last time: thermodynamics of atomic states
Q: ratio of $2p$ *to* $1s$ *states in hydrogen at* T*?*
Q: what is hydrogen ionization fraction x_e*?*
Q: in thermodynamic equilibrium, what parameters determine x_e*?*

ratio of $2p$ to $1s$ in hydrogen:

$$\frac{n(2p)}{n(1s)} = \frac{g(2p)}{g(1s)} e^{-[E(2p)-E(1s)]/kT} = 3e^{-3B/4kT} \tag{1}$$

define *ionization fraction*

$$x_e = \frac{n_e}{n_{\rm tot}} 4 \tag{2}$$

with total electron number density $n_{\rm tot} = n_e + n_{\rm H}$
using $n_e = n_p$ (charge neutrality): **Saha equation**

$$\frac{x_e^2}{1 - x_e} \approx \frac{2(2\pi m_e kT/h^2)^{3/2}}{n_{\rm tot}} e^{-B_{\rm H}/kT} = \frac{n_{{\rm Q},e}}{n_{\rm tot}} e^{-B_{\rm H}/kT} \tag{3}$$

ionization depends on T but also particle density $n_{\rm tot}$

Radiative Transitions

Radiative Transitions

so far: thermal populations of bound states
now: *transitions* between states
leading to emission/absorption

we want a qualitative and quantitative understanding

qualitatively:
- what is the basic physics?
- selection rules: which transition are allowed?

quantitatively:
Q: what do we want to know?

quantitatively:

we want to describe the *strength* of transitions

in particular, the usual radiation transfer quantities

- emission coefficient j_ν
- absorption coefficient α_ν

these are closely related to Einstein coefficients

- A_{if} *spontaneous emission* rate per atom for $i \to f$
- B_{if} *stimulated emission* coefficient
- B_{fi} *true absorption* coefficient

recall: we found that, for $h\nu_{if} = E_i - E_f$

$$j_\nu = \frac{h\nu_{if}\ A_{if}}{4\pi}\ n_i\ \phi(\nu) \tag{4}$$

$$\alpha_\nu = \frac{h\nu_{if}}{4\pi}\ \left(B_{fi}n_f - B_{if}n_i\right)\ \phi(\nu) \tag{5}$$

(6)

with $\phi(\nu)$ the *line profile* function

The Semiclassical Approach

Deriving the general Einstein A and B coefficient
for transitions between two atomic states
from first principles
is a big job

we will take a "first-ish" principles approach
sketch what goes into the final result

we will work in the *semiclassical limit*

- treat the atomic states quantum mechanically
- but treat the radiation classically
  $\rightarrow$ i.e., in the limit of large photon occupation f

good for getting Einstein B, bad for A *Q: why?*
Q: but what's the workaround if we know B?

classical radiation $\leftrightarrow$ large photon occupation f

absorption and stimulated emission: rate proportional to $\bar{J}_\nu = \int I_\nu \, d\Omega$

and recall $I_\nu = 2\nu^2/c^2 \; f$

$\rightarrow$ so rate $\propto \int f \; d\Omega$ works even down to small f

spontaneous emission: involves single photons

correct analysis demands quantum treatment of radiation field

but luckily Einstein says: $A_{if} = (2h\nu_{if}^3/c^2) B_{fi}$

so if we find B, then use this to get A

thus: we will calculate *absorption*

So we will:

- treat atoms quantum mechanically, and
- treat radiation as a perturbation, in the form of an *external classical* EM field

Q: how do we describe formally the unperturbed system?

Q: how do we introduce the perturbation?

The Electromagnetic Hamiltonian

recall quantum mechanics: stationary atomic states $|n\rangle$
are governed by the time-independent Schrödinger equation

$$H_0 \; |n\rangle = E_n \; |n\rangle \tag{7}$$

in terms of wavefunctions $\psi_n(x) = \langle x|n\rangle$,

$$H_0 \; \psi_n = E_n \; \psi_n \tag{8}$$

with H_0 the Hamiltonian operator for the atom
and includes the e-nucleus EM interactions
and E_n is the energy of state n

add an external classical field with 4-potential $(\phi, \vec{A})$
the relativistic Hamiltonian for an electron is

$$H = \sqrt{\left(c\vec{p} + e\vec{A}\right)^2 + (m_e c^2)^2} - e\phi \tag{9}$$

for experts: gives right equation of motion in Hamilton's eqs
Q: limit of no field? non-relativistic limit?

The Relativistic Hamiltonian

full relativistic Hamiltonian for an electron

$$H = \sqrt{\left(c\vec{p} + e\vec{A}\right)^2 + (m_e c^2)^2} - e\phi \tag{10}$$

non-relativistic limit: $cp \ll m_e c^2$

$$\begin{aligned} H &= \frac{1}{2m_e}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 - e\phi & (11)\\ &= \frac{p^2}{2m_e} + \frac{e}{m_e c}\vec{A}\cdot\vec{p} + \frac{e^2A^2}{2m_e c^2} - e\phi & (12)\end{aligned}$$

plus a constant term $m_e c^2$ which we ignore *Q: why?*

note: we have used the "Coulomb gauge" for the perturbation
$\nabla \cdot \vec{A} = 0 = \phi$

we can write the non-relativistic Hamiltonian as

$$H = H_0 + H_1 + H_2 \tag{13}$$

where the *unperturbed atomic Hamiltonian* is H_0,
the perturbation *first order in A* is

$$H_1 = \frac{e}{m_e c} \vec{A} \cdot \vec{p} \tag{14}$$

and the perturbation *second order in A* is

$$H_2 = \frac{e^2 A^2}{2 m_e c^2} \tag{15}$$

there is a beautiful physical interpretation of the terms:

- H_1 describes one-photon emission processes
- H_2 describes two-photon emission processes

Q: relative importance of the two terms?

order-of-magnitude estimate of the ratio of terms, in H atom:

$$\eta = \frac{H_1}{H_2} \sim \frac{epA/m_e c}{e^2 A^2/m_e c^2} \sim \frac{ev/c}{\alpha^2 a_0 A} \tag{16}$$

external electric field $E \sim 1/c \; partial_t A \sim \nu/c \; A$
and in H: $v/c \sim \alpha$, and $h\nu \sim e^2/a_0$ so $h\nu/c \sim \alpha/a_0$

$$\eta^2 \sim \frac{h\nu}{a_0^3 E^2} \tag{17}$$

but $E^2/h\nu \sim n_{\rm ph}$, the photon density in the external field

$$\eta^2 \sim \frac{1}{n_{\rm ph} a_0^3} \sim \left(\frac{10^{25} \text{ photons/cm}^3}{n_{\rm ph}} \right) \tag{18}$$

at the Sun's surface $n_{\rm ph} \sim 10^{12}/\text{cm}^3$

lesson: $\eta \gg 1$ for (almost) all astro applications
$\rightarrow$ *ignore the two-photon term H_2*

The Transition Probability

we want the *probability* for transition $i \to f$
where the unperturbed wavefunctions satisfy $H_0\ \psi_k = E_k\ \psi_k$ this probability is *time-dependent*

the perturbing field generates nonzero amplitude for states $n \neq i$
so write time-dependent wavefunction as

$$\psi(t) = \sum_k a_k(t)\ \psi_k\ e^{-iE_k t/\hbar} \tag{19}$$

Q: $a_k(t)$ for system without perturbation? behavior with perturbation?

for at time-dependent potential, standard quantum mechanics gives
the probability P_{fi} to go from state $i \to f$

$$P_{fi} = w_{fi} \; t \tag{20}$$

with t the time the perturbation acts
and the *transition probability per unit time*

$$w_{fi} = \frac{4\pi^2 \; |H(\omega_{fi})|^2}{\hbar^2 \; t} \tag{21}$$

where $H_{fi}(\omega) = (2\pi)^{-1} \int_0^t H_{fi}(t) \;\; e^{i\omega t'}$
with the *matrix element* $H_{fi} = \int \psi_f^* \; H_1 \; \psi_i \; d^3x$
and where $\hbar\omega_{fi} = E_f - E_i$

if we have multiple atomic electrons, them perturbation is sum

$$H_1 = \frac{e}{m_e c} \sum_j \vec{A} \cdot \vec{p}_j = \frac{ie\hbar}{m_e c} \vec{A} \cdot \sum_j \nabla_j \tag{22}$$

let the perturbing field have:

- $\vec{A}(\vec{r},t) = \vec{A}(t)\ e^{i\vec{k}\cdot\vec{r}}$, with
- $\vec{A}(t') = 0$ outside of $(0,t)$

then the Fourier transform of the matrix element is

$$H_{fi} = \vec{A}_{fi}(\omega_{fi}) \cdot \ \frac{ie\hbar}{c}\ \langle f|\ e^{i\vec{k}\cdot\vec{r}} \sum_j \nabla_j |i\rangle \tag{23}$$

where $\langle f|\ e^{i\vec{k}\cdot\vec{r}} \sum_j \nabla_j |i\rangle = \sum_j \int \psi_f^*\ \nabla_j\ \psi_i\ d^3x$ is *time-independent*

write $\vec{A} = A\ \mathbf{e}$ with unit polarization vector $\mathbf{e}$:

$$w_{fi} = \frac{4\pi^2 e^2}{m_e c^2\ t} \left|A(\omega_{fi})\right|^2\ \left|\langle f|e^{i\vec{k}\cdot\vec{r}}\mathbf{e}\cdot\sum_j \nabla_j |i\rangle\right|^2 \tag{24}$$

note that $w_{fi} \propto |A(\omega_{fi})|^2$; related to intensity recall: *integrated* intensity is

$$I = \left\langle \vec{S} \cdot \vec{n} \right\rangle = \frac{c}{4\pi\ t} \int E^2(t)\ dt = \frac{c}{t} \int |E(\omega)|^2\ dt \tag{25}$$

to *monochromatic intensity*

$$J_\omega = \frac{c\ |E(\omega)|^2}{t} \tag{26}$$

and since $\vec{E} = -1/c\ \partial_t \vec{A} = -i\omega/c\vec{A}$

$$J_\omega = \frac{\omega^2}{c\ t} |A(\omega)|^2 \tag{27}$$

and thus we see that $w_{fi} \propto |A(\omega)|^2$
implies $w_{fi} \propto J_\omega$, as expected for absorption!

also: what about w_{if}, for $f \to i$?

finally, for the transition probability per unit time for $i \to f$ we have

$$w_{fi} = \frac{4\pi^2 e^2}{m_e c^2} \frac{J(\omega_{fi})}{\omega_{fi}^2} \left| \langle f | e^{i\vec{k}\cdot\vec{r}} \mathbf{e} \cdot \sum_j \nabla_j | i \rangle \right|^2 \tag{28}$$

about the probability for $f \to i$?
the same except now $\langle i | e^{i\vec{k}\cdot\vec{r}} \mathbf{e} \cdot \sum_j \nabla_j | i \rangle$
but integrating by parts, can show

$$w_{if} = w_{fi} \tag{29}$$

principle of detailed balance