Astro 501: Radiative Processes
Lecture 21
October 17, 2018

Announcements:

- **Problem Set 6** due next time
- Problem 1 is simplified view of intracluster medium
  real data more complex, as noted in paper
  can view HW problem as test of simple model
- Perseus fig 5 plots flux as $\epsilon F_\epsilon = \nu F_\nu$
- Part 1 (e): for optical depth, pick 1-2 observed energies
  where you expect the *highest* effect
- Problem 2(b): only 40 lowest energy states
  2(c): can plot instead of sketch!
- Midterm: grading elves still hard at work

Last Time: Building Atoms

big picture: need to understand atomic states
to understand transitions between then:
$\rightarrow$ there are lines we may observe

thus far: ignoring spin, levels depend on n, ℓ

Q: what do these measure?

Q: rules for filling states?

Energy Level Rankings

electron configuration = set of single-electron states
for atom ground state is the set that places electrons
in the lowest possible energies consistent with Pauli
each subshell filled before beginning next shell

empirical rules of thumb: good for atoms of low Z
  most of interest to astrophysics

"*Aufbau principle*" $- (n, \ell)$ ordering
▷ states filled in order of increasing $n + \ell$
▷ when two states have same $n + \ell$
   filled in order of increasing n, i.e., lowest n first

Q: Li states ($Z = 3$)? C ($Z = 6$?) Si ($Z = 14$)?

$\triangleright$ states filled in order of increasing $n + \ell$

$\triangleright$ when two states have same $n + \ell$
filled in order of increasing n

lithium: $Z = 3$
filled $1s^2 = 2$ states, $2s^1$ half-filled: $\boxed{1s^2 2s}$

carbon: $Z = 6$
filled: $1s^2 2s^2 = 4$ states, $2p^2$ partial $= 2$ states
$\boxed{1s^2 2s}$

silicon: $Z = 14$
filled: $1s^2 2s^2 2p^6 3s^2 = 12$ states, $3p^2$ partial $= 2$ states
$\boxed{1s^2 2s^2 2p^6 3s^2 3p^2}$

www: online data

Aufbau principle gives ordering of (n, ℓ) subshells

further splitting at fixed (n, ℓ) depending on electron spins

recall: total atomic angular momentum $\vec{J} = \vec{L} + \vec{S}$ sums
- total e orbital angular momenta $\vec{L}$, eigenstates $\hbar L$
  total e spins $\vec{S}$, eigenstates $\hbar S$
- filled subshells have $L_{\mathsf{shell}} = 0 = S_{\mathsf{shell}}$
  so L and S set only by *unfilled subshells*

Hund's Rule

Hund's rule: energy level orderings in (n, ℓ) subshell
for a fixed electron configuration = fixed unfilled (n, ℓ) subshell
then the *lowest energy* state(s) are the one(s) with

▷ the *largest possible* total spin S

▷ the *largest possible* total L for this maximal S

▷ for subshells half-filled our less: pick lowest J
otherwise pick highest J

Q: for np^2, which L, S has lowest energy? what J does this have?

for np^2: 2 electrons, each with $\ell = 1$
possible states: $m = -1, 0, +1$, $s_z = \pm 1/2$

lowest energy is
▷ the *largest possible* total spin S
this is $S = 1$, gotten for $s_{z1} = s_{z1}$ and so $S_z = \pm 1$

▷ the *largest possible* total L
Pauli: cannot both be $m = \pm 1$, not same m, s_z: can't have $L = 2$
maximal L when $m_1 = 1$ and $m_2 = 0$ (or $m_1 = -1$ and $m_2 = 0$)
$\rightarrow L = 1$

▷ for subshells half-filled our less: pick lowest J
since $J \in (|L - S|, L + S)$, here min at $J = 0$

Spectroscopic Notation for (L, S, J) states or "terms"
$^{2S+1}\mathcal{L}_J$, with $\mathcal{L} = S, P, D, \ldots$ for $L = 0, 1, 2, \ldots$
here: np^2 lowest-energy state has $(L, S, J) = (1, 1, 0) = {}^3P_0$
www: online data

Hund's Rules: Physical Origin

then the *lowest energy* state(s) are the one(s) with

▷ the *largest possible* total spin S

largest $S \rightarrow$ preference for spins aligned

but then Pauli demands different m

$\rightarrow$ fill m states with one e each before "doubling up"

$\rightarrow$ "*bus seat rule*"

▷ the *largest possible* total L for this maximal S

largest $L \rightarrow$ preference for orbit planes aligned

orbit in "same direction" and not opposite

$\rightarrow e$ avoid each other, have nucleus in between

$\rightarrow$ decrease e screening of nuclear charge, and e repulsion

Atomic Fingerprints

atomic wavefunctions, states are complex function of
nuclear charge and number of electrons
$\rightarrow$ resulting energy levels *unique* to each atom
  and to each ionization state, e.g., $C^{3+} \equiv C$ IV

lesson: atomic spectra are "fingerprints"
observed lines can pin down identity and ionization state
of emitting atom

sometimes even the mere existence of an element
tells an important story
1950's: technetium (Tc) detected in some AGB stars
Q: what's an AGB star?
Q: why is it s Big Deal to find Tc in them?

Thermal Population of Atomic States

if atoms can interact, e not necessarily all in ground state

in general: a big job to calculate population of atomic states

but as usual: much simplification if *thermodynamic equilibrium*

Boltzmann: consider a single atomic state having energy E_i

for an ensemble of n_{tot} atoms in thermodynamic equilibrium at T

the population = numbers n_i of atoms in state i is

$$n_i = \frac{n_{\text{tot}}}{Z} e^{-E_i/kT} \tag{1}$$

interpret $p_i = e^{-E_i/kT}/Z$ as the probability that an atom is found in state i

Q: how do we find the normalization constant Z?

each state has population n_i, and if we sum all states must recover total population n, so

$$n_{\text{tot}} = \sum_{\text{states } i} n_i \frac{n_{\text{tot}}}{Z} \sum_{\text{states } i} e^{-E_i/kT} \qquad (2)$$

and thus we find the **partition function**

$$Z = \sum_{\text{states } i} e^{-E_i/kT} \qquad (3)$$

and thus $p_i = e^{-E_i/kT} / \sum_j e^{-E_j/kT}$ and clearly $\sum_i p_i = 1$

in many cases, more than one atomic state has energy E_i

let the number of states with E_i be g_i

  i.e., g_i counts the "degeneracy" at level E_i

then the number of states with energy E_i is

$$n(E_i) = g_i \frac{n}{Z} e^{-E_i/kT} \tag{4}$$

and the partition function can be written

$$Z = \sum_{\text{levels } E_i} g_i e^{-E_i/kT} \tag{5}$$

consider two states of energies E_1, $E_2 > E_1$

for an ensemble of atoms in thermodynamic equilibrium at T

the populations = numbers n_1, n_2 of atoms the states

is given by

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-(E_2 - E_1)/kT} \tag{6}$$

note that for a given atomic system and temperature T
the partition function $Z = \sum_{\text{states}} g_i e^{-E_i/kT}$ is *a number*

Q: physical dimensions of Z?

*Q: what does this number represent physically? hint: roughly at
what levels does the sum effectively terminate?*

Q: what is Z as $kT \to 0$?

roughly:

the partition function counts all states with $E_i \lesssim kT$

so $Z \approx$ number of states with $E_i \lesssim kT$

$\rightarrow$ i.e., "partitions" full set of atomic states
into those "accessible" at T

as $kT \rightarrow 0$: all states suppressed except ground state $E_1 = 0$
so $Z \rightarrow g_1$, the degeneracy of the ground state

consider the partition function for *atomic hydrogen*
where $E_n = -B/n^2$, with $B = |E_1| = e^4 m_e / 2\hbar^2$, the binding
energy
recalling that the shell each n has degeneracy $g_n = 2n^2$:

$$Z(\mathsf{H}) = 2 \sum_{n=1}^{\infty} n^2 e^{\beta B / n^2} \qquad (7)$$

where $\beta = 1/kT$

Q: roughly what is the value of $Z(\mathsf{H})$? why? implications?

neutral hydrogen partition function, with $\beta = 1/kT$

$$Z(\mathsf{H}) = 2 \sum_{n=1}^{\infty} n^2 e^{\beta B/n^2} \tag{8}$$

$e^{\beta B/n^2} \to 1$ for large n, so

$$Z(\mathsf{H}) \approx 2 \sum_{\text{large } n}^{\infty} n^2 \sim n_{\text{max}}^3 \to \infty \tag{9}$$

infinite partition function!

but what does this mean?!
strictly: probability to be in state i is $p_i \propto 1/Z = 0$?!
that is: high probability to be at high n

physically: if H atoms in equilibrium with a thermal bath at T
and all states n are accessible
then eventually all atoms fluctuate to high $n \to$ *ionized!*

this can't be right! atoms do exist! *Q: what's the fix?*

Partition Function Cutoff

We implicitly assumed that we could carry our sum
out to *arbitrarily large n*

While it is true that atomic H has such states
recall $r_n = n^2 a_0$: high-n states are physically large!

physically, real e orbits in an H atom cannot extend
beyond the nearest-neighbor H atom
which typically lies at distance d_{max} such that $n_{\mathsf{H}} d^3 \sim 1$
or $d_{\mathsf{max}} \sim n_{\mathsf{H}}^{-1/3}$

setting $d_{\mathsf{max}} = n_{\mathsf{max}}^2 a_0$, we estimate

$$n_{\mathsf{max}} \sim \sqrt{d_{\mathsf{max}}} a_0 \sim \left(a_0^3 n_{\mathsf{H}} \right)^{-1/6} \sim 10^4 \left(\frac{n_{\mathsf{h}}}{1 \text{ atom/cm}^3} \right)^{-1/6} \qquad (10)$$

but: a very Wild West estimate! real physics is more complex…