Astro 501: Radiative Processes
Lecture 29
April 3, 2013

Announcements:

- **Problem Set 9** due 5pm next Monday
- Special guest lecturer: *Prof. Dr. Charles F. Gammie*
  theoretical astrophysicist extraordinarie
  expert in black holes, relativistic magnetohyrodynamics
  accretion disks, and spectroscopic notation
- Physics Colloquium today:
  Dan Hooper, Fermilab and U. Chicago
  "Searching for Dark Matter in the Discovery Age"

Last time: atomic structure

Today: thermodynamics of atomic states

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 atoms in thermodynamic equilibrium at T
the population = numbers n_i of atoms in state i is

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

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

$$n = \sum_{\text{states } i} n_i \frac{n}{Z} \sum_{\text{states } i} e^{-E_i/kT} \tag{2}$$

and thus we find the **partition function**

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

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

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

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" 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 $g_n = 2n^2$:

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

where $\beta = 1/kT$

Q: roughly what is the value of Z(H)? why? implications?

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

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

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

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

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 → *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 $d_{\rm max}$ such that $n_{\rm H} d^3 \sim 1$
or $d_{\rm max} \sim n_{\rm H}^{-1/3}$

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

∞

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

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

Thermodynamics of Ionization

consider a hydrogen gas in thermodynamic equilibrium at T
ionization and recombination both occur

$$\mathrm{H} + \gamma \leftrightarrow p + e \tag{11}$$

and the number densities n_e, n_p, and n_{H} adjust themselves
until the recombination and ionization rates are equal

this equilibrium determines a relationship among the densities
which we want to find

Method I (R&L):
starting point–the ratio of free electrons at speed v
to neutral hydrogen atoms in the ground state

$$\frac{\delta n_e(v)}{n_1} = \frac{\delta g_e(v)}{g_0} e^{-[E_e(v)-E_1]/kT} = \frac{\delta g_e(v)}{g_0} e^{-(B+m_e v^2/2)/kT} \tag{12}$$

where $B = -E_1$ is hydrogen binding energy

Method II:

recall that the number of states for a particle is related to its *distribution function* f via

$$dN = \frac{g}{h^3} f \; d^3x \; d^3p \tag{13}$$

where f counts states in phase space
  i.e., *translational* degrees of freedom
and where g counts *internal* degrees of freedom
  e.g., for a free electron, $g_e = 2s_e + 1 = 2$

a particle species in thermal (in fact, kinetic) equilibrium at T has

$$f = \frac{1}{e^{(E-\mu)/kT} \pm 1} \tag{14}$$

where $\pm \leftrightarrow$ fermion/boson
and $E(p) = \sqrt{(cp)^2 + (mc^2)^2} \overset{\text{nonrel}}{=} mc^2 + p^2/2m$
and where μ is the chemical potential (more on this soon)

distribution function, ± ↔ fermion/boson

$$f = \frac{1}{e^{(E-\mu)/kT} \pm 1} \tag{15}$$

for nonrelativistic, nondegenerate gasses of interest, $f \ll 1$
$\rightarrow e^{(E-\mu)/kT} \gg 1$, and thus we get
Maxwell-Boltzmann, same for fermions and bosons

$$f \approx f_{\mathrm{MB}} = e^{(mc^2-\mu)/kT} e^{-p^2/2mkT} \tag{16}$$

and thus *number density* is

$$n = \frac{g}{h^3} \int d^3p \; f = g \left(\frac{2\pi mkT}{h^2} \right)^{3/2} e^{(mc^2-\mu)/kT} \tag{17}$$

thus $n(T,\mu)$: density depends not only on T
but also on chemical potential(?)

nonrelativistic particle density

$$n(T,\mu) = \frac{g}{h^3}\int d^3p\ f = g\left(\frac{2\pi mkT}{h^2}\right)^{3/2} e^{(mc^2-\mu)/kT} \tag{18}$$

if chemists invented μ, isn't it boring? Fair question, but no!

chemical potential μ: bad name, important quantity

consider a particle species with $\mu = 0$
Q: effect on n if T changes?
Q: what would it be like if air in this room obeyed this rule?

Q: so what does it mean physically if $\mu = 0$?
Q: so what does it mean physically if $\mu \neq 0$?

Chemical Potential

if $\mu = 0$:

density obeys $n(T) = g\ n_{\rm q}(T)\ e^{-mc^2/kT}$
with the *quantum concentration* $n_{\rm q} = (2\pi mkT/h^3)^{3/2}$
$\rightarrow$ density is a fixed, universal function of T
$\rightarrow$ all $\mu = 0$ gasses have *same density at same* T!?

furthermore:

- since nonrel, $kT \ll mc^2 \rightarrow n$ small!
- but n is an increasing function of T
  $\rightarrow$ so in fixed volume, *raising* T *adds new particles*!

lesson: particles with $\mu = 0$ are *not conserved!*

in fact, we already saw a (relativistic) example: photons!
recall Planck dist func $f = 1/(e^{E/kT} - 1)$: boson with $\mu = 0$

we are usually interested in species that *are* conserved
e.g., protons, neutrons conserved due to baryon number
electrons conserved due to charge and lepton number

in that case: non-relativistic equilibrium density
determined not by temperature, but by conservation law

$$n_{\mathrm{cons}} = g \; n_{\mathrm{q}} \; e^{-(mc^2-\mu)/kT} \tag{19}$$

this sets value of μ

Why is all of this useful?!
because in a reaction $a + b \leftrightarrow c + d$
the chemical potentials of each species
are related by

$$\mu_a + \mu_b = \mu_c + \mu_d \tag{20}$$

Q: so what about the case $p + e \leftrightarrow \mathrm{H} + \gamma$*?*

for $p + e \leftrightarrow \mathrm{H} + \gamma$, we have

$$\mu_p + \mu_e = \mu_{\mathrm{H}} \tag{21}$$

because $\mu_\gamma = 0$

using this and $n_i = g_i n_{\mathrm{Q}} e^{-(m_i c^2 - \mu_i)/kT}$, we have
the **Saha equation**

$$\frac{n_e n_p}{n_{\mathrm{H}}} = \frac{g_e g_p}{g_{\mathrm{H}}} \left(2\pi \frac{m_e m_p}{m_{\mathrm{H}}} \frac{kT}{h^2} \right)^{3/2} e^{-B_{\mathrm{H}}/kT} \tag{22}$$

where *hydrogen binding energy*
$B_{\mathrm{H}} = (m_e + m_p - m_{\mathrm{H}})c^2 = 13.6\ \mathrm{eV}$

Q: behavior at high T? low T? does this make sense?

The Saha Equation

define *ionization fraction*

$$x_e = \frac{n_e}{n_{\mathrm{tot}}} \tag{23}$$

with total electron number density $n_{\mathrm{tot}} = n_e + n_{\mathrm{H}}$

using $n_e = n_p$ (charge neutrality):

$$\frac{x_e^2}{1 - x_e} \approx \frac{2(2\pi m_e kT/h^2)^{3/2}}{n_{\mathrm{tot}}} e^{-B_{\mathrm{H}}/kT} = \frac{n_{\mathrm{Q},e}}{n_{\mathrm{tot}}} e^{-B_{\mathrm{H}}/kT} \tag{24}$$

for $kT \gg B_{\mathrm{H}}$, $x_e \to 1$: (nearly) fully ionized

for $kT \ll B_{\mathrm{H}}$, $x_e \ll 1$: (nearly) fully neutral

but note that, e.g., temperature at which $x_e = 1/2$

also depends on particle density n_{tot}

Awesome Saha Example: Cosmic Recombination

the early universe: *hot!*
$kT \gg B_{\mathrm{H}} \rightarrow$ totally ionized, $x_e \rightarrow 1$

present-day universe: on average, *cold!*
$T = 2.725$ K → if no stars, U would be neutral, $x_e \rightarrow 0$

thus there was a transition: **(re)combination**
our mission: estimate $T_{\mathrm{rec}} =$ when cosmic $x_e = 1/2$

Q: naïve, zeroth order estimate?
Q: how to improve?

naïvely, expect recombination when $kT_{\rm rec} \sim B_{\rm H}$
with $B_{\rm H} = 13.6$ eV, this gives
$T_{\rm rec,naive} = B_{\rm H}/k \sim 120,000$ K

but we can do better using Saha
exponential dependence on $B_{\rm H}$, but also
dependence on $n_{\rm tot}$

big-bang nucleosynthesis teaches* us that
the cosmic baryon-to-photon ratio is

$$\eta \equiv \frac{n_{\rm b}}{n_\gamma} = 6 \times 10^{-10} \tag{25}$$

most baryons are hydrogen, so $n_{\rm tot} \sim n_{\rm b}$
and thus there are *many photons for each* p *and* e

Q: anticipated effect on $T_{\rm rec}$*? higher or lower than* $T_{\rm rec,naive}$*?*

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*How? find out the next time Nuclear and Particle Astrophysics is taught!

many photons per p and $e \rightarrow$ very easy to ionize H

- when $kT < B_{\mathrm{H}}$, there are still many photons in Wien tail with $h\nu > B_{\mathrm{H}}$
- thus expect $T_{\mathrm{rec}} < T_{\mathrm{rec,naive}}$

in detail:
recall that $n_\gamma \sim (kT/hc)^3$, so

$$n_{\mathrm{tot}} \sim \eta n_\gamma \sim \eta (kT/hc)^3 \tag{26}$$

and so Saha becomes

$$\frac{x_e^2}{1-x_e} \sim \frac{1}{\eta}\left(\frac{m_e c^2}{kT}\right)^{3/2} e^{-B_{\mathrm{H}}/kT} \tag{27}$$

note: $1/\eta \gg 1$ and $m_e c^2/kT \gg 1$

so when $x_e = 1/2$ we have (PS 8)
$T_{\mathrm{rec}} \simeq T_{\mathrm{rec,naive}}/40 \sim 3000$ K
$kT_{\mathrm{rec}} \simeq 0.3$ eV $\ll B_{\mathrm{H}}$
and thus $1 + z_{\mathrm{rec}} = T_{\mathrm{rec}}/T_0 \sim 1000$

Saha Generalized

can generalize Saha to get ionization equilibrium for any species having $a^+ + e \leftrightarrow a^0 + \gamma$

$$\frac{n_+ n_e}{n_0} = \frac{g_+ g_e}{g_0} \left(2\pi \frac{m_e m_+}{m_0} \frac{kT}{h^2} \right)^{3/2} e^{-B/kT} \tag{28}$$

with B the binding energy