Astronomy 501: Radiative Processes

Lecture 24

Oct 19, 2022

Announcements:

- **Problem Set 7 due Friday**
- Midterm exams scores posted after class
  see Chris to pick up graded exam

Last time: the thermodynamics of ionization

case study: hydrogen $p + e \leftrightarrow \mathsf{H} + \gamma$

Saha: number densities linked via

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

Q: what is B_{H}?

Q: behavior at low T? high T? what sets high and low?

The Saha Equation

define *ionization fraction*

$$x_e = \frac{n_e}{n_{\text{tot}}} \tag{1}$$

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

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

with H binding $B_{\text{H}} = 13.6$ eV and $n_{\text{Q},e} = 2(2\pi m_e kT/h^2)^{3/2}$

for $kT \gg B_{\text{H}}$, $x_e \to 1$: (nearly) fully ionized
for $kT \ll B_{\text{H}}$, $x_e \ll 1$: (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!*

$kT \gg B_{\mathsf{H}} \rightarrow$ totally ionized, $x_e \rightarrow 1$

present-day universe: on average, *cold!*

$T = 2.725$ K $\rightarrow$ if no stars, U would be neutral, $x_e \rightarrow 0$

thus there was a transition: **(re)combination**

our mission: estimate $T_{\mathsf{rec}} =$ when cosmic $x_e = 1/2$

Q: naïve, zeroth order estimate?

Q: how to improve?

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

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

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

$$\eta \equiv \frac{n_{\text{b}}}{n_\gamma} = 6 \times 10^{-10} \tag{3}$$

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

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

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*How? find out next semester in Physical Cosmology!

many photons per p and $e \rightarrow$ very easy to ionize H
- when $kT < B_\mathsf{H}$, there are still many photons
  in Wien tail with $h\nu > B_\mathsf{H}$
- thus expect $T_\mathsf{rec} < T_\mathsf{rec,naive}$

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

$$n_\mathsf{tot} \sim \eta n_\gamma \sim \eta(kT/hc)^3 \tag{4}$$

and so Saha becomes

$$\frac{x_e^2}{1 - x_e} \sim \frac{1}{\eta}\left(\frac{m_e c^2}{kT}\right)^{3/2} e^{-B_\mathsf{H}/kT} \tag{5}$$

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

so when $x_e = 1/2$ we have (PS 7)
$T_\mathsf{rec} \simeq T_\mathsf{rec,naive}/40 \sim 3000$ K
$kT_\mathsf{rec} \simeq 0.3$ eV $\ll B_\mathsf{H}$
and thus $1 + z_\mathsf{rec} = T_\mathsf{rec}/T_0 \sim 1000$

Saha Generalized

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

$$\frac{n_+ n_e}{n_0} = \frac{g_+ g_e}{g_0} \left(2\pi \frac{m_e m_+}{m_0} \frac{kT}{h^2} \right)^{3/2} e^{-B/kT} \qquad (6)$$

with B the binding energy

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?

• how are tehse written on the sky `www: awesome examples`

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 $h\nu_{if} = E_i - E_f$

$$j_\nu = \frac{h\nu_{if}\ A_{if}}{4\pi}\ n_i\ \phi(\nu) \tag{7}$$

$$\alpha_\nu = \frac{h\nu_{if}}{4\pi}\ \left(B_{fi}n_f - B_{if}n_i\right)\ \phi(\nu) \tag{8}$$

$$\tag{9}$$

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

Radiative Transitions: Eigenstates are Forever?

Reall the quantum mechanics of bound systems, e.g., H atom
controlled by Hamiltonian operator $\hat{H} = \hat{p}^2/2m + V(\hat{r})$
with V the *potential* binding the constituents

wavefunctions are *energy eigenstates* $H\Psi_n = E_n\Psi_n$
with $\Psi_n(\vec{r}, t) = \psi_n(\vec{r})e^{-iE_h t/\hbar}$

Note:
- electron probability density in space $dP/dV = |\Psi(\vec{r})|^2$
  for eigenstate: $dP/dV = |\psi_n(\vec{r})|^2$ is *independent of time*
- expectation values within eigenstate also *time independent*
  e.g., $\langle \vec{r} \rangle = \int |\psi(\vec{r})|^2 \ \vec{r} \ d^3\vec{r}$
- thus *expected dipole moment* $\langle \vec{d} \rangle = e \langle \vec{r} \rangle$
  also *time independent*

Q: implications for eigenstate evolution? for radiation?
Q: Wut? how can it be that atoms radiate at all??

Spontaneous Emission: Dipole Approximation

for *unperturbed bound* system: once in *any* eigenstate
- stay there forever! including in excited states!
- no changing dipole moment (or change in any higher moments)
  $\rightarrow$ no radiation!

but *if an external perturbation is present*
wavefunction *mixes states*

Q: what could be the source of perturbation?

A Quantum Vacuum is Not Boring!

External perturbation needed to drive transitions in bound states
but luckily: one source is guaranteed!

the electrogmagnetic field is quantized!
- closely analogous to *simple harmonic oscillator*
  where $H = p^2/2m + m\omega^2 x^2/2$ leads to
  quantized states $E_n = (n + 1/2)\hbar\omega$
  ground state $n = 0$: $\psi_0 \neq 0$! zero point energy $E_0 = \hbar\omega/2$!
- EM field Hamiltonian $H = (E^2 + B^2)/8\pi$

  for experts, true analogy is potentials: $H \sim \dot{A}^2 + (\nabla A)^2 \sim \dot{A}_\omega^2 + \omega^2 A_\omega^2$

  leads to quantized states, each with $E = \hbar\omega$
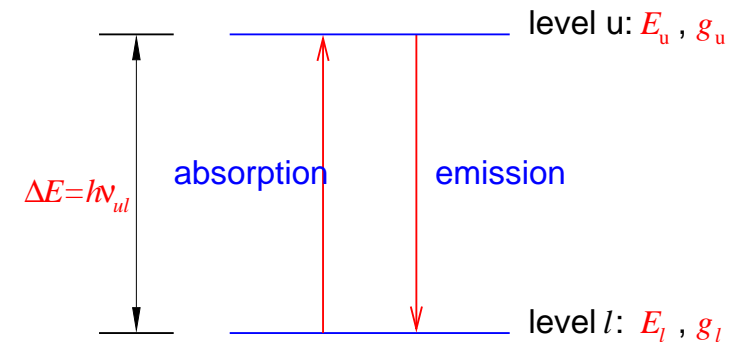 but also **zero point** fluctuations for $n = 0$ quanta!

Lessons:
- *EM vacuum: ground state $(n = 0)$. Not empty!*
- vacuum fluctuations inevitable, always present
- perturbs bound systems, drives transitions

Feeling Perturbed

consider two eigenstates:
upper level E_u and *lower level* E_ℓ

when perturbed $V \to V + \delta V$, new wavefunction

$$\Psi = a_\ell e^{-iE_\ell t/\hbar}\psi_\ell + a_u e^{-iE_u t/\hbar}\psi_u \tag{10}$$

with nonzero amplitudes a_i

this changes expectations values

$$\left\langle \vec{d} \right\rangle = |a_\ell|^2 \left\langle \vec{d} \right\rangle_\ell + |a_u|^2 \left\langle \vec{d} \right\rangle_u + 2\mathrm{Re}\left(a_\ell * a_u e^{i\omega_{\ell u}t}\right) \tag{11}$$

creates *time changing dipole* and thus **radiation**
at frequency $\omega_{\ell u} = (E_u - E_\ell)/\hbar$!!

Spontaneous Dipole Emission: Wild West Derivation

Full derivation: requires quantum electrodynamics
i.e., quantum treatment of electromagnetic field
Sketched in R&L and in Extras below
Here: cowgirl/cowboy "horseback" derivation

consider a transition from an *upper level* E_u
to a *lower level* E_ℓ
expected time-changing dipole component is

$$\vec{d} \equiv \left\langle \vec{d} \right\rangle \sim e \ e^{-i\omega_{\ell u} t} \ \langle u|\vec{r}|\ell \rangle \qquad (12)$$

and so dipole acceleration is

$$\ddot{\vec{d}} \sim e \ \omega_{\ell u}^2 \ e^{-i\omega_{\ell u} t} \ \langle u|\vec{r}|\ell \rangle \qquad (13)$$

Q: and so?

in dipole approximation, **Larmor power per atom** is

$$P_{u\ell} = \frac{2}{3}\frac{|\ddot{d}|^2}{c^3} \sim \frac{\omega_{\ell u}^4}{c^3}|d_{u\ell}|^2 \qquad (14)$$

- transition driven by dipole operator

$$\vec{d}_{u\ell} = e \int \psi_\ell^* \; \vec{r} \; \psi_u \; dV$$

  between initial and final states
- zero when dipole moment vanishes—*forbidden* transitions!
  but higher multipole transitions may still go

now we are ready for Einstein $A_{u\ell}$! *Q: how?*

Spontaneous Dipole Emission

the *power* emitted in $u \rightarrow \ell$ transition:

$$P_{u\ell} \sim \frac{\omega_{\ell u}^4}{c^3} |d_{u\ell}|^2 \qquad (15)$$

energy released per transition $E_{u\ell} = \hbar \omega_{\ell u}$
so estimate transition rate per atom as

$$\frac{d\mathcal{N}_{u\ell}}{dt} \sim \frac{P_{u\ell}}{E_{u\ell}} \sim \frac{\omega_{\ell u}^3}{\hbar c^3} |d_{u\ell}|^2 \qquad (16)$$

exact Einstein coefficient for *spontaneous emission*

$$A_{u\ell} = \frac{64\pi^4 \, \nu_{u\ell}^3 \, |d_{u\ell}|^2}{3c^3 h} \qquad (17)$$

Q: what about absorption and stimulated emission?

Einstein Coefficients

the Einstein coefficients in the electric dipole approximation are:

- *spontaneous emission*

$$A_{u\ell} = \frac{64\pi^4 \ \nu_{u\ell}^3 \ |d_{u\ell}|^2}{3c^3h} = \frac{2\nu^3}{c^2h}B_{\ell u} \qquad (18)$$

- true *absorption*

$$B_{\ell u} = \frac{8\pi^2}{3c\hbar^2}|d_{\ell u}|^2 = \frac{32\pi^4}{3ch}|d_{\ell u}|^2 \qquad (19)$$

for *non-degenerate atomic levels* with $g_\ell = g_u = 1$ we have

- *stimulated emission*

$$B_{u\ell} = B_{\ell u} \qquad (20)$$

this gives (at least in principle) a direct means to connect
the radiative coefficients j_ν and α_ν
to the atomic properties encoded in the dipole moment $d_{u\ell}$

recall that the absorption coefficient is

$$\alpha_\nu = \frac{h\nu}{4\pi} \ n_\ell \ B_{\ell u} \ \phi(\nu) \tag{21}$$

and so writing this in terms of the *absorption cross section* $\sigma_{\ell u}$

$$\alpha_\nu = n_\ell \ c \ \sigma_{\ell u}(\nu) \tag{22}$$

so that the cross section and Einstein coefficient are related by

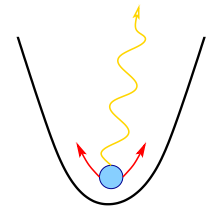$$\sigma_{\ell u}(\nu) = \frac{h\nu}{4\pi \ c} \ B_{\ell u} \ \phi(\nu) \tag{23}$$

integrating and using $\int \phi(\nu) \ d\nu = 1$, we have

$$B_{\ell u} = \frac{4\pi \ c}{h\nu_{\ell\nu}} \int \sigma_{\ell u}(\nu) \ d\nu \tag{24}$$

and thus our expressions for $B_{\ell u}$ also give $\sigma_{\ell u}$

Oscillator Strength

If the electron moves as a *damped classical oscillator*
with natural (resonant) frequency ω_0
then (PS7) absorption rate is $B_{\ell u}^{\text{classcial}} \ J(\nu_{\ell u})$ with

$$B_{\ell u}^{\text{classical}} = \frac{4\pi^2 e^2}{h\nu_{\ell u} \ m_e c} \tag{25}$$

it is thus convenient write

$$B_{\ell u} \equiv f_{\ell u} \ B_{\ell u}^{\text{classical}} \tag{26}$$

$$\sigma_{\ell u}(\nu) = \frac{\pi e^2}{m_e c} \ f_{\ell u} \ \phi(\nu) \tag{27}$$

where the dimensionless **oscillator strength** is

$$f_{\ell u} = \frac{m_e}{\pi e^2} \int \sigma_{\ell u}(\nu) \ d\nu = \frac{2m_e}{3\hbar^2 g_\ell e^2}(E_u - E_\ell) \sum |d_{\ell u}|^2 \tag{28}$$

Q: what about $f_{u\ell}$?

Einstein $g_\ell B_{\ell u} = g_u B_{u\ell}$, and since we have absorption

$$g_u \; f_{u\ell} = - \; g_\ell f_{\ell u} \tag{29}$$

so *emission oscillator strengths are negative*

if we sum over all transitions from $i \to j$,
can show that *one-electron atoms have*

$$\sum_{j \; \text{final}} f_{ij} = 1 \tag{30}$$

where strong transitions have $f_{ij} \sim 1$
and *N-electron atoms have*

$$\sum_{j \; \text{final}} f_{ij} = N \tag{31}$$

the *Thomas-Riche-Kuhn sum rule*

Q: What if two states have no dipole moment: $d_{if} = 0$?

Director's Cut Extras

The Road to Saha: Method II–Chemical Equilibrium

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

$$dN = \frac{g}{h^3} f \; d^3x \; d^3p \qquad (32)$$

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

$$f = \frac{1}{e^{(E-\mu)/kT} \pm 1} \qquad (33)$$

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, $\pm \leftrightarrow$ fermion/boson

$$f = \frac{1}{e^{(E-\mu)/kT} \pm 1} \tag{34}$$

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

$$f \approx f_{\mathsf{MB}} = e^{(mc^2-\mu)/kT} e^{-p^2/2mkT} \tag{35}$$

and thus *number density* is

$$n = \frac{g}{h^3} \int d^3p \ f = g \left(\frac{2\pi mkT}{h^2} \right)^{3/2} e^{(mc^2-\mu)/kT} \tag{36}$$

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

nonrelativistic particle density

$$n(T,\mu) = \frac{g}{h^3} \int d^3p \; f = g \left(\frac{2\pi m kT}{h^2} \right)^{3/2} e^{(mc^2-\mu)/kT} \qquad (37)$$

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 $n(T) = g \; n_{\mathsf{q}}(T) \; e^{-mc^2/kT}$

with the *quantum concentration* $n_{\mathsf{q}} = (2\pi mkT/h^3)^{3/2}$

$\rightarrow$ 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

$$n_{\text{cons}} = g \; n_{\text{q}} \; e^{-(mc^2 - \mu)/kT} \tag{38}$$

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

$$\mu_a + \mu_b = \mu_c + \mu_d \tag{39}$$

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

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

$$\mu_p + \mu_e = \mu_{\mathsf{H}} \tag{40}$$

because $\mu_\gamma = 0$

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

$$\frac{n_e n_p}{n_{\mathsf{H}}} = \frac{g_e g_p}{g_{\mathsf{H}}} \left(2\pi \frac{m_e m_p}{m_{\mathsf{H}}} \frac{kT}{h^2} \right)^{3/2} e^{-B_{\mathsf{H}}/kT} \tag{41}$$

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

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