

Astro 501: Radiative Processes  
Lecture 19  
October 10, 2018

Announcements:

- good news: no Problem Set due this week  
bad news **Miderm Exam in class Friday**

# Midterm Exam

**Time** In class **Friday October 12.**

You will have the usual class time, 50 minutes

## Topics

Everything up to and including Thomson scattering.

All material in Lectures 1–16 and Problem Sets 1-5 is fair game.

## What to Bring

something to write with. won't need a calculator.

**You may bring any notes**, but exam is *closed book* and *closed internet*.

## Question Format

The homework questions point to important topics and questions. Given the exam time constraints, the problems will generally be less involved than in homework, but rather the questions will emphasize an understanding of how to apply and interpret the tools we have developed.

## Bremstrahlung Summary

for a *fixed electron velocity*  $v$

$$4\pi j_{\omega}(\omega, v) = \frac{16\pi Z^2 e^6}{3\sqrt{3} m_e^2 c^3 v} n_i n_e g_{\text{ff}}(\omega, v) \quad (1)$$

for a **thermal distribution of velocities** = Maxwell-Boltzmann

$$4\pi j_{\nu, \text{ff}}(T) = \frac{2^5 \pi Z^2 e^6}{3 m_e c^3} \left( \frac{2\pi}{3m_e kT} \right)^{1/2} \bar{g}_{\text{ff}}(\nu, T) e^{-h\nu/kT} n_e n_i \quad (2)$$

with *Gaunt factor*  $g_{\text{ff}} \sim 1$

Q: *spectral features?*

Q: *all of this was for emission—what about*

$\omega$  *the thermal bremsstrahlung absorption coefficient  $\alpha_{\nu}(T)$ ?*

## Thermal Bremsstrahlung Absorption

for *thermal* system, *Kirchoff's law*:  $S_\nu = B_\nu(T) = j_\nu/\alpha_\nu$

thus we have

$$\alpha_{\nu,\text{ff}} = \frac{j_{\nu,\text{ff}}}{B_\nu(T)} = \frac{4 Z^2 e^6}{3 m_e h c} \left( \frac{2\pi}{3 m_e k T} \right)^{1/2} \bar{g}_{\text{ff}}(\nu, T) \nu^{-3} \left( 1 - e^{-h\nu/kT} \right) n_e n_i$$

limits:

- $h\nu \ll kT$ :  $\alpha_{\nu,\text{ff}} \propto \nu^{-2}$
- $h\nu \gg kT$ :  $\alpha_{\nu,\text{ff}} \propto \nu^{-3}$

Q: sketch optical depth vs  $\nu$ ? implications?

## Bremsstrahlung Self-Absorption

bremsstrahlung optical depth at small  $\nu$ :

$$\tau_\nu \propto \alpha_{\nu, \text{ff}} \propto \nu^{-2} \quad (3)$$

*guaranteed optically thick* below some  $\nu$

→ free-free emission is absorbed inside plasma:

### bremsstrahlung self-absorption

thus observed plasma spectra should have three regimes

- small  $\nu$ :  $\tau_\nu \gg 1$ , optically thick,  $I_\nu \rightarrow B_\nu \propto \nu^3$
- $h\nu < kT$ : optically thin,  $I_\nu \rightarrow j_\nu s$  *flat* vs  $\nu$
- $h\nu \gg kT$ : thermally suppressed,  $I_\nu \rightarrow j_\nu s \sim e^{-h\nu/kT}$

<sup>51</sup> Q: expected X-ray *count* spectrum for galaxy cluster?

www: observations

## Bremsstrahlung and Stellar Interiors

in stellar interiors, bremsstrahlung known as **free-free** emission

stellar flux transfer depends on **frequency-averaged opacity**

*Q: what's opacity?*

*Q: how do we perform frequency average?*

## Bremsstrahlung and Stellar Interiors

**opacity** defined via

$$\alpha_\nu = n\sigma_\nu = \rho\kappa_\nu \quad (4)$$

and in thermal radiation field, frequency avg is **Rosseland mean**

$$\frac{1}{\alpha_R} = \frac{\int (\alpha_\nu + \varsigma_\nu)^{-1} \partial_T B_\nu d\nu}{\int \partial_T B_\nu d\nu} \quad (5)$$

for bremsstrahlung at  $h\nu < kT$

$$\alpha_\nu \sim \frac{Z^2 \nu^2}{T^{3/2}} n_e n_i \quad (6)$$

Q: and so what do we expect for  $\alpha_R(\rho, T)$ ?

## Free-Free Opacity

free-free = bremsstrahlung:  $\alpha_\nu \sim \nu^2/T^{3/2} n_e n_i$   
scalings in Rosseland mean for bremsstrahlung:

- $h\nu \sim kT$
- $n_i \propto \rho$ , and  $n_e \propto \rho/\mu_e$

gives **Kramer's Law** for opacity

$$\kappa_{\text{ff}}(\rho, T) \sim \frac{\rho}{\mu_e T^{7/2}} \quad (7)$$

appears in local flux expression

$$F(z) = -\frac{16\sigma T^3}{3\kappa\rho} \frac{\partial T}{\partial z} \quad (8)$$

important for stellar interiors

<sup>∞</sup> bonus: same scaling works for bound-free!



## Build Your Toolbox: Bremsstrahlung

microphysics: matter-radiation interactions

*Q: physical origin of bremsstrahlung?*

*Q: physical nature of sources?*

*Q: spectrum characteristics?*

*Q: frequency range?*

real/expected astrophysical sources of Thomson scattering

*Q: where do we expect this to be important?*

*Q: relevant EM bands? temperatures?*

# Toolbox: Bremsstrahlung

## emission physics

- **physical origin:** non-relativistic Coulomb acceleration in free electrons and ions interactions
- **physical sources:** need free  $e^-$  and ions  $\rightarrow$  ionized gas = plasma
- **spectrum:** continuum emission  
for thermal plasma,  $j_\nu \sim \text{const}$  vs  $\nu$   
up to *exponential cutoff*  $e^{-h\nu/kT}$

## astrophysical sources of bremsstrahlung emission/absorption

- **sites** are highly ionized gas: stellar interiors, stellar coronæ, hot nebulæ (Hii regions), early Universe
- **EM bands** radio to X-ray
- **temperatures** up to  $\sim 10^6$  K

# Radiation and Bound States

# Radiation and Bound States

In the course up until now, focused largely on *continuum* radiation

i.e., processes that emit/absorb across a wide range of  $\nu$  and (mostly) involve *unbound* electrons

- blackbodies
- bremsstrahlung
- Thompson scattering

But what about *lines*!?

these arise from transitions involving electrons in *bound states*

→ atoms and molecules

To discuss these, begin with refresher on atoms and molecules

# Atomic Structure

## Gossip Break: Wiesskopf's Pauli Story

# Atomic Structure: Order of Magnitude

Atoms and molecules inherently *quantum* systems

Cowgirl/cowboy view of hydrogen:

*quantum* bound state of electron around proton, with energy

$$E = \frac{p^2}{2m_e} - \frac{e^2}{r} \quad (9)$$

but Heisenberg:  $rp \geq \hbar/2$

Wild West: cowgirl/cowboy approximation  $p \sim \hbar/r$

$$E = \frac{\hbar^2}{2m_e r^2} - \frac{e^2}{r} \quad (10)$$

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Q: so how to find ground state?

Heisenberg-ized sketch of hydrogen energy

$$E = \frac{\hbar^2}{2m_e r^2} - \frac{e^2}{r} \quad (11)$$

ground state:  $E$  is *minimum*

$$\partial_r E = -\frac{\hbar^2}{m_e r^3} + \frac{e^2}{r^2} = 0 \quad (12)$$

gives electron radius  $r_{\min} \equiv a_0$ :

$$a_0 = \frac{\hbar^2}{e^2 m_e} = 0.05 \text{ nm} \quad (13)$$

and electron energy  $E(r_{\min}) \equiv E_1$ :

$$E_1 = -\frac{e^4 m_e}{2\hbar^2} = -\frac{1}{2}\alpha^2 m_e c^2 = 13.7 \text{ eV} \quad (14)$$

16 where  $\alpha = e^2/\hbar c \approx 1/137$

Q: how do these compare with results of honest calculation?



# Hydrogen Atom: Honest Non-Relativistic Results

*non-relativistic* Schrödinger ignores relativistic effects

- electron (and proton) spins absent from Hamiltonian  
→ electron orbit properties independent of spin

for **hydrogen-like species**: single electron, nuclear charge  $Z$

*ground state* properties

- energy  $E_1 = -Z^2 e^4 m_e / 2\hbar^2$
- mean radius  $\langle r_1 \rangle = a_0 / Z$
- electron expected speed  $\langle v_1 \rangle = Ze^2 / \hbar = Z\alpha c$   
so that  $\beta_1 = v_1 / c = Z\alpha \approx Z / 137 \ll 1$  for most atoms  
if not: non-relativistic is bad approximation!

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Q: what about excited states: how many?

Q: how do  $E_n, r_n, v_n$  vary with  $n$ ?

excited states, ignoring spin effects (*non-relativistic*):

for each integer  $n = 1, 2, 3, \dots$

- $E_n = E_1/n^2$
- $\langle r \rangle_n = n^2 r_1$
- $\langle v \rangle_n = v_1/n$

## Lessons

- H has an infinite “tower” of bound states
- $\langle r \rangle_n \propto n^2$ : *principal quantum number*  $n$   
controls *radial* part of wavefunction
- as  $n \rightarrow \infty$ : bigger radius, slower, more weakly bound

*hydrogen wavefunction*: 3-D system  $\rightarrow$  need 3 quantum numbers

Q: *what are the other two?*

Non-relativistic hydrogen wavefunction: states specified by

- *principal* quantum number  $n = 1, 2, \dots$   
controls wavefunction dependence on  $r$
- *orbital angular momentum*  $l = 0, 1, \dots, n - 1$   
 $\hat{L}^2\psi = l(l + 1)\hbar^2\psi$   
controls wavefunction dependence on  $\theta$
- *z-projection*  $\hat{L}_z\psi = m\hbar\psi$  with  $m = -l, \dots, +l$   
controls wavefunction dependence on  $\phi$

in non-relativistic case: energy only depends on  $n$

all states with fixed  $n$  are *degenerate* (same energy)

- at each  $l$  value:  $2l + 1$  “substates” of different  $m$
- each of which has 2 possible  $e$  spin states:  $s_z = \pm 1/2$
- at each  $n$ : a total of  $2 \sum_{l=0}^{n-1} 2l + 1 = 2n^2$  states  
all with the same energy

Q: *effect of full relativistic treatment?*

## Realistic Atoms

for *hydrogen*

Schrödinger:  $v_n/c = \alpha/n \ll 1$ ,  $|E_n| = \alpha m_e c^2 / 2 \ll m_e c^2$

→ electron motion is (very) non-relativistic: approx justified!

→ expect relativistic corrections to be small

Full relativity: Dirac equation

Hamiltonian includes spins of electron and proton

new interactions are  $\propto \beta = v/c$  or  $\beta^2 \rightarrow$  small corrections

→ lifts degeneracy of levels at same  $n$

# Multi-Electron Atoms

in **first (i.e., non-relativistic) approximation**

- principal quantum number  $n$  still appears
- spins do not appear in Hamiltonian  $\rightarrow$  atom state only depends on total orbital angular momentum quantum number  $L$
- due to Pauli  $\rightarrow$  atom state still does depends on total electron spin quantum number  $S$
- states with same  $n$ ,  $L$  and  $S$  are degenerate

for **realistic multi-electron atoms**

spin interactions are relativistic perturbations  
break (“lift”) degeneracy at same  $n$ ,  $L$ ,  $S$

To a good first approximation:

- wavefunction (state) of each electron is **independent** of other electrons
- except that Pauli principle is crucial  $Q$ : *how?*

# Building Atoms

Pauli: no two (or more) fermions  
can occupy the same quantum state

electrons are fermions, each with  $s = 1/2$

→ projection  $s_z = \pm 1/2$  adds one last quantum number

“assembly” of multi-electron atoms, to first approximation,

- state of *each* electron has fixed  $n$  and  $\ell$   
with  $\ell = 0, 1, \dots, n - 1$  (like H-atom)
- but order of state energies *not* always like H-atom
- states “filled” from lowest energy up, according to Pauli
- fill by “subshells” = states with same  $(n, \ell)$
- ∞ while “shells” are *all* states at fixed  $n$
- atom ground state: electrons in lowest possible states

**electron configuration:** distribution of states in atom

- notation:  $(n, \ell)$  electron state (“subshell”) is  $n\Upsilon$   
with  $\Upsilon = s, p, d, f, \dots$  for  $\ell = 0, 1, 2, 3, \dots$
- multiplicity: if  $k$  electrons in subshell:  $n\Upsilon^k$

for example:

- lowest shell is  $(n, \ell) = (1, 0)$   
 $\ell = 0$  has only  $m = 0$ ; so filled shell is  $1s^2$
- next subshell is  $(n, \ell) = (2, 0)$ ; filled is  $2s^2$
- then  $(n, \ell) = (2, 1)$ :  $\ell = 1$ ,  $p$  state  
 $m = -1, 0, 1$  allowed, so filled subshell is  $2p^6$

www: sketches of  $\ell$  states in 3D

*Q: how do we know the order of filling states?*

*that is: what determines the ranking of energy levels?*

## 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  $n$

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



- ▷ states filled in order of increasing  $n + l$
- ▷ when two states have same  $n + l$   
filled in order of increasing  $n$

lithium:  $Z = 3$

filled  $1s^2 = 2$  states,  $2s^1$  half-filled:  $1s^2 2s$

carbon:  $Z = 6$

filled:  $1s^2 2s^2 = 4$  states,  $2p^2$  partial = 2 states

$1s^2 2s$

silicon:  $Z = 14$

filled:  $1s^2 2s^2 2p^6 3s^2 = 12$  states,  $3p^2$  partial = 2 states

$1s^2 2s^2 2p^6 3s^2 3p^2$

Aufbau principle gives ordering of  $(n, \ell)$  subshells  
further splitting at fixed  $(n, \ell)$  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  $L_{\text{shell}} = 0 = S_{\text{shell}}$   
so  $L$  and  $S$  set only by *unfilled subshells*

## Hund's Rule

Hund's rule: energy level orderings in  $(n, \ell)$  subshell for a fixed electron configuration = fixed unfilled  $(n, \ell)$  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 or 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  $s_{z1} = s_{z2}$  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  $m_2 = 0$ )  
→  $L = 1$

▷ for subshells half-filled or 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  $\mathcal{L} = S, P, D, \dots$  for  $L = 0, 1, 2, \dots$

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  $S$  → preference for spins aligned

but then Pauli demands different  $m$

→ fill  $m$  states with one  $e$  each before “doubling up”

→ “*bus seat rule*”

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

largest  $L$  → preference for orbit planes aligned

orbit in “same direction” and not opposite

→  $e$  avoid each other, have nucleus in between

→ decrease  $e$  screening of nuclear charge, and  $e$  repulsion

# Atomic Fingerprints

atomic wavefunctions, states are complex function of nuclear charge and number of electrons

→ resulting energy levels *unique* to each atom

and to each ionization state, e.g.,  $C^{3+} \equiv C\text{ iv}$

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?*