# Physics of the Diffuse Universe

Professor Crystal L. Martin
UC Santa Barbara

"I ask you to look both ways. For the road to a knowledge of the stars leads through the atom; and important knowledge of the atom has been reached through the stars."

-- Sir Arthur Eddington (Stars & Atoms, 1928)

# Outline for Week 2 & 3

- T & $\rho$ diagnostics (cont'd)
- Spectroscopic Notation
  - Selection rules
  - Spacing of molecular lines
- Radiative Transfer
  - Definitions (Rybicki & Lightman)
  - Interstellar/Intergalactic Absorption (Spitzer)
  - Radio Astronomy (DS ch 4; Spitzer; Dyson & Williams)
- Main concepts/tools
  - Statistical Equilibrium
  - Equation of Radiative Transfer

# Atomic Spectra

- Governed by rules of quantum mechanics
  - Wave function of individual electrons (in a spherically symmetric potential)

    $\Psi(r,\theta,\phi) = R_{nl}(r)\,\Theta_{lm}(\theta)\,\Phi_{m}(\phi)$
  - Principal n = 1, 2, 3, …
  - Electron spin s = 1/2
  - Angular momentum l = 0, 1, 2, …, (n–1)
  - Magnetic m = –l, –(l–1), …, 0, …, (l–1), l

# Spectroscopic Notation

- Notation for ions
- Electron configuration
- Spectroscopic term
- Pauli exclusion principle
  - One active electron (e.g., Mg II, Na I)
  - Two electrons with LS coupling (e.g., Mg I)
  - Heavier ions can have JJ coupling
  - Real coupling usually intermediate to these limiting cases

# Temperature diagnostics via $p^2$ and $p^4$ ions

- **Three (five) Level Atom** describes many of the strong lines in spectra of ionized nebulae (and late-type galaxies) used to infer physical conditions.
- The states have different spin-orbit interactions but the same principle quantum number, so these are forbidden lines
- **$E_{32}$ ~ $E_{21}$ and Low Density** [BB]
- $F_{32}/F_{21} = E_{32}/E_{21} * A_{32}/(A_{32} + A_{31}) * \Omega_{12}/\Omega_{12} * \exp(-E_{32}/kT)$

# Density diagnostics via $p^3$ ions

- $E_{32} << E_{21}$
- LDL -- all collisional excitations result in radiative decays
- [BB] $F_{31}/F_{21} = \Omega_{13}/\Omega_{12}$
- See sum rule for collision strengths
- HDL -- Radiative decay rate matters because collision deexcitation may occur
- [BB] $F_{31}/F_{21} = A_{13}/A_{12} * g_3/g$
- At what densities is the line ratio a good indicator of the electron density? [BB]

# Infrared Line Diagnostics

- Transitions between fine-structure levels of $p^2$ and $p^4$ ions are dominant coolants of gas at 100 - 3000 K. See DS Table 3.3.
- E.g., [CII] 158 um; [OIII] 88.36, 51.81 um
- Atmospheric water vapor blocks 25-300 um
- Infrared Space Observatory (ISO)
- Spitzer IRS
- Herschel
- Sofia
- ALMA (these lines for high redshift galaxies)

# Terms for ns and np Subshells

| E config. | Terms | Examples |
|---|---|---|
| $...ns^1$ | $^2S_{1/2}$ | H I, He II, C IV, N V, O VI |
| $...ns^2$ | $^1S_0$ | He I, C III, N IV, O V |
| $...np^1$ | $^2P_{1/2,\ 3/2}$ | C II, N III, O IV |
| $...np^2$ | $^3P_{0,1,2}\ \ ^1D_2\ \ ^1S_0$ | C I, N II, O III, Ne V, S III |
| $...np^3$ | $^4S_{3/2}\ \ ^2D_{3/2/,5/2}\ \ ^2P_{1/2,3/2}$ | N I, O II, Ne IV, S II, Ar IV |
| $...np^4$ | $^3P_{2,1,0}\ \ ^1D_2\ \ \ ^1S_0$ | O I, Ne III, Mg V, Ar III |
| $...np^5$ | $^2P_{3/2,1/2}$ | Ne II, Na III, Mg IV, Ar IV |
| $...np^6$ | $^1S_0$ | Ne I, Na II, Mg III, Ar III |

# Addendum (T & n diagnostics)

- HII regions: T and density diagnostics
  - Real ISM is clumpy; measure $n_{e,c}$
  - Emission measure ~ $\langle n_e^2 \rangle$ * length
  - Define a volume filling factor for the clumps such that $\langle n_e^2 \rangle \sim f * n_{e,c}^2$
- f ~ 0.01 to 0.1 typically

# Resonance Lines

- Electric dipole transition selection rules
  - Only 1 electron involved in the transition
  - Initial and final states have different parity
  - Emitted photon carries 1 unit of angular momentum, so $\Delta l = +/- 1$
  - Electron spin does not change
  - Change in the total angular momentum of the active electron is $\Delta J = +/- 1, 0$ (with J=0 to J=0 forbidden)
- Statistical weight of any level is $g = 2J + 1$

# Selection Rules

| | | Electric dipole (E1) | Magnetic dipole (M1) | Electric quadrupole (E2) | Mag quadru |
|---|---|---|---|---|---|
| **Rigorous rules** | (1) | $\Delta J = 0, \pm 1$ $(J = 0 \not\leftrightarrow 0)$ | | $\Delta J = 0, \pm 1, \pm$ $(J = 0 \not\leftrightarrow 0, 1; \frac{1}{2}$ | |
| | (2) | $\Delta M_J = 0, \pm 1$ | | $\Delta M_J = 0, \pm 1,$ | |
| | (3) | $\pi_\mathrm{f} = -\pi_\mathrm{i}$ | $\pi_\mathrm{f} = \pi_\mathrm{i}$ | | |
| **LS coupling** | (4) | One electron jump $\Delta l = \pm 1$ | No electron jump $\Delta l = 0$, $\Delta n = 0$ | None or one electron jump $\Delta l = 0, \pm 2$ | One ele $\Delta l$ |
| | (5) | If $\Delta S = 0$ $\Delta L = 0, \pm 1$ $(L = 0 \not\leftrightarrow 0)$ | If $\Delta S = 0$ $\Delta L = 0$ | If $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm$ $(L = 0 \not\leftrightarrow 0, 1$ | |
| **Intermediate coupling** | (6) | If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2$ | | If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ $\pm 2, \pm 3$ $(L = 0 \not\leftrightarrow 0)$ | If $\Delta$ $\Delta L =$ $(L =$ |

# Intercombination or Semi-forbidden Lines

- Departure from pure LS coupling means that electric quadrupole transitions between states of different multiplicity can occur
- But at much lower probability, A ~ $10^2$ to $10^3$ $s^{-1}$
- At typical ISM density and temperature, these transitions are still more probable than a collision with another atom.
- Example: CIII]

# Forbidden Lines

- Magnetic dipole transitions
- A of 1 to $10^{-4}$ $s^{-1}$
- How long do electons involved in forbidden transitions rest in their excited states?
- Clearly the densities must be very low indeed for the atom to avoid a collision on this timescale.
- The emitted photon is very unlikely to be reabsorbed by another ion. Why?
- Forbidden line photons usually escape from a nebula, so they are very important coolants.
- Examples [OIII] 4959, 5007; [OII] 3726,29,
  - **What makes $^1D_2 \rightarrow {}^3P_2$ forbidden?**

# Pure Recombination Lines

- Recombination of an ion and electron forms an ion an excited state.
- The electron cascades through many possible energy levels back down to the ground state
- Why is this more complicated than the two-level resonance line transitions?
- Calculation of the cascade process requires precision; See [DS] 2.1.2 for the QM approach.
- Hydrogen recombination spectrum [BB]

# Molecular Spectra

- Rotating Molecules
- Vibrating Molecules
- Ro-Vibrational Spectra
- Electronic Molecular Spectra

# Rotating Molecules

- Quantized rotational energy levels related to the moments of inertia of the molecules along the various axes of symmetry
- Example: Linear (Diatomic) molecules
  - Roughly a rigid rotator with constant spacing between atoms
  - Solutions quantized in the z component of the angular momentum, $m_j$, and the rotational quantum number, J, analogous to "l" in one electron atoms [BB]
  - $E_J \sim J(J+1)$
  - Lines are linearly spaced

# Molecular Hydrogen

- Does H2 radiate strongly?
- To produce electric dipole line emission in these rotational transitions requires a heterogeneous linear molecule like CO.
- Transitions occur via electric quadrupole interaction. The least energetic transition is J=0 to J=2
- Lifetimes of excited states are much, much longer than for the ions, e.g., about 1000 years for the J=2 level.
- Hence the rotational levels are populated by collisions

# Vibrating Molecules

- Equilibrium distance $r_0$ at potential minimum, I.e., repulsion of the nuclei vs. attractive force of the bond [BB]
- Stretching
- 1 frequency!
- Higher E

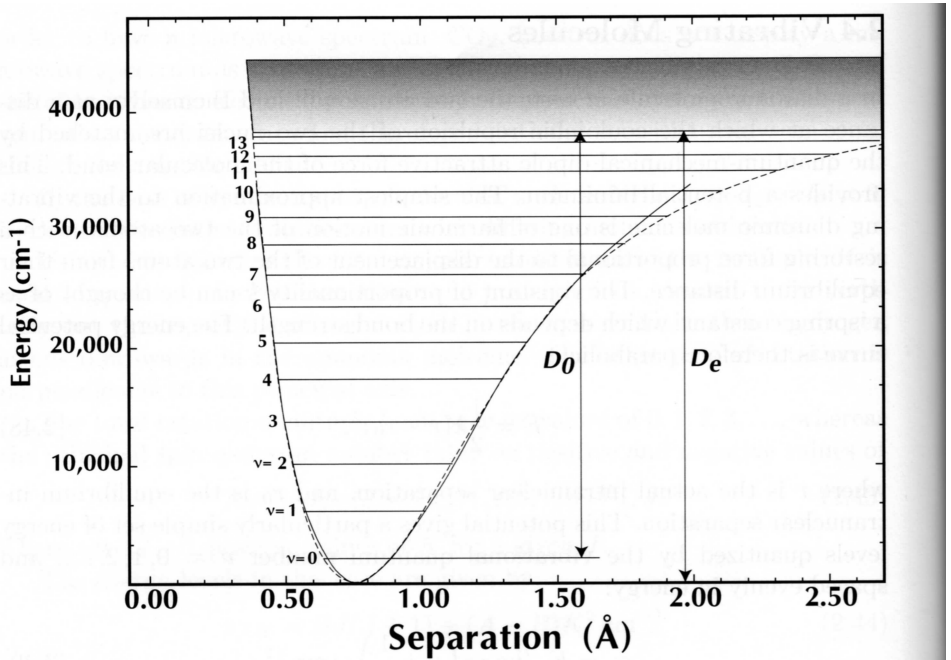



**Fig. 2.6.** The Morse potential for $H_2$. The actual potential inferred from detailed spectroscopy is the solid curve, the Morse potential is given by the dashed curve.

# Ro-vibrational levels

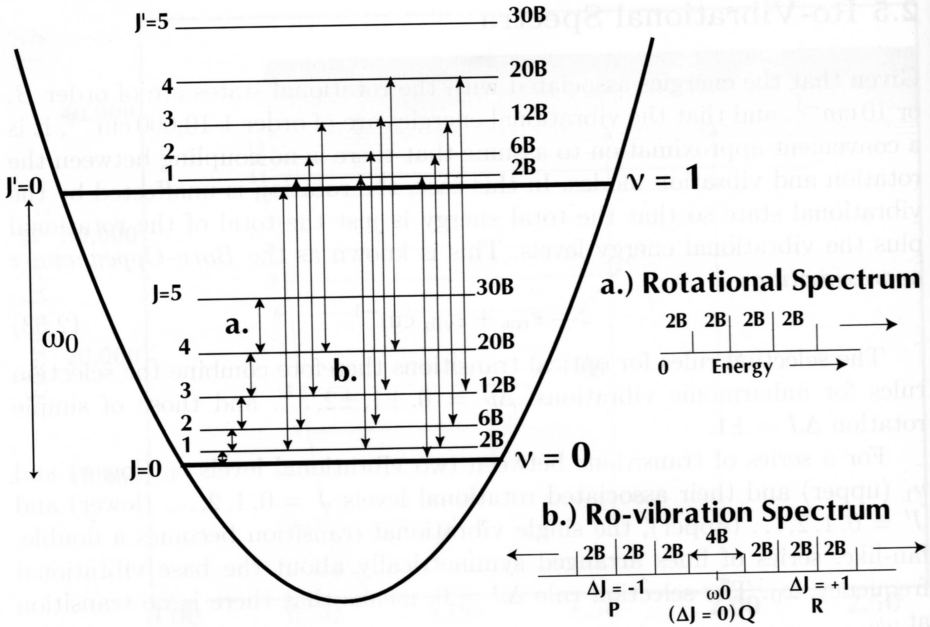



**Fig. 2.7.** Rotational-vibrational levels. Within each vibrational level of a diatomic molecule, a series of rotational levels occur, here magnified by a factor of several hundred for illustrative purposes. Transitions within the rotational levels (a.) produce a microwave spectrum with a spacing of $2B$ in energy. Transitions between rotational levels across vibrational levels, (b.), produce an infrared line at $\omega_0$ that is split into rotational series spectral lines ($P$- and $R$- branches) that are also separated by an energy of $2B$. If $\Delta J = 0$ is permitted by out-of-line bending vibrations, a series of lines called the $Q$ branch can appear at $\omega_0$ with zero spacing because the energy differences for $\Delta J = 0$ are constant.

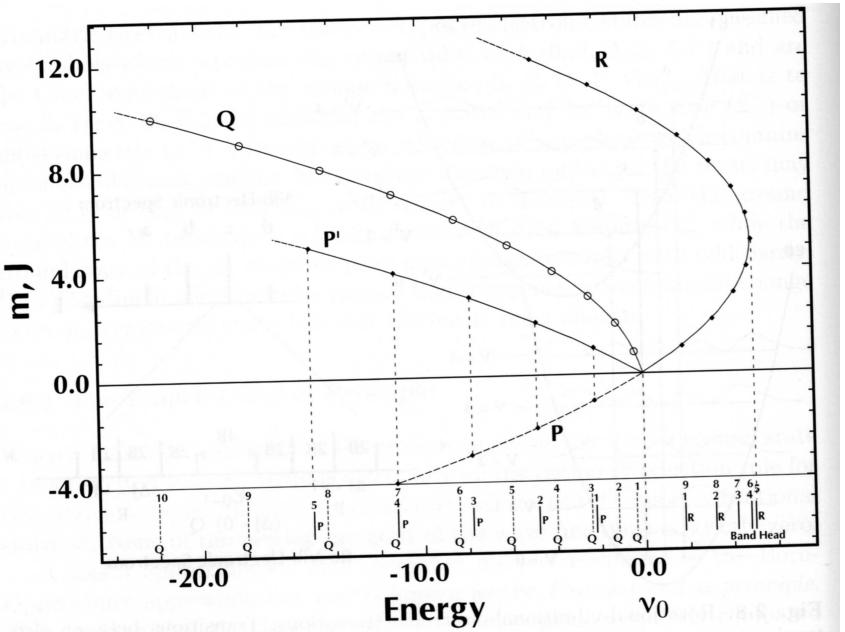



**Fig. 2.9.** Fortrat diagram for a Rotational-vibrational-electronic spectrum.

# Electronic Transitions

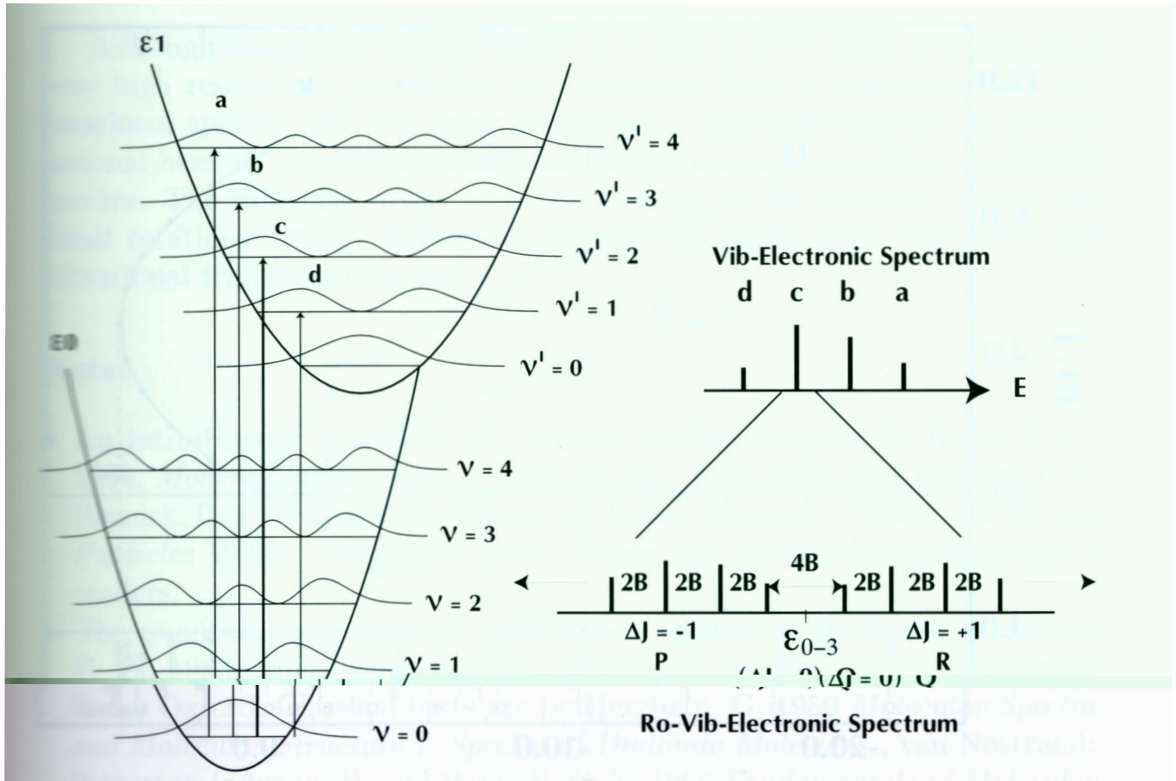



**Fig. 2.8.** Rotational-vibrational-electronic transitions. Transitions between electronic states are essentially instantaneous compared to vibrational or rotational timescales, and therefore are vertical transitions with no change in the separation of the atoms. Transitions are possible between different $\nu$ levels, with transition probabilities determined by the overlap of the vibrational wave functions. The line intensities are determined by the level populations and the transition probabilities. Each vibrational-electronic transition is also split by rotational levels, resulting in a ro-vib-electronic spectrum with $P$-, $Q$- and $R$- rotational branches.

Electric Quadrupole (E2) - Intercombination Trans.

$\Delta M = 0, \pm 1, \pm 2$

$\Delta J = 0, \pm 1, \pm 2$ $\quad 0 \not\to 0,\ \frac{1}{2} \to \frac{1}{2},\ 0 \to 1$

$\Delta l = 0, \pm 2$ $\quad$ no parity change

$\Delta n$ arbitrary

$\Delta L = 0, \pm 1, \pm 2$ $\quad 0 \not\to 0 \quad 0 \to 1$

$\Delta S = 0$

Magnetic Dipole (M1) - Forbidden Transitions

$\Delta M = 0, \pm 1$

$\Delta J = 0, \pm 1$ $\quad J=0 \not\to J=0$

$\Delta l = 0$

$\Delta n = 0$

$\Delta L = 0$ $\quad$ If $\Delta S = 0$

$\Delta L = 0, \pm 1, \pm 2$ $\quad$ If $\Delta S = \pm 1$

Possible rotational energy levels in rigid rotator


$\mu = \frac{m_1 m_2}{m_1 + m_2}$ reduced mass

$I = \mu r^2$ Inertia

$$\frac{d^2\Phi(\phi)}{d\phi^2} = -m_j^2 \Phi(\phi)$$

Wave eqn. contrains J to integers with $J = -m_j, \ldots, c, \ldots m_j$

The rotational energy $E = J(J+1)\frac{h^2}{8\pi^2 I}$

Radiative transitions change $\Delta J$ by $\pm 1$,

So $\Delta E = \left[(J+1)(J+2) - J(J+1)\right]\frac{h^2}{8\pi^2 I}$

$= (J+1)(J+2-J)\frac{h^2}{8\pi^2 I}$

$= (J+1)\frac{2h^2}{8\pi^2 I}$

$\Delta E$ = 1 unit, 2 units, 3 units $\Rightarrow$

Linearly spaced spectrum

w/ spacing that decreases as $I$ increases

$\Delta J = \pm 1$ $A_r$ are all equal

Level populations determine relative intensities

$$\nu = \frac{2B}{h}(J+1) \quad , \quad J = 0, 1, 2$$

CO: $J = 1-0$ $\quad 110,204.338\ MH_2$

$$B = \frac{\nu h}{2} = \frac{110,204.338 \times 10^6\ H_2\ (6.63 \times 10^{-27}\ erg \cdot s)}{2}$$

$$= 3.65 \times 10^{-16}\ erg$$

Level populations $N_J \propto (2J+1)\, e^{-E_J/kT}$

$$\frac{dN_J}{dT} = 0 \quad \Rightarrow \text{Maximum Population in Level}$$

$$J(\max N_J) = \left(\frac{kT}{2B}\right)^{1/2} - \frac{1}{2}$$

@ 1000K $\quad J = \left(\frac{1.38 \times 10^{-16}\ \frac{erg}{K}\ (10^3 K)}{2\ (3.65 \times 10^{-16} erg)}\right)^{1/2} - \frac{1}{2}$

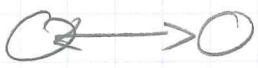
$J = 13$

@ 100K $\quad J = 4$

@ 10K $\quad J = 1$

# Vibrating Molecules

Harmonic motion of the two atoms



PE curve is parabolic $E = \frac{1}{2} k_2 (r - r_0)^2$

$k_2$ depends on bond strength

$\varepsilon_\nu = E_\nu = (\nu + \frac{1}{2})\,\omega$ , $\nu = 0, 1, 2$ ← units need hc?

Selection rule $\Delta\nu = \pm 1$ ⇒ simple spectrum with 1 line!

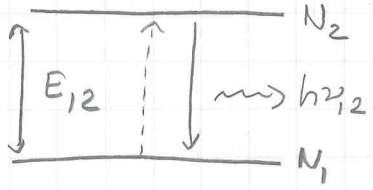
$$\Delta E = (\nu + 1 + \tfrac{1}{2})\omega - (\nu + \tfrac{1}{2})\omega$$

$$= \omega \ [cm^{-1}]$$

Can also have $\Delta\nu = \pm 2, \pm 3 \ldots$ but with decreasing P

## Oscillator Strength

Idealized two-level atom




$g$ = statistical weight
$J$ = total angular momentum quantum number

- Transition strength describes the probability that an excited atom will emit a photon in unit time

(1) $$N_2(t) = N_2(0)\, e^{-A_{21}t}$$

$A_{21}$ $\propto$ electric dipole matrix element $= e^2 |\langle \psi_1 | r | \psi_2 \rangle|^2$

i.e. The overlap of the wavefunctions

or the strength of the electric dipole during the transition

Line Emissivity [energy/volume] $= n_2 h\nu_{21} A_{21}$

- Atom in ground state has a probability

$$B_{12}\, U(\nu_{12})$$ Einstein coefficient for absorption

of absorbing a photon of frequency $\nu_{12}$.

- Einstein coefficient for stimulated emission

$$B_{21}\, g_2 = g_1 B_{12}$$

- Absorption oscillator strength, $f_{12}$, treats the transition as if it were a bound harmonic oscillator.

Picture a classical electron oscillating between the two levels.

$f_{12}$ is the effective number of classical oscillators involved in the transition. It can be calculated quantum mechanically.

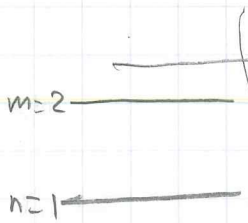
strongest transitions have $f \sim 1$.

$$g_1 f_{12} = g_2 f_{21}$$

Transition probability

$$A_{12} = \frac{8\pi^2 e^2}{m_e c^3} \nu_{12}^2 f_{12}$$

The sum of the $f$ values for all the transitions in the atom cannot exceed the number of optically active e's.




$$P_{21} = A_{21} + B_{21} U_\nu$$

↑ spontaneous emission ↑ induced emission

$$U = \frac{4\pi}{c} B$$

$$\frac{\text{energy}}{\text{area} \cdot \text{time}} \cdot \frac{s}{cm} = \frac{\text{energy}}{\text{volume}}$$

$$P_{12} = B_{12} U_\nu$$

↑ absorption

the Einstein coeff's are properties of the atom.

steady state # transitions up = # transitions down

In LTE $g_1 e^{-E_n/kT} B_{nm_{12}} U_\nu = g_2 e^{-E_m/kT} (A_{21} + B_{21} U)$

↑ level population

and $U_\nu = \frac{4\pi}{c} B_\nu$

$h\nu = E_2 - E_1$

$$\Rightarrow \boxed{A_{21} = \frac{8\pi h\nu^3}{c^3} B_{21}}$$

and $\boxed{g_2 B_{21} = g_1 B_{12}}$