

- Solution of the Schrödinger equation for the hydrogen atom leads to the same energy quantization as in the Bohr model, but with total angular momentum quantized according to

$$L = \hbar\sqrt{l(l+1)} \quad , \quad l = 0, 1, 2, 3, \dots \quad (9)$$

and the azimuthal component of L quantized according to $L_z = m_l\hbar$ for $m_l = 0, 1, \dots, 2l + 1$. There is a degeneracy of energy levels with l and m_l .

- Introducing an external magnetic field \mathbf{B} defines a preferred direction, breaking the isotropy symmetry and thereby splitting the energy degeneracy. The fine structure of lines is described by the splitting

$$\Delta E = \pm \frac{eB\hbar}{2\mu c} \quad , \quad (10)$$

which applies to the atomic electrons. This effect is called the **Zeeman effect** and is used to measure solar and stellar magnetic fields.

Plot: Zeeman Splitting of Atomic Lines

- Where does this energy splitting estimate come from? A semi-classical treatment suffices to answer this. Energy differences can be obtained by computing the work done by moving a charge a distance $\Delta\mathbf{r}$ under the Lorentz force:

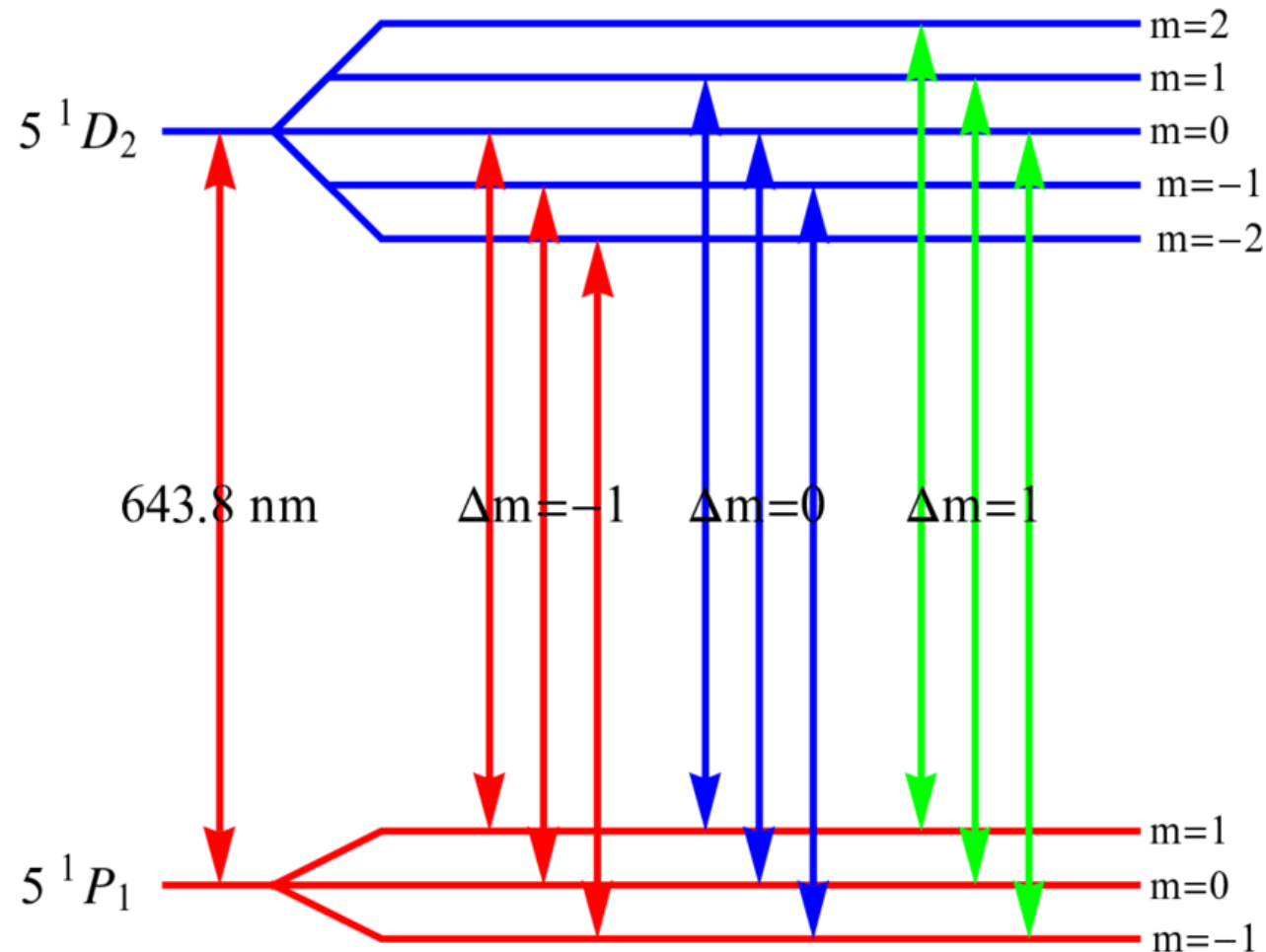
$$|\Delta E| = \Delta\mathbf{r} \cdot \frac{d\mathbf{p}}{dt} = \frac{e}{c} \Delta\mathbf{r} \cdot (\mathbf{v} \times \mathbf{B}) \rightarrow eB |\Delta\mathbf{r}| \frac{|\mathbf{v}|}{c} \quad . \quad (11)$$

The Bohr model of the atom can be used to estimate the kinetic energy of the electron through $\mu v^2/2 \approx |E_{\text{tot}}| = \mu e^4/(2\hbar^2)$. Thus, one estimates the orbital speed of a Schrödinger electron to be $v/c \sim e^2/(\sqrt{2}\hbar c) \approx 5.1 \times 10^{-3}$, which is *non-relativistic*. The displacement of a bound orbital electron is on the scale of the Bohr radius $a_0 = \hbar^2/(\mu e^2)$. Accordingly,

$$|\Delta E| \rightarrow eB |\Delta\mathbf{r}| \frac{|\mathbf{v}|}{c} \sim eB a_0 \frac{\alpha_f}{\sqrt{2}} = \frac{eB\hbar}{\sqrt{2}\mu c} \quad . \quad (12)$$

This derivation clearly connects to the physical elements of the Bohr atomic model. Yet we note that a quick way to derive this estimate is just to multiply the cyclotron frequency $eB/\mu c$ by \hbar .

Zeeman Effect: Line Splitting by B



- Splitting of atomic lines by magnetic fields was first observed by **P. Zeeman** (1897) in Cadmium, shown here. *Credit: I. Suzuki*

6. STELLAR SPECTRA AND ATMOSPHERES

Matthew Baring – Lecture Notes for ASTR 350, Fall 2021

1 Spectral Classification

Spectral classification started as an organized taxonomy with the work at Harvard of Pickering — stars were labelled by letters according to the strength of their H absorption lines (AFGKM)

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- Annie Jump Cannon (1901) revised this classification by sequencing them according to temperature:

$$OBAFGKM \tag{1}$$

- * O stars: hot, blue, young and massive (labelled *early-type*)
- * M stars: cool, red, old and less massive (labelled *late-type*)

Subdivisions are numbered: e.g. $B1 \rightarrow B9$.

Temperature strongly influences the state of atoms, whether they are ionized or not, hence we expect a strong coupling between spectral type and line characteristics. States critically depend on species, so line spectra give powerful indicators of “real temperatures” as opposed to effective temperature.

- Ionization states are classified observationally via Roman numerals:
 - * H I = neutral hydrogen; H II = ionized hydrogen
 - * He I = neutral helium; He II = singly-ionized helium; He III = doubly-ionized helium. e.g. Si IV, OVII, MgII

2 Atom Excitation: the Boltzmann Equation

Spectral classification depends on (i) in what orbitals are electrons most likely to reside? and (ii) what are the relative states of ionization?

- Answers are governed by statistical mechanics of thermal gases, which indicate that the velocity distribution of a gas of non-relativistic particles of mass m at temperature T is given by

$$n_v dv = 4\pi n \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left\{ -\frac{mv^2}{2kT} \right\} v^2 dv \quad , \quad (2)$$

where k is Boltzmann's constant. This is the famous **Maxwell-Boltzmann** distribution of statistical/thermal physics.

Plot: Maxwell-Boltzmann Distribution

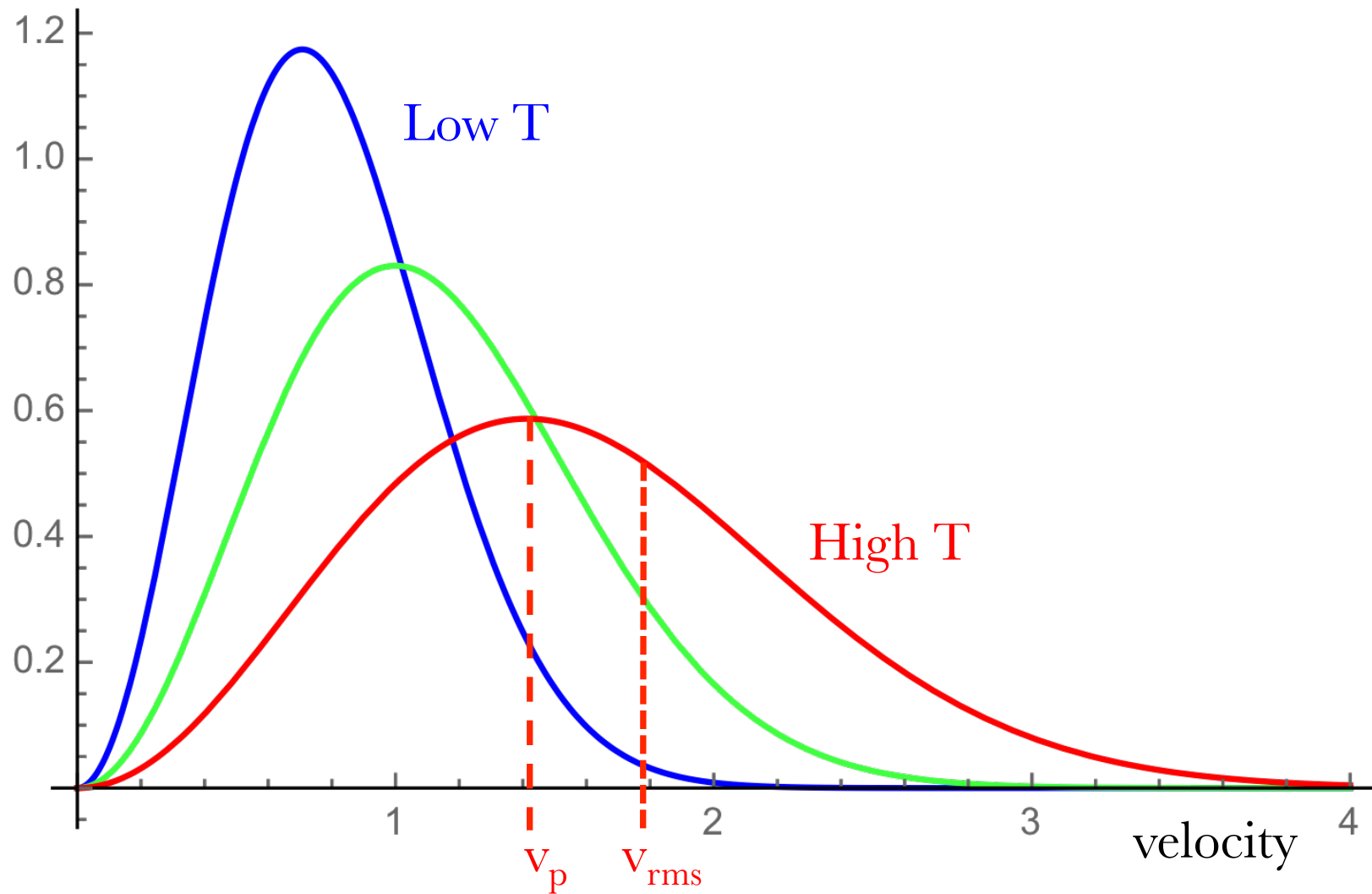
The peak velocity is $v_{\text{peak}} = \sqrt{2kT/m}$ and the rms value is $v_{\text{rms}} = \sqrt{3kT/m}$.

$$v_{\text{rms}}^2 = \langle v^2 \rangle = \int_0^\infty v^2 n_v dv \Big/ \int_0^\infty n_v dv = \frac{3kT}{m} \quad . \quad (3)$$

It then follows that the mean kinetic energy is $\langle K \rangle = mv_{\text{rms}}^2/2 = 3kT/2$, which is the ideal gas equation of state.

- Thermonuclear reaction rates in stellar interiors critically depend on such distributions, in detailed balance similar to the atomic considerations below.
- In the atomic context, v represents atom speeds in a hot or cool gas, which then impacts the distribution of electrons in atomic states via a collisional excitation/de-excitation. In this way, the exponential in the M-B distribution maps over to an $\exp(-E/kT)$ factor that can apply to both the atom kinetic energies and also the orbital excitation energies.

Maxwell-Boltzmann Distributions



Let E_a and E_b be two energy levels of an atom, each with g_a and g_b degenerate sub-states; i.e. $g_{a,b} \geq 1$. If $P(E_a)$ and $P(E_b)$ are the probabilities of finding e^- in these respective energy levels, then statistical mechanics yields

$$\boxed{\frac{N_b}{N_a} \equiv \frac{P(E_b)}{P(E_a)} = \frac{g_b}{g_a} \exp\left\{-\frac{E_b - E_a}{kT}\right\}} \quad (4)$$

This is called the **Boltzmann equation**. The factor $e^{-E/kT}$ is called the **Boltzmann factor**. Note that $g_{a,b} \neq 1$ arises through spin and L and L_z degeneracies in the solution of the Schrödinger equation.

Ground States s_1				Energy E_1
n	ℓ	m_ℓ	m_s	(eV)
1	0	0	+1/2	-13.6
1	0	0	-1/2	-13.6
First Excited States s_2				Energy E_2
n	ℓ	m_ℓ	m_s	(eV)
2	0	0	+1/2	-3.40
2	0	0	-1/2	-3.40
2	1	1	+1/2	-3.40
2	1	1	-1/2	-3.40
2	1	0	+1/2	-3.40
2	1	0	-1/2	-3.40
2	1	-1	+1/2	-3.40
2	1	-1	-1/2	-3.40

Quantum Number Degeneracies for Hydrogen

- e.g. Consider the hydrogen atom and excitations from the ground state $n = 1$, with $g_1 = 2(1)^2 = 2$ to the first excited state $n = 2$ with $g_2 = 2(2)^2 = 8$. Here $E_1 = -13.6\text{ eV}$ and $E_2 = -13.6\text{ eV}/4 = -3.4\text{ eV}$.

At what temperature does $N_2 = N_1$?

$$1 = \frac{N_2}{N_1} = \frac{8}{2} \exp\left\{-\frac{(-3.4\text{ eV}) - (-13.6\text{ eV})}{kT}\right\} \quad , \quad (5)$$

yielding $T = 8.54 \times 10^4\text{ K}$. This is clearly hotter than effective temperature of sunlight, implying that most hydrogen atoms at the solar surface are in the ground state.

* Yet hydrogen Balmer lines achieve maximum intensity at much lower temperatures, around 10^4 K . Something else must be in play!

Plot: Boltzmann Equation for Hydrogen

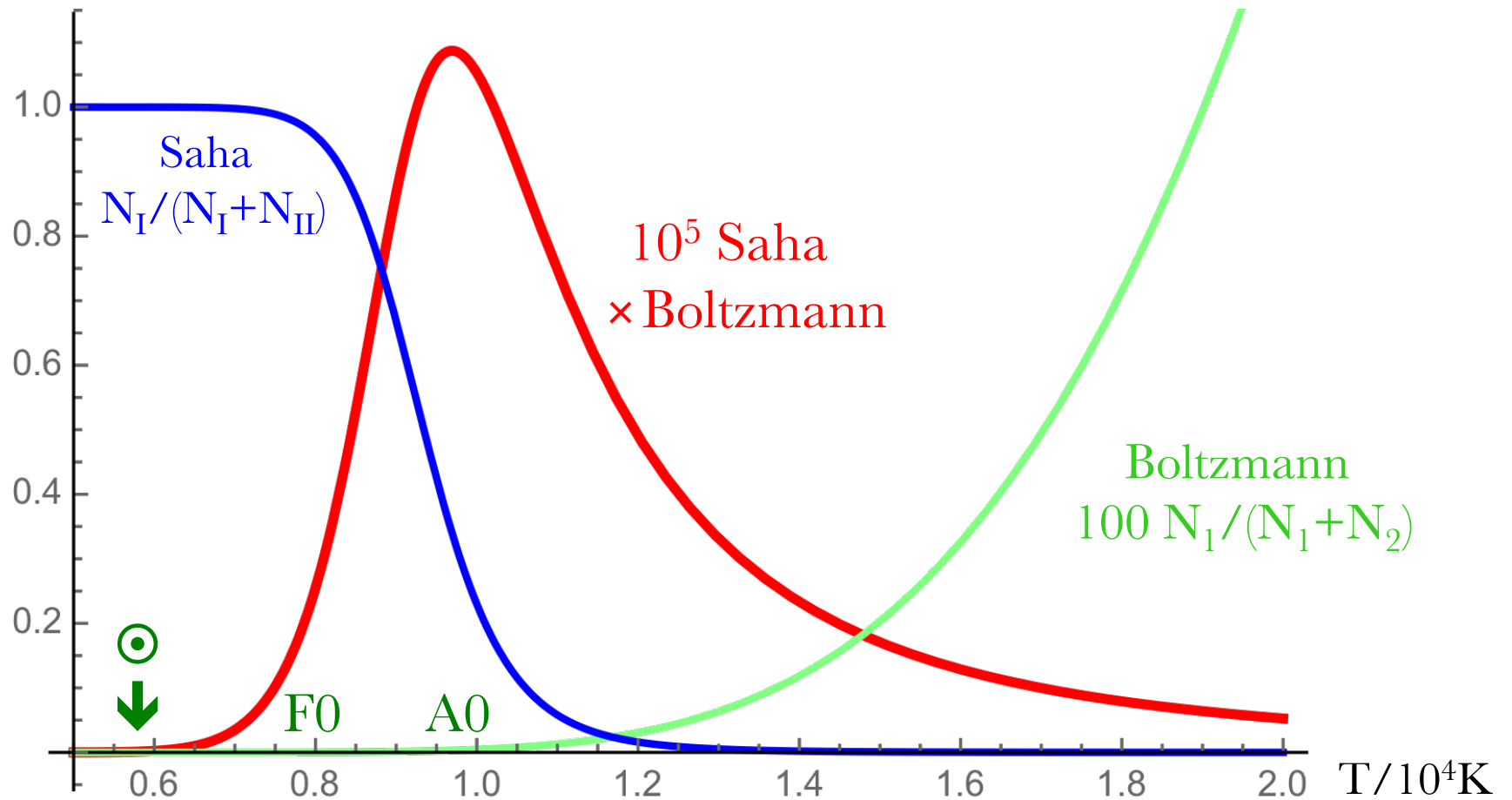
- Now consider singly-ionized helium, which will require a significant temperature to realize such a state. The Schrödinger equation applies to it, and the solution scales like the hydrogen atom. Yet, now the nuclear charge is Ze for $Z = 2$, and $\mu \approx m_e$. The Bohr model tells us that $E_1 = -54.4\text{ eV}$ and $E_2 = -54.4\text{ eV}/4 = -13.6\text{ eV}$.

At what temperature does $N_2 = N_1$ now?

$$1 = \frac{N_2}{N_1} = \frac{8}{2} \exp\left\{-\frac{(-13.6\text{ eV}) - (-54.4\text{ eV})}{kT}\right\} \quad , \quad (6)$$

yielding $T = 3.4 \times 10^5\text{ K}$, i.e. 4 times larger than for the hydrogen example. This case pertains to white dwarf stars, and again is much hotter than their typical surface temperatures.

Boltzmann and Saha Equations



- Boltzmann excitation (green, 1-2) and Saha (neutral fraction, blue, I-II) ionization solutions for **hydrogen** for temperatures T in units of 10^4K . Here $n_e = 10^{14}\text{cm}^{-3}$.
- Combined (red) illustrates peak Balmer H_α line signal at $T \sim 10^4\text{K}$.

3 Ionization and the Saha Equation

Ionization balance also critically affects the strengths of atomic de-excitation lines, constraining the number of states available for de-excitation. Such ionization balance also depends strongly on Boltzmann factors.

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Let χ_i be the ionization energy for transitioning from ionization state i to state $i + 1$. Thus, for $HI \rightarrow HII$, $\chi_I = 13.6 \text{ eV}$.

- We define the **partition function** Z_i to be the weighted sum of the number of ways an atom or ion ionization state i can arrange its electrons among excitation states. Boltzmann statistics then gives

$$Z_i = g_1 + \sum_{j=2}^{\infty} g_j e^{-(E_{i,j} - E_{i,1})/kT} \quad (7)$$

for the g_i being the degeneracy factors ($g_1 = 2$, $g_2 = 8$, etc.; $g_n = 2n^2$).

- The ratio of the number N_{i+1} of atoms in ionization state $i + 1$ to the number N_i in state i is given by detailed balance and is

$$\boxed{\frac{N_{i+1}}{N_i} = \frac{2Z_{i+1}}{n_e Z_i} \left(\frac{m_e kT}{2\pi\hbar^2} \right)^{3/2} e^{-\chi_i/kT} .} \quad (8)$$

This is the **Saha Equation**, derived in 1920. The factor of 2 accommodates the two spin states of free electrons, and represents their partition function (i.e. no bound states).