

Ionization

$$\frac{n_s}{n_0} = \frac{g_s}{g_0} e^{-\psi_s/kT}, \quad \dots \text{ Boltzmann formula}$$

which describes the distribution of particles over states of different energy.

With the **total number of atoms** $n = \sum_s n_s$ the Boltzmann formula becomes, after summation of all energy (excitation) $_s$ States

$$g_0 \frac{n}{n_0} = g_0 \sum_{s=0}^{\infty} \frac{n_s}{n_0} = g_0 + g_1 e^{-\psi_1/kT} + g_2 e^{-\psi_2/kT} + \dots := u_p,$$

where $u_p = u_p(T)$ is the so-called partition function.

Boltzmann's formula can than be rewritten as

$$\frac{n_s}{n} = \frac{g_s}{u_p} e^{-\psi_s/kT}.$$

We have to distinguish between **excited states** s (bound electrons distributed over discrete states) and **ionization** (free electrons with a continuous manifold of states).

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- We have to distinguish between **excited states** s (bound electrons distributed over discrete states) and **ionization** (free electrons with a continuous manifold of states).

- ions (atoms) that already lost **electrons** are said to be in the r^{th} ionization state.

- the **energy necessary** to remove the next electron (e^-) from the **ground state** is then χ_r .

- the free e^- will have a kinetic energy $p_e^2/(2m_e)$ relative to the atom, so its total energy relative to its bound state is therefore $\chi_r + p_e^2/(2m_e)$, where p_e is (free) electron's momentum relative to the **ion**, which is now in the **ionization state** $r+1$.

- consider the **lower states** as an r -times **ionized** ion in the **ground state**, and the **upper state** be that of the $(r+1)$ -times ion plus free e^- with p_e in $[p_e, p_e + dp_e]$.

- with number densities n_r and dn_{r+1} of the two states and with the statistical weight for the **upper state** being the product of g_{r+1} of the ion and $dg(p_e)$ of the free e^- , we have in TDE

$$\frac{dn_{r+1}}{n_r} = \frac{g_{r+1} dg(p_e)}{g_r} \exp\left(-\frac{\chi_r + p_e^2/(2m_e)}{kT}\right).$$

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- **What is the statistical weight** $dg(p_e)$ in the momentum interval $[p_e, p_e + dp_e]$?

Pauli principle: (6-dim.) phase space of volume $dq_1 dq_2 dq_3 dp_1 dp_2 dp_3 = dV d^3 p$ can only contain up to $2dV d^3 p/h^3$ electrons, i.e. up to 2 e^- /quantum cell of volume h^3 .
 $\rightarrow dg(p_e) = \frac{2dV d^3 p_e}{h^3}$.

- the volume available per e^- is $dV = 1/n_e$, while the volume available in the momentum interval $[p_e, p_e + dp_e]$ is $d^3 p_e = 4\pi p_e^2 dp_e$, since all these points are on a spherical shell with radius p_e and thickness dp_e

$$\rightarrow dg(p_e) = \frac{8\pi p_e^2 dp_e}{n_e h^3} \quad \text{and} \quad \frac{dn_{r+1}}{n_r} = \frac{g_{r+1}}{g_r} \frac{8\pi p_e^2 dp_e}{n_e h^3} \exp\left(-\frac{\chi_r + p_e^2/(2m_e)}{kT}\right).$$

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$$dg(p_e) = \frac{8\pi p_e^2 dp_e}{n_e h^3} \quad \text{and} \quad \frac{dn_{r+1}}{n_r} = \frac{g_{r+1}}{g_r} \frac{8\pi p_e^2 dp_e}{n_e h^3} \exp\left(-\frac{\chi_r + p_e^2/(2m_e)}{kT}\right).$$

All upper states (ions of ionization degree $r+1$ in the **ground state** and free e^- of all momenta) are than obtained from integrating over p_e :

$$\frac{n_{r+1}}{n_r} = \frac{g_{r+1}}{g_r} \frac{8\pi}{n_e h^3} e^{-\chi_r/kT} \int_0^{\infty} p_e^2 \exp\left(-\frac{p_e^2}{2m_e kT}\right) dp_e.$$

With $\int_0^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{4a^3}$ for $a > 0$ we obtain

$$\frac{n_{r+1}}{n_r} n_e = \frac{g_{r+1}}{g_r} f_r(T), \quad \text{where } f_r(T) = \frac{2(2\pi m_e kT)^{3/2}}{h^3} e^{-\chi_r/kT}.$$

Saha equation (Meghnad Saha, 1920) [only for the **ground state**].

Ionization

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Saha equation (Meghnad Saha, 1920) (only for the ground state).

In order to be more precise, i.e. indicating only the ground state $s=0$, we use the quantities

$$n_{r+1,0}, n_r, g_{r+1,0}, g_r,$$

where the second subscript indicates the ground state for which these quantities are defined.

all states of excitation @ r+1 ionization

$$n_{r+1}, n_r, g_{r+1}, g_r$$

By the notation n_{r+1} we mean **from now on** the number densities of ions and statistical weights of **all states of excitation**, where as

A particular state of excitation is indicated by a second subscript such that
 $n_{r,k}$ is the number density of atoms in the stage i of ionization and in state k of excitation,
and $g_{i,k}$ is the corresponding statistical weight.

$$\begin{array}{c} \text{state of ionization} \\ \downarrow \\ n_{i,k} \end{array} \quad \begin{array}{c} \text{state of excitation} \\ \nearrow \end{array}$$

The **Saha equation** (for the ground state only) is then written more precisely as

$$\frac{n_{r+1,0}}{n_{r,0}} n_e = \frac{g_{r+1,0}}{g_{r,0}} f_r(T), \quad \text{where } f_r(T) = \frac{(2\pi m_e k T)^{3/2}}{h^3} e^{-\chi_r/kT}.$$

The number density of ions in the ionization state r (and in all excitation states s) is

$$n_r = \sum_s n_{r,s},$$

and, as before with the definition for all ions n , the **Boltzmann formula for ions of state r** becomes

$$\frac{n_{r,s}}{n_{r,0}} = \frac{g_{r,s}}{g_{r,0}} e^{-\psi_{r,s}/kT},$$

where $\psi_{r,s}$ is the **excitation energy of (one single) state s of ions in ionization state r** .

Ionization

Ionization of Hydrogen

$$\text{Def.: degree of ionization: } \frac{x}{n_0 + n_1}, \quad \begin{array}{c} \nearrow \text{number of ionized H atoms} \\ \downarrow \end{array} \quad [n_1/n_0 = x/(1-x)].$$

If the gas is neutral, then $x = 0$;
if it is completely ionized, $x = 1$.

With this definition, the l.h.s. of Saha equation can be replaced by

$$\frac{n_{r+1}}{n_r} P_e = \frac{x P_e}{1-x},$$

and if $n = n_0 + n_1$ is the total number of H atoms, we obtain for the partial pressure P_e of the e- to the **total gas pressure** P_{gas} :

$$P_e = n_e k T = (n + n_e) k T \frac{n_e}{n + n_e} = P_{\text{gas}} \frac{n_e}{n + n_e}.$$

Ionization

the **Boltzmann formula for ions of state r** becomes

$$\frac{n_{r,s}}{n_{r,0}} = \frac{g_{r,s}}{g_{r,0}} e^{-\psi_{r,s}/kT}, \quad \text{where } \psi_{r,s} \text{ is the excitation energy of (one single) state } s.$$

The number density of ions of ionization state r , $n_r = \sum_s n_{r,s}$, can then be written as

$$\begin{aligned} \frac{g_{r,0}}{n_{r,0}} n_r &= g_{r,0} \sum_s \frac{n_{r,s}}{n_{r,0}} \\ &= g_{r,0} + g_{r,1} e^{-\psi_{r,1}/kT} + g_{r,2} e^{-\psi_{r,2}/kT} + \dots := u_r, \end{aligned}$$

where $u_r = u_r(T)$ is the partition function for the ion in state r .

With $n_r g_{r,0} = n_{r,0} u_r$ the **Saha equation** eventually becomes for **all stages of excitation**

$$\frac{n_{r+1}}{n_r} n_e = \frac{u_{r+1}}{u_r} f_r(T), \quad f_r(T) = \frac{(2\pi m_e k T)^{3/2}}{h^3} e^{-\chi_r/kT}.$$

And finally with $P_e = n_e k T$

$$\frac{n_{r+1}}{n_r} P_e = \frac{u_{r+1}}{u_r} \frac{2(2\pi m_e)^{3/2}}{h^3} (k T)^{5/2} e^{-\chi_r/kT}.$$

Ionization

Ionization of Hydrogen

$$P_e = n_e kT = (n + n_e) kT \frac{n_e}{n + n_e} = P_{\text{gas}} \frac{n_e}{n + n_e}$$

For each ionized atom there is just one electron ($n_e = n_1$): therefore $x := \frac{n_e}{n}$ & number of ionized H atoms

$$P_e = \frac{x}{1+x} P_{\text{gas}}$$

and the **Saha equation** can be written in the form with $n_{r+1}/n_r = n_1/n_0 = x/(1-x)$

$$\frac{x^2}{1-x^2} = K_H, \quad \text{with} \quad K_H = \frac{u_1}{u_0} \frac{2}{P_{\text{gas}}} \frac{(2\pi m_e)^{3/2}}{h^3} (kT)^{5/2} e^{-\chi_H/kT},$$

where $\chi_H = 13.6$ eV is the ionization energy of hydrogen;

quadratic equation for x , which can be solved for given T and P_{gas} :

We still need, however, the **partition function** u .

Ionization

$$\frac{x^2}{1-x^2} = K_H, \quad \text{with} \quad K_H = \frac{u_1}{u_0} \frac{2}{P_{\text{gas}}} \frac{(2\pi m_e)^{3/2}}{h^3} (kT)^{5/2} e^{-\chi_H/kT}.$$

Partition function u :
statistical weights from quantum mechanics (e.g. Cox, 2000, pp. 2-34):

$$\begin{aligned} \text{ground state: } u_0 &\approx g_{0,0} = 2, \\ \text{ionized H : } u_1 &= 1 \end{aligned}$$

$$\text{Example: solar atmosphere : } \left. \begin{aligned} P_{\text{gas}} &= 1.01 \times 10^5 \text{ dyn cm}^2 \\ T &= 5779 \text{ K} \end{aligned} \right\} x = 5 \times 10^{-5},$$

$$\text{deeper layers : } \left. \begin{aligned} P_{\text{gas}} &= 3.35 \times 10^{12} \text{ dyn cm}^2 \\ T &= 7.17 \times 10^5 \text{ K} \end{aligned} \right\} \begin{aligned} x &= 0.985, \\ \text{H is nearly} \\ \text{completely} \\ \text{ionized.} \end{aligned}$$

Because K_H increases with T (decreases with P_{gas}) \rightarrow x increases with T
and l.h.s. increases with x :

Ionization

In order to determine mean mol weight μ for the H gas with ionization degree x , we define E as the **number of free electrons per atom** (neutral or ionized), which is here (for H) simply

$$E = \frac{n_e}{n} = x = \frac{\mu_0}{\mu_e} \rightarrow \frac{1}{1+E} = \frac{n}{n+n_e}.$$

$$\text{The density } \varrho = (n + n_e) \mu m_u = n \mu_0 m_u = n_e \mu_e m_u \rightarrow \mu = \frac{\rho}{m_u(n+n_e)}.$$

With the definition of E and $n = n_0 + n_1$ we obtain for the mean mol(lcular) weight

for a neutral gas ($E=0$)

$$\mu = \frac{\varrho}{m_u n} \frac{1}{1+E} = \frac{\mu_0}{1+E} = \mu_e \frac{E}{1+E},$$

where we have neither replaced μ_0 by its value 1 for hydrogen nor E by x , since above expression(s) also holds for a mixture of gases.

Ionization

Ionization

TD quantities for a pure hydrogen gas

$$\delta = -(\partial \ln \varrho / \partial \ln T)_P : \left. \begin{aligned} \text{for } x = 0 &\rightarrow \delta = 1 \\ x = 1 &\rightarrow \delta = 1 \end{aligned} \right\} \text{because } \mu = \text{constant in both cases.}$$

$$\text{for any } x \rightarrow \delta = 1 + \frac{1}{1+E} \left(\frac{\partial E}{\partial \ln T} \right)_P, \quad (\mu_0 = \text{constant})$$

which also holds for a mixture of gases.

For pure hydrogen $E = x$

$$\delta = 1 + \frac{1}{2} x (1-x) \left(\frac{5}{2} + \frac{\chi_H}{kT} \right), \quad [f(\beta) \propto (1-\beta)/\beta].$$

Note: for this last expression we needed the derivative of x : obtained from diff. Saha equ.

Ionization

TD quantities for a pure hydrogen gas

$$c_P := \left(\frac{dq}{dT} \right)_P = \left(\frac{\partial u}{\partial T} \right)_P + P \left(\frac{\partial v}{\partial T} \right)_P$$

ionization/
recombination
energy

Using $P = \Re \rho T / \mu$ provides $c_P = \left(\frac{\partial u}{\partial T} \right)_P + \frac{\Re}{\mu} \delta$,

for which we need the internal energy / unit mass $u = \frac{3}{2} \frac{\Re}{\mu_0} (1 + E) T + u_{\text{ion}}$,

kinetic energy of ions & e-

For pure hydrogen, $E = x$ and $u_{\text{ion}} = x \chi_H / (\mu_0 m_u) = x \chi_H / m_u$,

$\xrightarrow{x=1 \text{ for H}}$

$$c_P \frac{\mu_0}{\Re} = \frac{5}{2} (1 + x) + \frac{\phi_H^2}{G(x)}$$

with $\phi_H := \frac{5}{2} + \frac{\chi_H}{kT}$

and $G(x) := \frac{1}{x(1-x)} + \frac{1}{x(1-x)^2} = \frac{2}{x(1-x^2)}$.

Ionization

TD quantities for a pure hydrogen gas

$$\nabla_{\text{ad}} = \frac{P\delta}{T \alpha c_P} = \frac{2+x(1-x)\phi_H}{5+x(1-x)\phi_H^2}.$$

Ionization

Hydrogen-helium mixtures

- weight fractions X, Y
- six types of particles: neutral and ionized hydrogen; neutral, ionized, and double ionized helium; and electrons.
- three types of ionization energy: χ_H^0 for hydrogen ($\chi_H^0 = 13.598 \text{ eV}$), $\chi_{\text{He}}^0, \chi_{\text{He}}^1$ for neutral and single ionized helium ($\chi_{\text{He}}^0 = 24.587 \text{ eV}, \chi_{\text{He}}^1 = 54.418 \text{ eV}$).

By $x_{\text{H}}^0, x_{\text{H}}^1, x_{\text{He}}^0, x_{\text{He}}^1, x_{\text{He}}^2$ we define degrees of ionization, i.e. x_i^r gives the number of atoms of type i in ionization state r ($= r$ electrons lost) divided by the total number of atoms (irrespective of their state of ionization):

$x_{\text{H}}^0 = \frac{n_{\text{H}}^0}{n_{\text{H}}}$,	$x_{\text{H}}^1 = \frac{n_{\text{H}}^1}{n_{\text{H}}}$,	$x_{\text{He}}^0 = \frac{n_{\text{He}}^0}{n_{\text{He}}}$,
$x_{\text{He}}^1 = \frac{n_{\text{He}}^1}{n_{\text{He}}}$,	$x_{\text{He}}^2 = \frac{n_{\text{He}}^2}{n_{\text{He}}}$,	

contribute to u_{ion}

Contribution to internal energy / unit mass:

$$u_{\text{ion}} = \frac{1}{m_u} \left\{ X x_{\text{H}}^1 \chi_{\text{H}}^0 + \frac{1}{4} Y [x_{\text{He}}^1 \chi_{\text{He}}^0 + x_{\text{He}}^2 (\chi_{\text{He}}^0 + \chi_{\text{He}}^1)] \right\},$$

since $X/m_u, Y/(4m_u)$ are the numbers of hydrogen and helium atoms (neutral and ionized) per unit mass.

Ionization

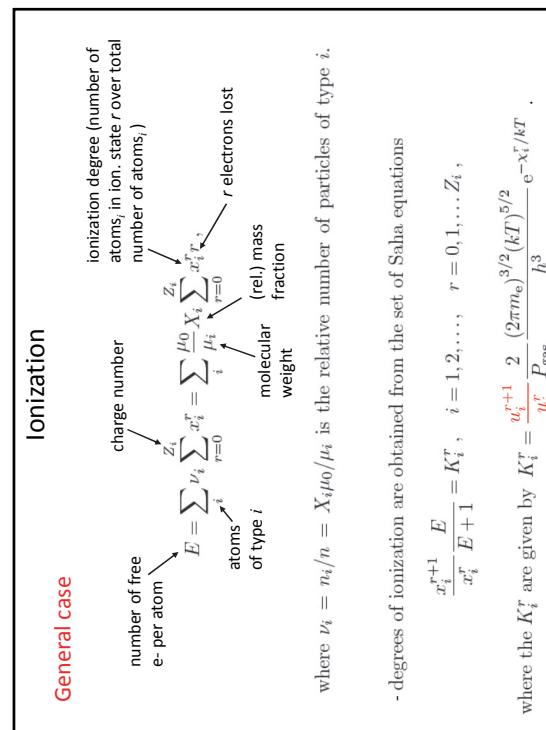
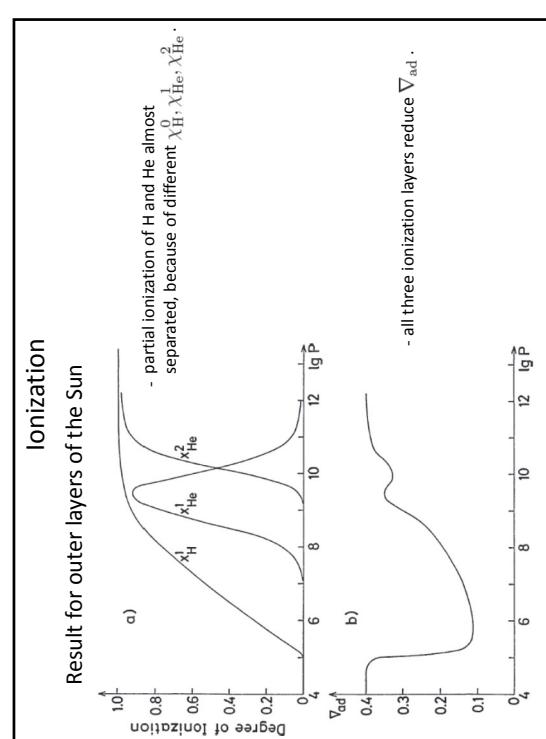
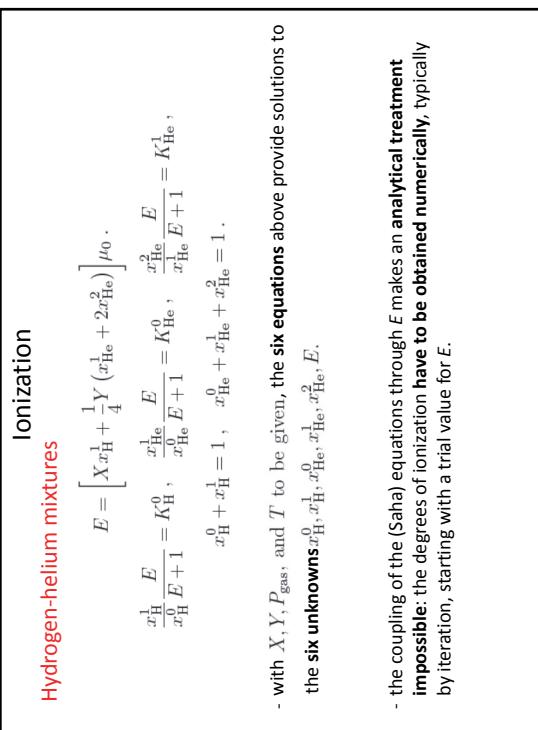
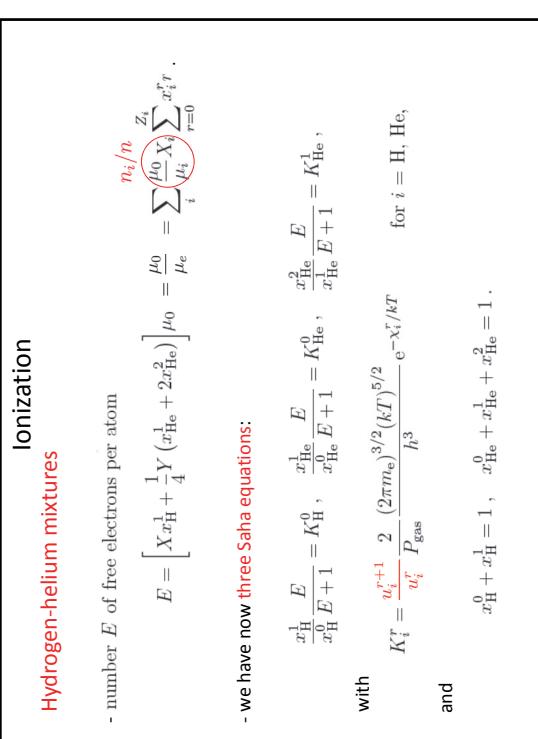
Hydrogen-helium mixtures

$$x_{\text{H}}^0 = \frac{n_{\text{H}}^0}{n_{\text{H}}}, \quad x_{\text{H}}^1 = \frac{n_{\text{H}}^1}{n_{\text{H}}}, \quad x_{\text{He}}^0 = \frac{n_{\text{He}}^0}{n_{\text{He}}},$$

$$x_{\text{He}}^1 = \frac{n_{\text{He}}^1}{n_{\text{He}}}, \quad x_{\text{He}}^2 = \frac{n_{\text{He}}^2}{n_{\text{He}}},$$

with $n_{\text{H}} = n_{\text{H}}^0 + n_{\text{H}}^1$,
 $n_{\text{He}} = n_{\text{He}}^0 + n_{\text{He}}^1 + n_{\text{He}}^2$,

and where the n_i^r are number densities of ions of type i in ionization state r .



Ionization

General case

$$E = \sum_i \nu_i \sum_{r=0}^{Z_i} x_i^r = \sum_i \frac{\mu_0}{\mu_i} X_i \sum_{r=0}^{Z_i} x_i^r,$$

where $\nu_i = n_i/n = X_i \mu_0 / \mu_i$ is the relative number of particles of type i .

In addition we have the relations

$$\sum_{r=0}^{Z_i} x_i^r = 1, \quad i = 1, 2, \dots,$$

which for a given type i of atoms, together with the Z Saha equations, in which E is replaced by the expression given above, represent Z+1 equations for the Z+1 degrees r of ionization, i.e. there are as many equations as variables; the equations can be solved iteratively to obtain the degrees of ionization and eventually the mean molecular weight $\mu = \mu_0/(1+E)$.

Ionization

General case

$$E = \sum_i \nu_i \sum_{r=0}^{Z_i} x_i^r = \sum_i \frac{\mu_0}{\mu_i} X_i \sum_{r=0}^{Z_i} x_i^r,$$

where $\nu_i = n_i/n = X_i \mu_0 / \mu_i$ is the relative number of particles of type i .

The kinetic part of the internal energy u is

$$u_{\text{kin}} = \frac{3 \mathfrak{R}}{2 \mu} T = \frac{3 \mathfrak{R}}{2 \mu_0} (1 + E)T,$$

while the ionization energy per mass unit is

$$u_{\text{ion}} = \sum_i \frac{X_i}{\mu_i m_u} \sum_{r=0}^{Z_i} x_i^r \sum_{s=0}^{r-1} \chi_i^s,$$

$$u_{\text{ion}} = \frac{1}{m_u} \left\{ X x_{\text{H}}^1 \chi_{\text{H}}^0 + \frac{1}{4} Y [x_{\text{He}}^1 \chi_{\text{He}}^0 + x_{\text{He}}^2 (\chi_{\text{He}}^0 + \chi_{\text{He}}^1)] \right\}.$$

Ionization

Limitation of the Saha formula

Let's consider pure H only.

Example: solar atmosphere :

$P_{\text{gas}} = 1.01 \times 10^5 \text{ dyn cm}^{-2}$	$T = 5779 \text{ K}$	$x = 5 \times 10^{-5},$
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deeper layers :

$P_{\text{gas}} = 3.35 \times 10^{12} \text{ dyn cm}^{-2}$	$T = 7.17 \times 10^5 \text{ K}$	$x = 0.985.$ H is nearly completely ionized.
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solar center :

$P_{\text{c}} \simeq P_{\text{gas}} \simeq 2.32 \times 10^{17} \text{ dyn cm}^{-2}$	$T_{\text{c}} \simeq 1.57 \times 10^7 \text{ K}$	$x \simeq 0.8.$ 20% of H would be neutral (this must be wrong!!)
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Ionization

Limitation of the Saha formula

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$x \simeq 0.8.$
20% of H would be neutral (this must be wrong!!)

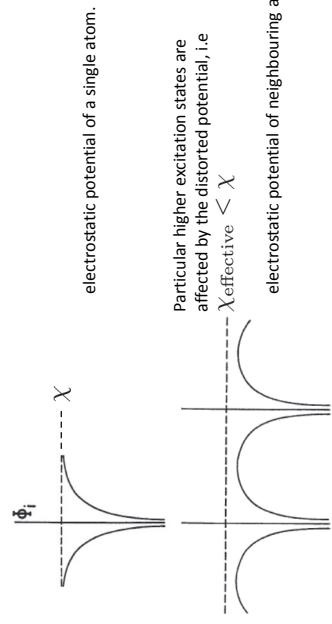
For $T >$, exponential ~ 1 and for $\nabla \equiv d \ln T / d \ln P_{\text{gas}} < 2/5$, x decreases inwards because of dominating increase of P_{gas} .

This is a result of the Saha equation of not knowing the size of the atoms!

Ionization

Limitation of the Saha formula

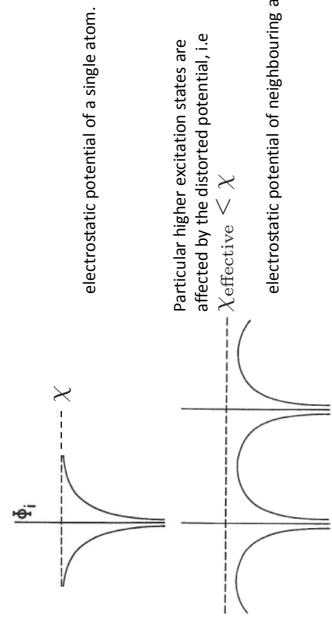
This is a result of the Saha equation of not knowing the **size of the atoms**!



Ionization

Limitation of the Saha formula

This is a result of the Saha equation of not knowing the **size of the atoms**!



Let's estimate the **mean distance d** between two atoms:

$$\frac{4d^3 \pi}{3} \simeq \frac{1}{n_{\text{H}}} \quad \rightarrow \text{number density of H atoms (cm}^{-3}\text{)}$$

We also know from quantum mechanics the orbital radius a of the (bound) electron:

$$a = a_0 \nu^2,$$

where $a_0 = 5.3 \times 10^{-9}$ cm is the Bohr radius, and ν the quantum number ($\nu = n$).

$$\text{Schr: } \varrho_c \approx 150 \text{ g/cm}^3,$$

$$n_{\text{H}} \approx \varrho_c / m_{\text{H}} \approx 10^{26} \text{ cm}^{-3}$$

$$\rightarrow \nu^2 < 0.13, \text{ i.e. even the ground state of H does not exist. Therefore}$$

\rightarrow all H atoms will be ionized:

$$\text{Saha equation valid for } d > 10a_0 \rightarrow \varrho = \mu_0 n_{\text{H}} n_{\text{ion}} < \frac{3\mu_0 \nu^2 n_{\text{H}}}{4\pi (10a_0)^3} = 2.66 \times 10^{-3} \mu_0 \text{ g cm}^{-3}.$$