

TALENT Summer School

Appendix on Statistical Mechanics

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Statistical Mechanics for Nuclear & Particle Astrophysics

Based on Fuller ECT*/Trento 2011 and NNPS 2012 lectures

references: Landau & Lifschitz *Statistical Mechanics*;
D. Goodstein's book *States of Matter* ;
S. Chandrasekar's book *Stellar Structure*

Thermodynamic and Notation Preliminaries

(1) non-relativistic (non-covariant) thermodynamics . . .

First Law – energy conservation $dE = TdS - PdV + \sum_i \mu_i dN_i$

$$dQ = TdS + \sum_i \mu_i dN_i$$

Second Law -- $dS \geq dQ/T$ ($dS = dQ/T$ if always in equilibrium)

Third Law – entropy zero when temperature is zero (system in ground state)

When possible refer all extensive quantities to quantities *per baryon*
e.g., heat flow per baryon dq , entropy per baryon s , and abundance . . .

abundance relative to baryons $Y_i \equiv \frac{n_i}{n_b}$

volume per baryon $1/n_b$

$$d\left(\frac{E}{n_b}\right) = Tds - Pd\left(\frac{1}{n_b}\right) + \sum_i \mu_i dY_i$$

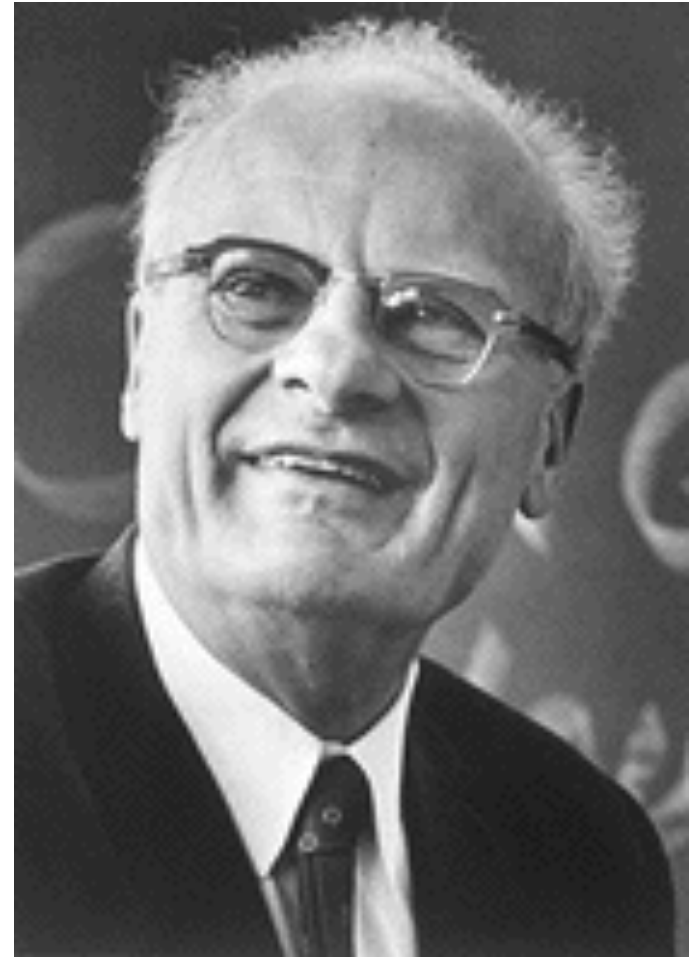
Thermal Equilibrium: *Temperature the same everywhere*

Chemical Equilibrium: $\sum_i \mu_i dY_i = 0$ *(the Saha equation)*

The man who discovered how stars shine made many other fundamental contributions in particle, nuclear, and condensed matter physics, as well as astrophysics.

In particular, Hans Bethe completely changed the way astrophysicists think about equation of state and nucleosynthesis issues with his 1979 insight on the role of entropy.

[Bethe, Brown, Applegate, & Lattimer \(1979\)](#)



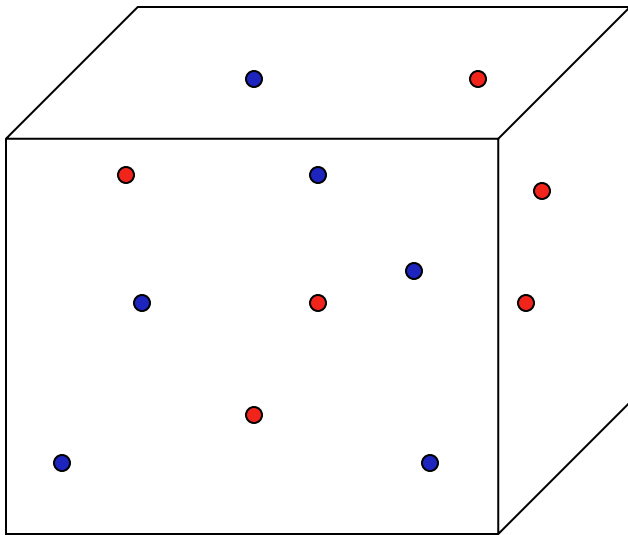
Hans Bethe

Entropy

$$S = k \log \Gamma$$

a measure of a system's **disorder/order**

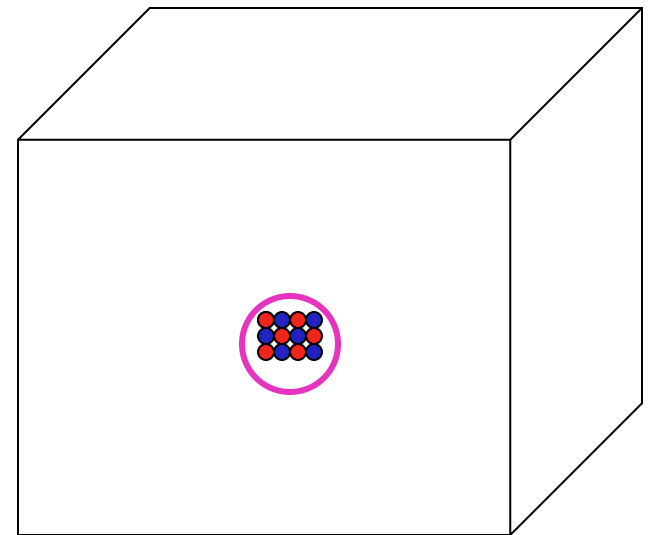
High Entropy



12 free nucleons



Low Entropy



^{12}C nucleus

Entropy

entropy per baryon (in units of Boltzmann's constant k)
of the air in this room $s/k \sim 10$

entropy per baryon (in units of Boltzmann's constant k)
characteristic of the sun $s/k \sim 10$

entropy per baryon (in units of Boltzmann's constant k)
for a 10^6 solar mass star $s/k \sim 1000$

entropy per baryon (in units of Boltzmann's constant k)
of the universe $s/k \sim 10^{10}$

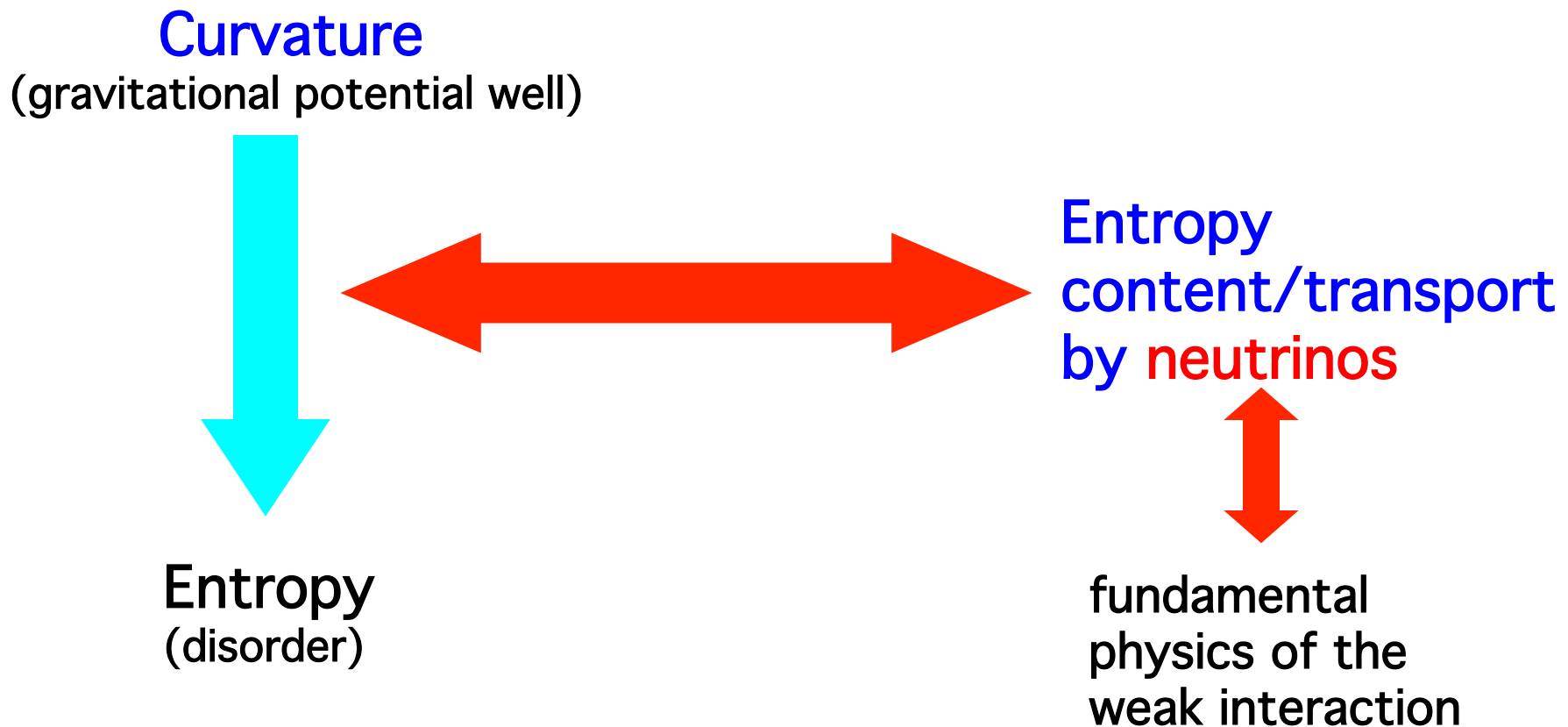
total entropy of a black hole of mass M

$$S/k = 4\pi \left(\frac{M}{m_{\text{pl}}} \right)^2 \approx 10^{77} \left(\frac{M}{M_{\text{sun}}} \right)^2$$

where the gravitational constant is $G = \frac{1}{m_{\text{pl}}^2}$

and the Planck mass is $m_{\text{pl}} \approx 1.221 \times 10^{22}$ MeV

There is a deep connection between
spacetime curvature and entropy



Statistical Mechanics

Follow Hans Bethe and *think entropy* $S(E, V, N) = k_B \log \Gamma$

$$E(S, V, N) = TS - PV + \mu N \qquad dE = TdS - PdV + \mu dN$$

think physically about
what these mean:

$$P = - \left. \frac{\partial E}{\partial V} \right|_{S, N} \qquad \mu = \left. \frac{\partial E}{\partial N} \right|_{S, V}$$

Define energy function with more “convenient” proper variables,
e.g., free energy-like combinations of variables. My favorite:

Thermodynamic Potential $\Omega(T, V, \mu) = E - TS - \mu N = -PV$

$$d\Omega = -SdT - PdV - Nd\mu$$

$$S = - \left. \frac{\partial \Omega}{\partial T} \right|_{V, \mu} \qquad P = - \left. \frac{\partial \Omega}{\partial V} \right|_{T, \mu} \qquad N = - \left. \frac{\partial \Omega}{\partial \mu} \right|_{T, V}$$

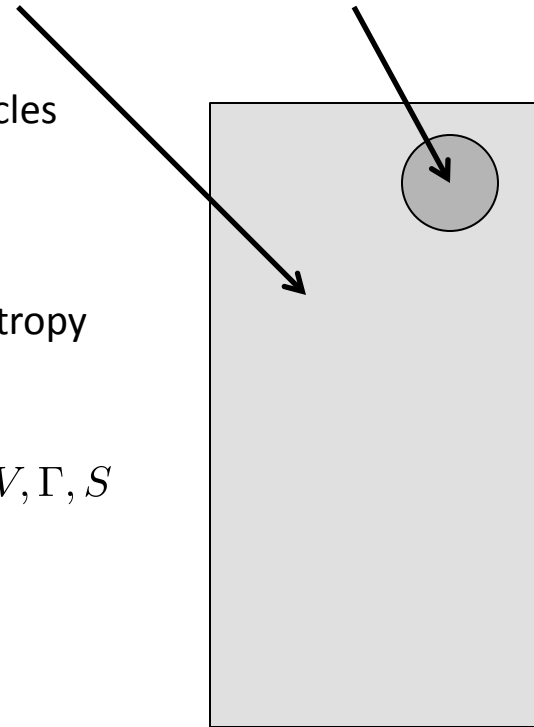
Micro Canonical Ensemble – counting states!

Consider a *system* consisting of a *medium* and a *subsystem*.

For *system* as a whole energy, volume and number of particles are fixed at E_0, V_0, N_0

medium has energy, number of particles, volume, number of quantum many-body states (number of choices), and entropy E', N', V', Γ', S'

While the *subsystem* has corresponding quantities E, N, V, Γ, S



subsystem+*medium*=*system*

Note that here we will fix the volumes, so we can define *system*, *subsystem*, and *medium*, and fix the temperature and chemical potentials common to all: V', V, V_0 are fixed; E_0, N_0 are fixed; T, μ are fixed

Entropy – counting many-body quantum states

Consider a *system* consisting of a *medium* and a *subsystem*.

Γ_0 possible many-body states in equilibrium for whole *system*

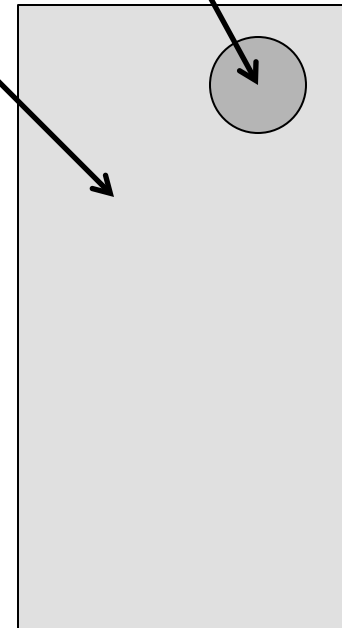
$S_0 = k_b \log \Gamma_0$ and probability of *system* as a whole being in any one state is $W_{\text{eq}} = \frac{1}{\Gamma_0}$

Note that all the *medium* (primed) quantities depend on the particular quantum state of the *subsystem*, α

If the *medium* has Γ' choices, *subsystem* Γ choices, then total number of choices is

$$\Gamma_{\text{tot}} = \Gamma' \cdot \Gamma \Rightarrow S_{\text{tot}} = S' + S$$

in equilibrium, $\Gamma_{\text{tot}} = \Gamma_0$ and $S_{\text{tot}} = S_0$



Entropy – counting many-body quantum states

Consider a *system* consisting of a *medium* and a *subsystem*.

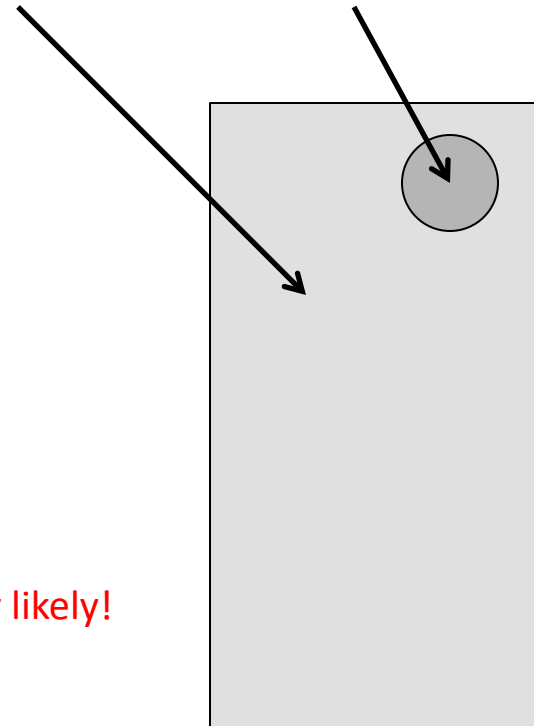
If we specify that the *subsystem* is in **one** particular quantum many-body state, α

$$\Rightarrow \Gamma'_\alpha = \text{\# of choices left to the } \textit{medium}$$

$$\Rightarrow \Gamma_{\text{tot } \alpha} = 1 \cdot \Gamma'_\alpha$$

So the probability in equilibrium that the subsystem is in a particular quantum many-body state α is

$$W_\alpha = \frac{\Gamma'_\alpha}{\Gamma_0} \quad \text{True since choices (states) are all equally likely!}$$



If f is an operator corresponding to some physical observable, then the expectation value of this in many-body state α is

$$f_\alpha \equiv \langle \Psi_\alpha | f | \Psi_\alpha \rangle$$

Average value of f in subsystem is then $\bar{f} = \sum_{\alpha} W_\alpha f_\alpha$

Entropy – counting many-body quantum states

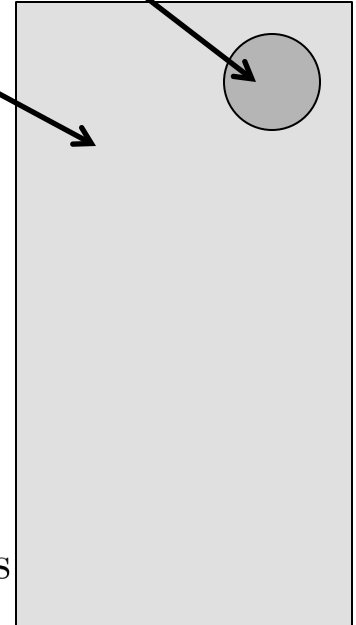
Consider a *system* consisting of a *medium* and a *subsystem*.

when *subsystem* is in state α ,
the *medium* has entropy $S'_\alpha = k_b \log \Gamma'_\alpha$

$$S_0 - S'_\alpha = k_b \log \Gamma_0 - k_b \log \Gamma'_\alpha = k_b \log \frac{\Gamma_0}{\Gamma'_\alpha} = -k_b \log W_\alpha$$

$$\Rightarrow W_\alpha = \exp\left(\frac{S'_\alpha - S_0}{k_b}\right) = A \exp\left(\frac{S'_\alpha}{k_b}\right)$$

where $A = \exp\left(-\frac{S_0}{k_b}\right)$ is a number fixed by the boundary conditions



$$S'_\alpha = S'(E_0 - E_\alpha, N_0 - N_\alpha) \approx S'(E_0, N_0) - E_\alpha \left. \frac{\partial S'}{\partial E'} \right|_{N'} - N_\alpha \left. \frac{\partial S'}{\partial N'} \right|_{E'}$$

$$\text{from } dE' = TdS' - P'dV' + \mu dN' = TdS' + \mu dN' \Rightarrow \left. \frac{\partial S'}{\partial E'} \right|_{N'} = \frac{1}{T} \text{ and } \left. \frac{\partial S'}{\partial N'} \right|_{E'} = -\frac{\mu}{T}$$

$$\Rightarrow S'_\alpha = S'(E_0, N_0) - \frac{E_\alpha}{T} + \frac{\mu N_\alpha}{T} = S'(E_0, N_0) - \left(\frac{E_\alpha - \mu N_\alpha}{T}\right)$$

Entropy – counting many-body quantum states

Consider a *system* consisting of a *medium* and a *subsystem*.

We got that when *subsystem* is in state α , the *medium* will have entropy

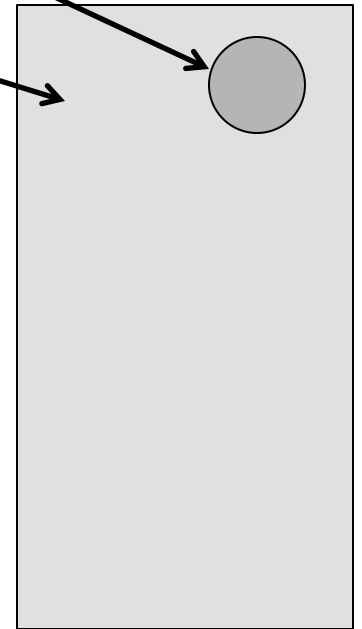
$$\Rightarrow S'_\alpha = S'(E_0, N_0) - \frac{E_\alpha}{T} + \frac{\mu N_\alpha}{T} = S'(E_0, N_0) - \left(\frac{E_\alpha - \mu N_\alpha}{T} \right)$$

some fixed number

$$W_\alpha = A \exp\left(\frac{S'_\alpha}{k_b}\right) = A \exp\left(\frac{S'(E_0, N_0)}{k_b} - \frac{E_\alpha}{k_b T} + \frac{\mu N_\alpha}{k_b T}\right) = B \exp\left[-\left(\frac{E_\alpha - \mu N_\alpha}{k_b T}\right)\right]$$

$$B = A \exp(S'(E_0, N_0)/k_b) = \exp[(S'(E_0, N_0) - S_0)/k_b] = \text{fixed}$$

$$\sum_\alpha W_\alpha = 1 \Rightarrow B = \frac{1}{\sum_\alpha \exp\left[-\left(\frac{E_\alpha - \mu N_\alpha}{k_b T}\right)\right]}$$



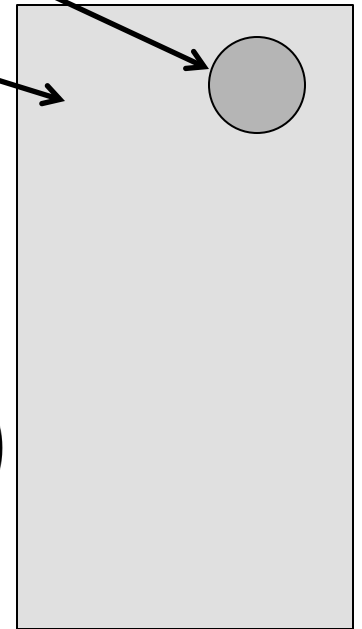
Now calculate average entropy of subsystem $S = \langle S_0 - S'_\alpha \rangle = \sum_\alpha W_\alpha (-k_b \log W_\alpha)$

since we showed that $S_0 - S'_\alpha = -k_b \log W_\alpha$

Entropy – counting many-body quantum states

Consider a *system* consisting of a *medium* and a *subsystem*.

So we calculate the average entropy of the *subsystem* in equilibrium



$$S = \langle S_0 - S'_\alpha \rangle = \sum_{\alpha} W_{\alpha} (-k_b \log W_{\alpha})$$

$$W_{\alpha} = A \exp\left(\frac{S'_\alpha}{k_b}\right) = A \exp\left(\frac{S'(E_0, N_0)}{k_b} - \frac{E_{\alpha}}{k_b T} + \frac{\mu N_{\alpha}}{k_b T}\right) = B \exp\left[-\left(\frac{E_{\alpha} - \mu N_{\alpha}}{k_b T}\right)\right]$$

$$S = \sum_{\alpha} W_{\alpha} \left(-k_b \log \left[B \exp\left(-\frac{E_{\alpha} - \mu N_{\alpha}}{k_b T}\right)\right]\right) = \sum_{\alpha} W_{\alpha} \left(-k_b \log B + \frac{E_{\alpha} - \mu N_{\alpha}}{T}\right)$$

$$\text{since } N = \sum_{\alpha} W_{\alpha} N_{\alpha}, \text{ etc., } \Rightarrow S = -k_b \log B + \frac{E - \mu N}{T}$$

$$\text{or } TS = -k_b T \log B + E - \mu N \quad \text{or} \quad E - TS - \mu N = \Omega = +k_b T \log B$$

$$\sum_{\alpha} W_{\alpha} = 1 \Rightarrow B = \frac{1}{\sum_{\alpha} \exp\left[-\left(\frac{E_{\alpha} - \mu N_{\alpha}}{k_b T}\right)\right]} \Rightarrow \Omega = E - TS - \mu N = -PV = -k_B T \log Z$$

$$\text{where the (grand) partition function is } Z = \sum_{\alpha} \exp\left[-\frac{(E_{\alpha} - \mu N_{\alpha})}{k_b T}\right]$$

Partition Functions

(grand) partition function is
$$Z = \sum_{\alpha} \exp \left[- \frac{(E_{\alpha} - \mu N_{\alpha})}{k_b T} \right] = \sum_{\alpha} \langle \Psi_{\alpha} | \exp \left[- \frac{(\hat{H} - \mu \hat{N})}{k_b T} \right] | \Psi_{\alpha} \rangle$$

where the sum is over the manybody states (wavefunctions) α (Ψ_{α})

if the number of particles is fixed use
$$z = \sum_{\alpha} e^{-E_{\alpha}/k_b T}, \quad \text{and} \quad F = E - TS = -k_b T \log z$$

note that partition function partitions! $\hat{H}_{\text{tot}} = \hat{H}_i + \hat{G}_j \Rightarrow E_{\alpha} = E_i + E_j$

$$\Rightarrow Z = \sum_{i,j} e^{\left(-\frac{E_i + E_j}{T}\right)} = Z_H \cdot Z_G$$

Identical Particles

Many-body wave functions must be either symmetric or antisymmetric under exchange of space and spin coordinates of particles

$$\Psi(1, 2, \dots, i, i + 1, \dots, n) = \pm \Psi(1, 2, \dots, i + 1, i, \dots, n)$$

BE \Rightarrow + \Rightarrow bosons

FD \Rightarrow - \Rightarrow fermions

Non-interacting Gases

Consider a *single* momentum mode \mathbf{q} for a system of non-interacting particles.
Two cases to consider:

I.) FD, occupation number $n_{\mathbf{q}} = 0, 1$

$$\text{partition function for this mode} \Rightarrow Z_{\mathbf{q}} = \sum_{\alpha} e^{-\frac{E_{\alpha} - \mu N_{\alpha}}{T}} = \sum_{n_{\mathbf{q}}} \exp \left[n_{\mathbf{q}} \cdot \frac{-\epsilon_{\mathbf{q}} + \mu}{T} \right] = 1 + e^{(-\epsilon_{\mathbf{q}} + \mu)/T}$$

where $\epsilon_{\mathbf{q}}$ = single particle energy

$$\text{thermodynamic potential for this mode } \Omega_{\epsilon_{\mathbf{q}}} = -k_{\text{b}} T \log Z_{\mathbf{q}} = -k_{\text{b}} T \log \left[1 + e^{(-\epsilon_{\mathbf{q}} + \mu)/T} \right]$$

$$\text{average occupation probability for this mode } n_{\mathbf{q}} = - \left. \frac{\partial \Omega_{\mathbf{q}}}{\partial \mu} \right|_{T, V} = \frac{1}{e^{(\epsilon_{\mathbf{q}} - \mu)/T} + 1}$$

$$\text{now sum over all modes } \Omega = \sum_{\mathbf{q}} \Omega_{\mathbf{q}} = -T \sum_{\mathbf{q}} \log \left[1 + e^{(-\epsilon_{\mathbf{q}} + \mu)/T} \right]$$

$$\Omega = -T V g \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \log \left[1 + e^{(-\epsilon_{\mathbf{q}} + \mu)/T} \right]$$

$$\Omega = -T V g \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \log \left[1 + e^{(-\epsilon_{\mathbf{q}} + \mu)/T} \right]$$

isotropy $\Rightarrow \Omega = \frac{-T g V}{2\pi^2} \int_0^\infty \underbrace{dq q^2}_{dv} \underbrace{\log \left[1 + e^{(-\epsilon_{\mathbf{q}} + \mu)/T} \right]}_u$

by parts $\Rightarrow \Omega = \frac{-g V}{6\pi^2} \int_0^\infty dq q^3 \cdot \frac{1}{e^{\frac{\epsilon_{\mathbf{q}} - \mu}{T}} + 1} \cdot \frac{\partial \epsilon_{\mathbf{q}}}{\partial q}$

where single particle energy dispersion relation is $\epsilon_{\mathbf{q}} = (\mathbf{q}^2 + m^2)^{1/2} \Rightarrow \frac{\partial \epsilon_{\mathbf{q}}}{\partial \mathbf{q}} = \frac{q}{\epsilon_{\mathbf{q}}}$

FD relativistic limit $\Rightarrow \epsilon_{\mathbf{q}} = q, \quad \text{where } q = |\mathbf{q}|$

$$\Rightarrow \Omega = \frac{-g V T^4}{6\pi^2} \int_0^\infty \frac{x^3}{e^{x-\eta} + 1} dx, \quad \text{where degeneracy parameter is } \eta \equiv \frac{\mu}{T}$$

$$\Rightarrow \Omega_{\text{FD,rel}} = -\frac{g V T^4}{6\pi^2} F_3 \left(\frac{\mu}{T} \right)$$

Define relativistic Fermi integral of order $k \Rightarrow F_k(\eta) \equiv \int_0^\infty \frac{x^k}{e^{x-\eta} + 1} dx$

$F_k(\eta) \approx k! e^\eta$ for $\eta < 0$ **non-degenerate**

$F_k(\eta) \approx \frac{\eta^{k+1}}{k+1} \left(\sum_{i=0}^{\infty} a_{2i} \eta^{-2i} \right)$ for $\eta > 0$ (Sommerfeld expansion) **degenerate**

slowly convergent since $a_0 = 1 \quad a_2 = \frac{\pi^2}{6} k(k+1) \quad a_4 = \frac{7\pi^4}{360} (k-2)(k-1)(k)(k+1)$

$$F_2(0) = \frac{3}{2} \zeta(3) \quad \text{where } \zeta(3) \approx 1.20206 \quad F_3(0) = \frac{7\pi^4}{120} \quad F_1(0) = \frac{\pi^2}{12}$$

more on Fermi Integrals . . .

can show (integrate by parts) that $\frac{dF_k(\eta)}{d\eta} = k F_{k-1}(\eta)$

$$\Rightarrow dF_k(\eta) = k F_{k-1}(\eta) d\eta \Rightarrow F_k(\eta) - F_k(0) = k \int_0^\eta F_{k-1}(\eta') d\eta'$$

but can integrate directly to find $F_0(\eta) = \ln(1 + e^\eta) = \eta + \ln(1 + e^{-\eta})$

and note that $F_0(-\eta) = \ln(1 + e^{-\eta})$

so that $F_0(\eta) - F_0(-\eta) = \eta$

Can now use the above integral identity and successively integrate to find the following identities. These are handy for fermions in the relativistic limit.

$$F_1(\eta) + F_1(-\eta) = \frac{1}{2}\eta^2 + 2F_1(0) = \frac{1}{2}\eta^2 + \frac{\pi^2}{6}$$

$$F_2(\eta) - F_2(-\eta) = \frac{1}{3}\eta^3 + \frac{\pi^2}{3}\eta$$

$$F_3(\eta) + F_3(-\eta) = \frac{1}{4}\eta^4 + \frac{\pi^2}{2}\eta^2 + 2F_3(0) = \frac{1}{4}\eta^4 + \frac{\pi^2}{2}\eta^2 + \frac{7\pi^4}{60}$$

Back to the thermodynamics of fermions in the relativistic limit . . .

$$\Rightarrow \Omega_{\text{FD,rel}} = -\frac{gVT^4}{6\pi^2} F_3\left(\frac{\mu}{T}\right)$$

$$N = -\frac{\partial\Omega}{\partial\mu}\bigg|_{V,T} \Rightarrow \text{number density } n = \frac{gT^3}{2\pi^2} F_2\left(\frac{\mu}{T}\right)$$

Example: relativistic electrons/positrons in equilibrium with the radiation field

$$\text{net number of ionization electrons } n_0 = n_{e^-} - n_{e^+} = \frac{T^3}{\pi^2} \left[F_2\left(\frac{\mu_{e^-}}{T}\right) - F_2\left(-\frac{\mu_{e^-}}{T}\right) \right]$$

$$\text{since } g = 2 \text{ for } e^\pm, \text{ and } e^- + e^+ \rightleftharpoons 2\gamma \Rightarrow \mu_{e^-} + \mu_{e^+} = 2\mu_\gamma = 0$$

Using the identities for the difference of relativistic Fermi integrals of order 2 (previous page)

$$n_0 = n_{e^-} - n_{e^+} = \frac{T^3}{\pi^2} [F_2(\eta) - F_2(-\eta)] = \frac{1}{3} T^3 \eta \left[1 + \frac{\eta^2}{\pi^2} \right]$$

Pressure (relativistic fermions): $P = -\frac{\Omega}{V} \Rightarrow P = \frac{gT^4}{6\pi^2} F_3\left(\frac{\mu}{T}\right)$

entropy (relativistic fermions) $S/k_b = -\frac{\partial \Omega}{\partial T} \Big|_{V,\mu} = \frac{gV}{6\pi^2} \left[4T^3 F_3\left(\frac{\mu}{T}\right) - 3\mu T^2 F_2\left(\frac{\mu}{T}\right) \right]$

Now divide by the number of particles to get the entropy per particle:

$$\frac{S}{N k_b} = \frac{4}{3} \frac{F_3\left(\frac{\mu}{T}\right)}{F_2\left(\frac{\mu}{T}\right)} - \frac{\mu}{T} \rightarrow \pi^2 \frac{T}{\mu} \quad \text{in degenerate limit } \frac{\mu}{T} \gg 1$$

dilute (non-degenerate), extreme relativistic limit for fermions $T \gg \mu \Rightarrow \eta \rightarrow 0, \mu \rightarrow 0$

$$F_3(0) = \int_0^\infty \frac{x^3}{e^x + 1} dx = 6 \sum_{n=1}^\infty \frac{(-1)^{n-1}}{n^4} = \frac{7}{8} \cdot \frac{\pi^4}{15}$$

$$\Omega_{\text{FD,ER,ND}} \Rightarrow -\frac{7}{8} g V \frac{1}{3} a T^4 \quad \text{where we define } a \equiv \frac{\pi^2}{30}$$

$$\text{energy density } \rho = \frac{E}{V} = \frac{TS - PV + \mu N}{V} = \frac{7}{8} g a T^4 \quad \text{pressure } P = \frac{1}{3} \rho$$

$$\text{entropy per unit volume } S = \frac{4}{3} g a T^3 = \frac{2\pi^2}{45} g T^3 \quad \text{in units of } k_b$$

fermions, relativistic and extreme relativistic dilute limits . . .

number density relativistic limit $n = \frac{g T^3}{2\pi^2} F_2(\eta)$

extreme relativistic, dilute limits $\eta = \frac{\mu}{T} \rightarrow 0, \quad n = \frac{g T^3}{2\pi^2} F_2(\eta) \quad \Rightarrow \quad n = \frac{3}{4} \frac{\zeta(3)}{\pi^2} g T^3$

Example: number density of Big Bang thermal background relic neutrinos at the current epoch.

Each spin-1/2 neutrino has $g=1$ and there are 6 kinds of neutrinos $\nu_e, \bar{\nu}_e, \nu_\mu, \bar{\nu}_\mu, \nu_\tau, \bar{\nu}_\tau$

Moreover, neutrinos decouple at $T \sim 1$ MeV, so they have relativistic FD blackbody energy spectra at the current epoch with “temperature” a factor of $(4/11)^{1/3}$ lower than the cosmic microwave background (photon) temperature $T_\gamma = 2.75$ K

$$n = 6 \cdot \frac{3}{4} \frac{\zeta(3)}{\pi^2} \cdot \frac{\left(\frac{4}{11}\right) (2.75 \text{ K} \cdot 8.617 \times 10^{-11} \text{ MeV/K})^3}{(\hbar c)^3} \approx 345 \text{ cm}^{-3}$$

where we use $\hbar c \approx 197.33 \text{ MeV fm}, \quad 1 \text{ fm} = 10^{-13} \text{ cm}$

Example: add thermodynamic potentials for relativistic particles (-) and anti-particles (+) in equilibrium. An example might be electrons and positrons in equilibrium with the radiation field. In either case, equilibrium implies (Saha equation) that the (total) chemical potentials for the particles and antiparticles are equal and of opposite sign, as in the above example for relativistic electrons/positrons: $\mu_+ = -\mu_-$

$$\Rightarrow \quad \Omega_{\text{tot}} = \Omega_- + \Omega_+ = -\frac{g V T^4}{6\pi^2} \left[F_3 \left(\frac{\mu_-}{T} \right) + F_3 \left(\frac{-\mu_-}{T} \right) \right]$$

using the identity for the appropriate sum of relativistic Fermi integrals this becomes

$$\Rightarrow \quad \Omega_{\text{tot}} = \Omega_- + \Omega_+ = -\frac{g V T^4}{6\pi^2} \left[\frac{7\pi^4}{60} + \frac{\pi^2}{2} \left(\frac{\mu_-}{T} \right)^2 + \frac{1}{4} \left(\frac{\mu_-}{T} \right)^4 \right]$$

From this can get pressure, entropy, number density, etc., for a gas of, e.g., electrons and positrons in equilibrium. Check against example for number density of electrons minus positrons.

An aside on electron Fermi energies/chemical potentials

This is a tricky and confusing issue in the literature and in books on stellar interiors and evolution.

The root of the confusion stems from whether or not the electron rest mass is included in the Fermi energy and chemical potentials

For example, some works (e.g., BBAL 1979) include rest mass in the chemical potentials for electrons but not for neutrons and protons.

We will use the following convention for electron/positron chemical potentials:

$$\text{total Fermi energy (chemical potential)} \quad \mu_{e^-} = W_F^{e^-} = U_F^{e^-} + m_e c^2$$

Here $U_F^{e^-}$ is the *kinetic* chemical potential (*kinetic* Fermi energy)

Taking as an example electrons and positrons in equilibrium with the radiation field (though the conclusions apply to any such particle/antiparticle pair)

$$e^- + e^+ \rightleftharpoons 2\gamma \quad \Rightarrow \quad \text{Saha equation} \quad \mu_{e^-} + \mu_{e^+} = 2\mu_\gamma = 0 \quad \Rightarrow \quad \mu_{e^+} = -\mu_{e^-}$$

$$\Rightarrow \quad W_F^{e^+} = -W_F^{e^-} \quad \Rightarrow \quad U_F^{e^+} = -U_F^{e^-} - 2m_e c^2$$

Example: in the very low density, high temperature (dilute) limit

$$\Rightarrow \quad \mu_{e^-} = W_F^{e^+} = -W_F^{e^-} = -\mu_{e^+} \rightarrow 0 \quad \Rightarrow \quad U_F^{e^-} = U_F^{e^+} = -m_e c^2 \approx -0.511 \text{ MeV}$$

More on electron Fermi energy (chemical potential):

Example:

For *any* density and **zero temperature** (arbitrary kinematics, but degenerate limit)

$$U_{\text{F}}^{e^-} \approx 0.511 \text{ MeV} \left[\left(1.02 \times 10^{-4} (\rho Y_e)^{2/3} + 1 \right)^{1/2} - 1 \right] \text{ with } \rho \text{ in } \text{g cm}^{-3}$$

$$\Rightarrow \mu_{e^-} \approx 11.1 \text{ MeV } (\rho_{10} Y_e)^{1/3} \text{ when } \rho Y_e \gg 10^9 \text{ g cm}^{-3}, \text{ where } \rho_{10} \equiv \rho / 10^{10} \text{ g cm}^{-3}$$

In this latter limit, at densities this high, the electrons are very relativistic and the electron rest mass is small compared to the Fermi energy

In general, for any temperature and density, but arbitrary kinematics for electrons/positrons

$$\text{net electron number density } n_0 = n_{e^-} - n_{e^+} = \rho Y_e N_{\text{A}} = \frac{1}{\pi^2} \left(\frac{m_e c^2}{\hbar c} \right)^3 \int_0^\infty dx x^2 (S_- - S_+)$$

$$\text{with } x = p/m_e c^2 \text{ and, e.g., } S_- = \left[\exp \left(\frac{U - U_{\text{F}}^{e^-}}{T} \right) + 1 \right]^{-1}$$

and where the kinetic energy is related to the momentum by $U = (p^2 c^2 + m_e^2 c^4)^{1/2} - m_e c^2$

fermions, nonrelativistic

The general thermodynamic potential for fermions was

$$\Omega = -\frac{gV}{6\pi^2} \int_0^\infty \frac{q^4}{\epsilon_{\mathbf{q}}} \cdot \frac{1}{e^{(\epsilon_{\mathbf{q}}-\mu)/T} + 1} dq = -\frac{gV}{6\pi^2} \int_m^\infty (\epsilon_{\mathbf{q}}^2 - m^2)^{3/2} \cdot \frac{1}{e^{(\epsilon_{\mathbf{q}}-\mu)/T} + 1} d\epsilon_{\mathbf{q}}$$

where we use $q dq = \epsilon_{\mathbf{q}} d\epsilon_{\mathbf{q}}$ and m is the particle rest mass

now define $\tilde{\epsilon}_{\mathbf{q}} \equiv \epsilon_{\mathbf{q}} - m$ and $\tilde{\mu} \equiv \mu - m$ and note that $\epsilon_{\mathbf{q}} - \mu = \tilde{\epsilon}_{\mathbf{q}} - \tilde{\mu}$ and $d\tilde{\epsilon}_{\mathbf{q}} = d\epsilon_{\mathbf{q}}$

neglecting kinetic energies relative to mass, we get

$$\Omega_{\text{FD,NR}} \approx -\frac{gV \sqrt{2} m^{3/2}}{3\pi^2} \int_0^\infty \frac{\tilde{\epsilon}_{\mathbf{q}}^{3/2}}{e^{(\tilde{\epsilon}_{\mathbf{q}}-\tilde{\mu})/T} + 1} d\tilde{\epsilon}_{\mathbf{q}} = -\frac{gV \sqrt{2} m^{3/2} T^{5/2}}{3\pi^2} F_{3/2}(\tilde{\eta})$$

$$\text{with } \tilde{\eta} \equiv \frac{\tilde{\mu}}{T}$$

$$\text{In this limit the pressure is } P = -\frac{\Omega}{V} = \frac{g \sqrt{2} m^{3/2} T^{5/2}}{3\pi^2} F_{3/2}(\tilde{\eta})$$

$$\text{and the number of particles per unit volume is } n = \frac{1}{V} \left(-\frac{\partial \Omega}{\partial \mu} \right) \Big|_{V,T} \Rightarrow \frac{g \sqrt{2} m^{3/2} T^{3/2}}{2\pi^2} F_{1/2}(\tilde{\eta})$$

To make contact with our previous notation for Fermi energies and chemical potentials, note that, e.g., for electrons,

$$\text{kinetic chemical potential (kinetic Fermi energy)} \quad U_{\text{F}}^{e^-} = \tilde{\mu}_{e^-}$$

and similarly for other particles, with all other notation generalized in obvious fashion.

fermions, non-relativistic: entropy

$$\text{entropy per particle} \quad \frac{S}{N k_b} = -\frac{1}{N} \left(\frac{\partial \Omega}{\partial T} \right) \Big|_{V, \mu} = \frac{5}{3} \frac{F_{3/2}(\tilde{\mu})}{F_{1/2}(\tilde{\mu})} - \frac{\tilde{\mu}}{T}$$

$$\text{entropy per particle completely degenerate limit} \quad \frac{\tilde{\mu}}{T} \gg 1 \Rightarrow \frac{S}{N k_b} = \frac{\pi^2}{2} \frac{T}{\tilde{\mu}}$$

Example: what is the entropy per baryon in an ^{56}Fe nucleus in a collapsing stellar core at a temperature $T=1$ MeV ?

First, we need the kinetic Fermi energy for the “seas” of both neutrons and protons in the nucleus – approximate these seas as non-interacting fermions at symmetric nuclear matter density. The radius of nuclei is given by $R=r_0 A^{1/3}$, where the nuclear mass number is A , and $r_0=1.07$ fm. The number of particles per unit volume is relatively independent of the size of the nucleus because of the saturation of nuclear forces:

$$\frac{A}{V} = \frac{3}{4\pi r_0^3} \approx 1.95 \times 10^{38} \text{ particles per cm}^3$$

Each momentum state has a degeneracy (weight) factor of 4 (neutrons, protons, spin up, spin down), so modeling as a zero temperature non-relativistic degenerate Fermi gas we get an expression for the Fermi momentum:

$$\frac{A}{V} = \frac{2}{3\pi^2} p_F^3 \Rightarrow p_F \approx 1.42 \text{ fm}^{-1} \Rightarrow \tilde{\mu} = \frac{p_F^2}{2m} \approx 42 \text{ MeV} \sim 40 \text{ MeV}$$

$$\text{entropy per baryon} \quad \frac{S}{N_b k_b} \approx \frac{\pi^2}{2} \frac{T}{\tilde{\mu}} \approx \frac{\pi^2}{2} \frac{1 \text{ MeV}}{40 \text{ MeV}} \approx 0.1$$

fermions . **Maxwell-Boltzmann Limit** - non-relativistic kinematics, non-degenerate

non – relativistic $T \ll m c^2$ and non – degenerate (dilute) $\tilde{\mu} < 0$

$$\begin{aligned}\Omega_{\text{MB}} &\equiv \lim_{\text{MB}} (\Omega_{\text{FD,NR}}) \rightarrow -\frac{\sqrt{2} g V m^{3/2}}{3\pi^2} \cdot e^{\tilde{\mu}/T} \cdot \int_0^\infty d\epsilon_{\mathbf{q}} \epsilon_{\mathbf{q}}^{3/2} e^{-\epsilon_{\mathbf{q}}/T} \\ &= -\frac{\sqrt{2} g V m^{3/2} T^{5/2}}{3\pi^2} \cdot e^{\tilde{\mu}/T} \cdot \int_0^\infty x^{3/2} e^{-x} dx\end{aligned}$$

$$\int_0^\infty x^n e^{-x} dx = \Gamma(n+1) = n \Gamma(n) \quad \text{and} \quad \Gamma\left(\frac{5}{2}\right) = \frac{3}{2} \Gamma\left(\frac{3}{2}\right) = \frac{3}{4} \Gamma\left(\frac{1}{2}\right) = \frac{3}{4} \sqrt{\pi}$$

$$\Rightarrow \Omega_{\text{MB}} = -g V T^{5/2} \cdot \left(\frac{m}{2\pi}\right)^{3/2} \cdot e^{\tilde{\mu}/T}$$

number density $n = \frac{N}{V} = -\frac{\partial \Omega}{\partial \mu} \Big|_{V,T} = g T^{3/2} \cdot \left(\frac{m}{2\pi}\right)^{3/2} \cdot e^{\tilde{\mu}/T}$

which we can re-arrange to get the kinetic chemical potential in terms of the number density, mass of particle, temperature, and statistical weight:

$$\tilde{\mu} = T \ln \left[\left(\frac{2\pi}{m T}\right)^{3/2} \frac{n}{g} \right]$$

We can shed some light on the chemical potential in the MB limit and flesh out its physical dependence on the underlying arrangement of matter and associated degrees of freedom. First start by putting in the dimensions (and leaving T and m inside the log in energy units!):

$$\tilde{\mu} = k_b T \ln \left[\frac{(2\pi)^{3/2}}{g} \frac{n (\hbar c)^3}{(m T)^{3/2}} \right]$$

Now define a measure of the inter-particle spacing as $\lambda = \frac{1}{n^{1/3}}$

and the particle Compton wavelength as $\lambda_{\text{comp}} = \frac{\hbar c}{m}$

Now we can re-express the kinetic chemical potential in this limit as

$$\tilde{\mu} = k_b T \ln \left[\frac{(2\pi)^{3/2}}{g} \left(\frac{\lambda_{\text{comp}}}{\lambda} \right)^3 \left(\frac{m}{T} \right)^{3/2} \right]$$

The Compton wavelength is a measure of the quantum mechanical “size” of the particle and we see that as the inter-particle spacing becomes smaller than this, or as the temperature gets very, very low, we will be in danger of driving the kinetic chemical potential positive, *i.e.*, invalidating our assumed “dilute” limit.

The entropy in the Maxwell-Boltzmann limit is $\frac{S}{k_b} = -\frac{\partial \Omega}{\partial T} \Big|_{V, \mu} = N \left(\frac{5}{2} - \frac{\tilde{\mu}}{T} \right)$

$$\Rightarrow \text{entropy per particle} \quad \frac{S}{N k_b} = \frac{5}{2} - \frac{\tilde{\mu}}{T} = \frac{5}{2} + \ln \left[\left(\frac{m T}{2\pi} \right)^{3/2} \frac{g}{n} \right]$$

Example: contribution of a given species to the entropy per baryon

if number densities are, *e.g.*, for baryons $n_b = \frac{N_b}{V}$ and for species i , $n_i = \frac{N_i}{V}$,

then the contribution of species i , with abundance relative to baryons Y_i , to the entropy per baryon is

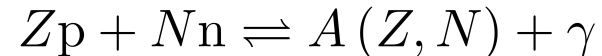
$$\frac{S}{N_b k_b} = \frac{S}{n_b V k_b} = \frac{n_i}{n_b} \left(\frac{S}{N_i k_b} \right) = Y_i \left(\frac{S}{N_i k_b} \right)$$

Example: What is the entropy per baryon of the air in this room? In the center of the sun?

Example: Nuclear Saha Equation

For temperatures in excess of $T_9 > 3$ the rates of the nuclear reactions that build-up and tear-down a nucleus with mass number $A=Z+N$ (here with Z =number of protons, N =number of neutrons) can become very large compared with material expansion/collapse rates and equal to each other, so that there is a steady state equilibrium abundance of nucleus $A(Z,N)$. This steady state condition is deemed **Nuclear Statistical Equilibrium** or **NSE**.

The beauty of equilibrium is that the details of the reaction sequences involved are unimportant and we can just summarize the net reaction sequence as, in this case,




From which we can derive the **Saha** equation relating the chemical potentials of these species (photons have zero chemical potential):

$$Z\mu_p + N\mu_n = \mu_A$$

These are *total* chemical potentials and we can convert this equation to one using the kinetic chemical potentials by subtracting the rest masses of the various nuclear species involved:

$$\mu_p = \tilde{\mu}_p + m_p \quad \mu_n = \tilde{\mu}_n + m_n \quad \mu_A = \tilde{\mu}_A + m_A$$


$$Z\tilde{\mu}_p + N\tilde{\mu}_n = \tilde{\mu}_A - Q(Z, N)$$

With the binding energy for nucleus $A=Z+N$ defined as $-Q(Z, N) \equiv -Zm_p - Nm_n + m_A$ (*i.e.*, very tightly bound nuclei correspond to large positive Q -values)

Example: nuclear Saha equation . . . continued . . .

Using the dilute Maxwell-Boltzmann limit expressions for the kinetic chemical potentials for free protons, free neutrons, and bound nucleus with mass number A , the Saha equation becomes

$$\ln \left[\left(\frac{2\pi}{T} \right)^{\frac{3}{2} \cdot Z} \frac{1}{m_p^{\frac{3}{2} \cdot Z}} \left(\frac{n_p}{g} \right)^Z \right] + \ln \left[\left(\frac{2\pi}{T} \right)^{\frac{3}{2} \cdot N} \frac{1}{m_n^{\frac{3}{2} \cdot N}} \left(\frac{n_n}{g} \right)^N \right] = \ln \left[\left(\frac{2\pi}{T} \right)^{\frac{3}{2}} \frac{1}{m_A^{\frac{3}{2}}} \left(\frac{n_A}{G(Z, A)} \right) \right] - \frac{Q}{T}$$

Where the number densities of protons, neutrons, and nucleus with mass number A , respectively, are n_p , n_n , n_A

and where the spin degeneracies (weights) for protons and neutrons are $g=2$ while the nuclear partition function at temperature T for the nucleus with mass number $A=Z+N$ is

$$G(Z, A) = \sum_i (2J_i + 1) e^{-E_i/T} \quad \text{-- which is just the *statistical weight* for the nucleus with energy levels } E_i \text{ and spins } J_i$$

This version of the Saha equation can be re-arranged to give the number density of the nucleus $A(Z, N)$

$$n_A = G(Z, A) \left[\frac{2\pi}{T} \right]^{\frac{3}{2}(A-1)} \left[\frac{m_A}{m_p^Z m_n^N} \right]^{\frac{3}{2}} \frac{1}{2^A} n_p^Z n_n^N \exp \left(+ \frac{Q}{T} \right)$$

We can put dimensions in this simply by adding the appropriate powers of $\hbar c$

$$n_A = G(Z, A) \left[\frac{2\pi (\hbar c)^2}{T} \right]^{\frac{3}{2}(A-1)} \left[\frac{m_A}{m_p^Z m_n^N} \right]^{\frac{3}{2}} \frac{1}{2^A} n_p^Z n_n^N \exp \left(+ \frac{Q}{T} \right)$$

Example: nuclear Saha equation . . . *continued* . . .

We can, in turn, re-express this as a mass fraction for nucleus $A(Z,N)$

$$X(Z, N) \approx G(Z, A) \frac{A^{5/2}}{2^A} \left[\frac{1.013 \times 10^{-10} \rho}{T_9^{3/2}} \right]^{(A-1)} \left(\frac{X_p}{A_p} \right)^Z \left(\frac{X_n}{A_n} \right)^N \exp \left(+ \frac{11.605 Q(Z, N)}{T_9} \right)$$

where the number densities for free protons, free neutrons, and nucleus $A(Z,N)$ are related to the corresponding mass fractions by

$$n_p = \rho N_A X_p, \quad n_n = \rho N_A X_n, \quad n_A = \rho N_A \frac{X(Z, N)}{A}$$

where ρ is density in g cm^{-3} and Avogadro's number is $N_A \approx 6.022 \times 10^{23}$
and the nucleon masses in terms of atomic mass units M_u are $m_p = A_p M_u$ $m_n = A_n M_u$,
with $A_p \approx 1.007825$ and $A_n \approx 1.00866$ and where $M_u \approx 931.494 \text{ MeV}$

Neglecting atomic electron binding energies, the nuclear Q -values are (in MeV)

$$Q(Z, N) \approx 8.0714 N + 7.2890 Z - \Delta(Z, N)$$

where $\Delta(Z,N)$ is the appropriate atomic mass excess in MeV

Example: nuclear Saha equation . . . *continued* . . .

There is yet another way to write the nuclear Saha equation that gives insight into what it means. First, define the baryon-to-photon ratio, a parameter familiar from cosmology which, unfortunately, has the same symbol as the one we have been using for degeneracy parameter. We will have to pay attention to context here!

baryon – to – photon ratio $\eta \equiv \frac{n_b}{n_\gamma}$ where the photon number density is $n_\gamma = g_\gamma \frac{\zeta(3)}{\pi^2} T^3$ and $g_\gamma = 2$

Using these and approximating non-exponential mass factors, we can write

$$X(Z, N) \approx G(Z, A) \left[2^{\frac{3A-5}{2}} (\zeta(3))^{A-1} \pi^{\frac{1-A}{2}} \right] A^{5/2} \left(\frac{T}{M_{\text{nuc}}} \right)^{\frac{3}{2}(A-1)} \eta^{A-1} X_p^Z X_n^N \exp\left(\frac{Q}{T}\right)$$

where M_{nuc} is a representative free nucleon mass and, *e.g.*, $m_A \approx A M_{\text{nuc}}$

In *radiation-dominated* conditions the entropy per baryon, s , and the baryon-to-photon ratio will be inversely proportional in regimes where statistical weights, g , are not changing,

$$\eta = \left[\frac{\pi^4}{45 \zeta(3)} \right] g s^{-1}$$

with the net result that in these environments the NSE mass fraction for nucleus $A=Z+N$ will be proportional to the product of the $1-A$ power of the entropy-per-baryon and the exponential of the nuclear binding energy to temperature ratio

$$X(Z, N) \propto G(Z, A) s^{1-A} X_p^Z X_n^N \exp\left(\frac{Q}{T}\right)$$

Example: nuclear Saha equation . . . *continued* . . .

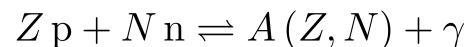
Repeating the result from the last page . . . $X(Z, N) \propto G(Z, A) s^{1-A} X_p^Z X_n^N \exp\left(\frac{Q}{T}\right)$

Therefore, in NSE the abundance of a nucleus is mostly determined by a *fight between binding and disorder*, with some dependence on the ratio of neutrons to protons.

In high entropy (*i.e.*, highly disordered) environments, the factor s^{1-A} will be very small for a big nucleus (large A), but this nucleus could be tightly bound, so that the exponential term could be large, depending on the temperature.

It is clear what is going on physically. Forcing $A=Z+N$ nucleons to move around as a unit reduces the translational degrees of freedom in the system from $3A$ to 3 , so that big nuclei are inherently ordered states and, therefore, disfavored when the entropy is high and favored when it is low.

Another way to view this result is to invoke Le Chatelier's principle and remember the original cartoon reaction sequence for NSE



Here it is clear that if we increase the photon number density (*i.e.*, increase the entropy in radiation-dominated conditions) we will drive the reaction balance to the left, favoring free nucleons and dismantling nuclei.

Problem: NSE obtains in the early universe when the temperature is $T=1$ MeV. Is there any ^{56}Fe around?

The mass excess Δ (in MeV) for ^{56}Fe can be found in the Table of Isotopes and this, combined with the formula for nuclear Q -values given above, implies $\Delta(^{56}\text{Fe}) \approx -60.6041 \Rightarrow Q \approx 492.2601$ MeV

and note that the term in the Saha equation for disorder, assuming WMAP entropy per baryon in units of k_b , $s=5.8945 \times 10^9$ is

$$(5.8945 \times 10^9)^{(1-56)} \approx 4.22 \times 10^{-538} \quad \text{and this easily beats the binding term} \quad \exp\left(\frac{492.2601 \text{ MeV}}{1 \text{ MeV}}\right) \approx 6.1 \times 10^{213}$$

Answer: not much iron around!

Example:

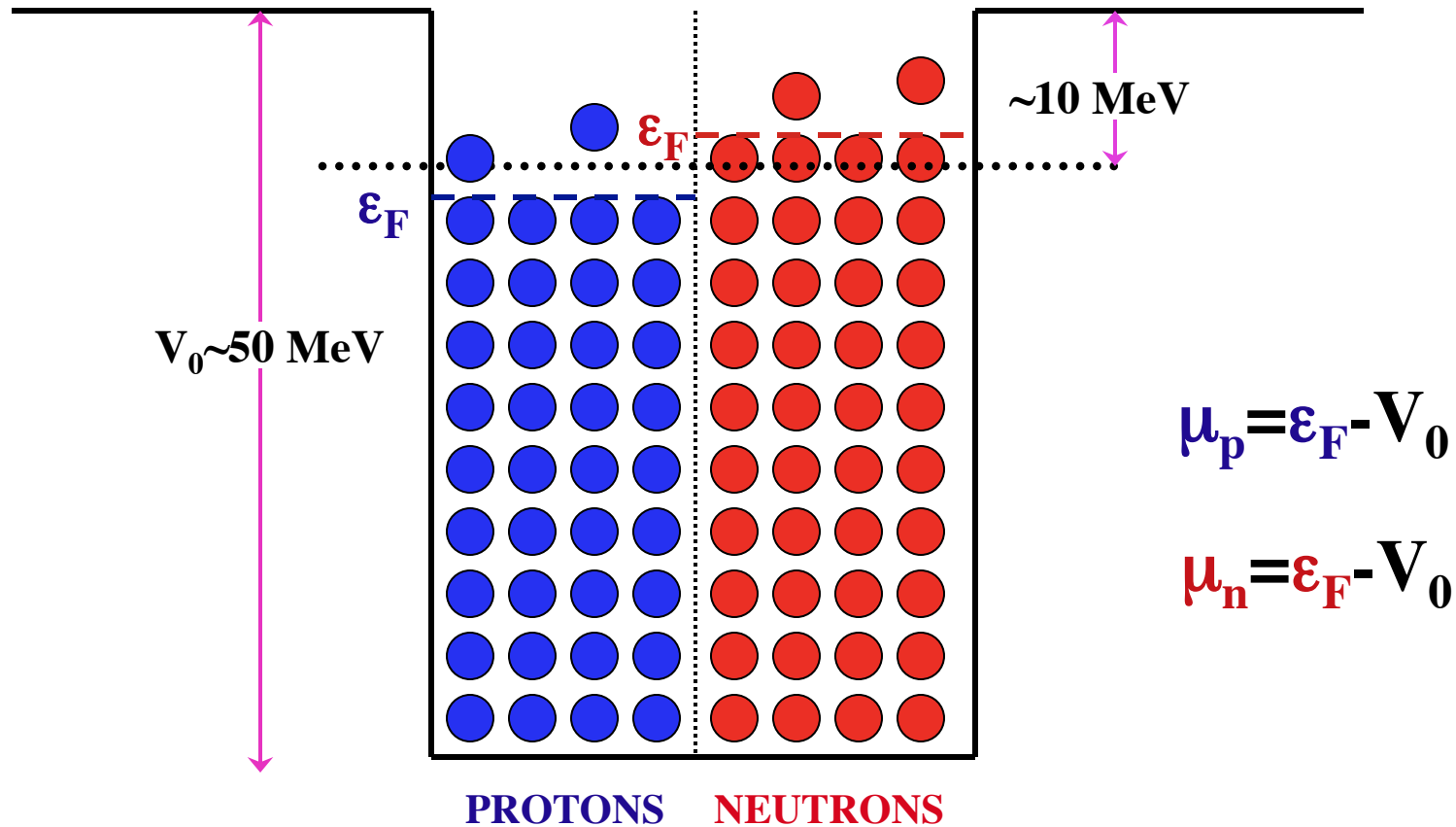
Big nuclei at high temperature,
but **low entropy**,
in a collapsing stellar core

Schematic “Nucleus” in Thermal Bath

(ignore Coulomb potential for protons)

Finite Temperature, excited states

Excited States: excitation of particles above the Fermi surface, leaving holes below



Nuclear Level Density

Bethe formula:

The level density for most all systems is exponential with excitation energy E above the ground state. Nuclei are no exception. A fit to experimental nuclear level data gives . . .

$$\rho(E) = \frac{\sqrt{\pi}}{12} \frac{\exp \left[2 (aU)^{1/2} \right]}{a^{1/4} U^{5/4}}$$

where $U = E - \delta$

and where the *back-shifting* parameter is δ

and the *level density* parameter is $a \approx \frac{A}{8 \text{ MeV}}$

nuclear mass number

Number of nucleons excited above the Fermi surface

$$N_{\text{nucleons}} \sim a T$$

where the level density parameter is $a \approx \frac{A}{8} \text{ MeV}^{-1}$

Each nucleon so excited has an excitation $\sim T$

so that the mean excitation energy of the nucleus is

$$\langle E \rangle \sim a T^2$$

For example, at a temperature $T = 2 \text{ MeV}$,

a nucleus with mass number $A \sim 200$,

which is typical during the late stages of infall/collapse,

will have mean excitation energy

$$\langle E \rangle \sim a T^2 \approx \frac{200}{8 \text{ MeV}} \cdot (2 \text{ MeV})^2 \approx 100 \text{ MeV}$$

Specific Heats and the Adiabatic Index

consider a Maxwell-Boltzmann gas . . . energy will be $E = \frac{f}{2} N k_b T$

f = number of degrees of freedom

$dE = dQ - PdV$ and $E = E(T)$ for a perfect gas

specific heats: $C_V = \left. \frac{\partial Q}{\partial T} \right|_V$ $C_P = \left. \frac{\partial Q}{\partial T} \right|_P$

equation of state: $P = \frac{N_A k_b}{\mu} \rho T$ μ = mean molecular weight (amu/particle)

$$\Rightarrow C_V = \frac{f}{2} N k_b \text{ and } C_P - C_V = N k_b$$

$$\gamma \equiv \frac{C_P}{C_V} = \frac{\frac{f}{2} + 1}{\frac{f}{2}} = 1 + \frac{2}{f}$$

e.g., $\gamma = \frac{5}{3}$ for a monatomic MB gas

Now consider MB gas plus radiation. Define ... $\Gamma_1, \Gamma_2, \Gamma_3$

$$\frac{dP}{P} + \Gamma_1 \frac{dV}{V} = 0$$

$$\frac{dP}{P} + \frac{\Gamma_2}{1 - \Gamma_2} \frac{dT}{T} = 0$$

$$\frac{dT}{T} + (\Gamma_3 - 1) \frac{dV}{V} = 0$$

$$E = VaT^4 + C_V T \quad a \equiv g_\gamma "a" \quad \beta \equiv P_{\text{gas}}/P_{\text{total}}$$

$$\Gamma_1 = \beta + \frac{(4 - 3\beta)^2(\gamma - 1)}{\beta + 12(\gamma - 1)(1 - \beta)}$$

In general . . .

$$\Gamma_1 \equiv \left. \frac{d \ln P}{d \ln \rho} \right|_S$$