Quantum Distribution Functions

for

Bosons, Fermions, & otherwise Objects

How to do the Lagrange Multiplier technique

Maximize a function subject to certain constraints on the dependent variables

- function $f(x_1, x_2, \ldots)$
- Constraint $g(x_1, x_2, \ldots)=c$

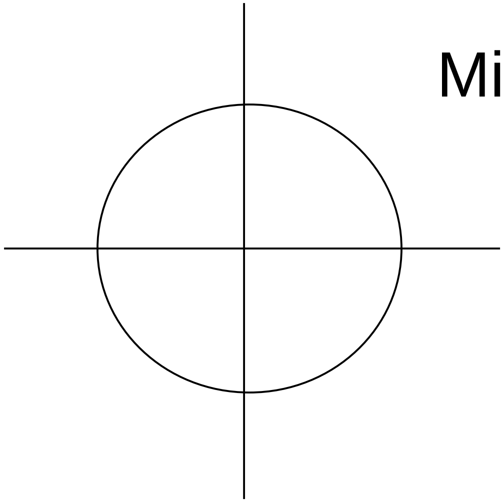
- Form new function $F = f + \lambda\ (g-c)$

- Maximize/Minimize it wrt $x_1, x_2, \ldots$

- Choose something for λ based upon other information

http://www.slimy.com/~steuard/teaching/tutorials/Lagrange.html
http://www.cs.berkeley.edu/~klein/papers/lagrange-multipliers.pdf

Example



Minimize $f = xy$ subject to constraint $x^2+y^2=1$

$$F = xy + \lambda (x^2+y^2-1)$$

$$set \quad \nabla F = 0$$

$dF/dx = y + 2\lambda x$

$dF/dy = x + 2\lambda y$

$$(y+2\lambda x) + (x+2\lambda y) = 0$$

$$(1+2\lambda)y + (1+2\lambda)x = 0$$

$$y = -x$$

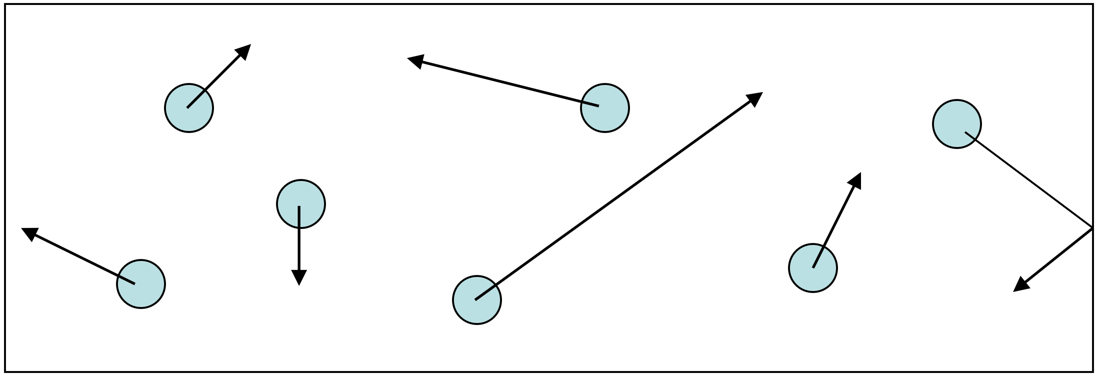
$$x^2+y^2=1 \rightarrow x^2+x^2=1 \rightarrow 2x^2 = 1 \rightarrow x=\pm 0.707$$

OUTLINE

- Harris 8.1
  - Quick Basic Probability Ideas
- Harris 8.4-8.5
  - Derivation of Boltzmann Distribution Fn
  - How to Use it
  - How to Normalize it
- Harris 8.2-8.3 Macroscopic Descriptions
  - Entropy and Temperature
  - Density of States
- Harris 8.6
  - Comparison of $\Psi_{tot}^* \Psi_{tot}$ for Bosons & Fermions
  - Detailed Balance
    - w/o special requirements
    - bosons
    - fermions
  - Distribution Fns
    - Interpreatations of the e^{α} factors
- Harris 8.7-8.10
  - 8.7 Density of States, Conduction Electrons, Bose-Einstein Condensation
  - 8.8 Photon Gasses
  - 8. Laser Systems
  - 8.10 Specific Heats

Harris 8.1
Thermodynamic Systems

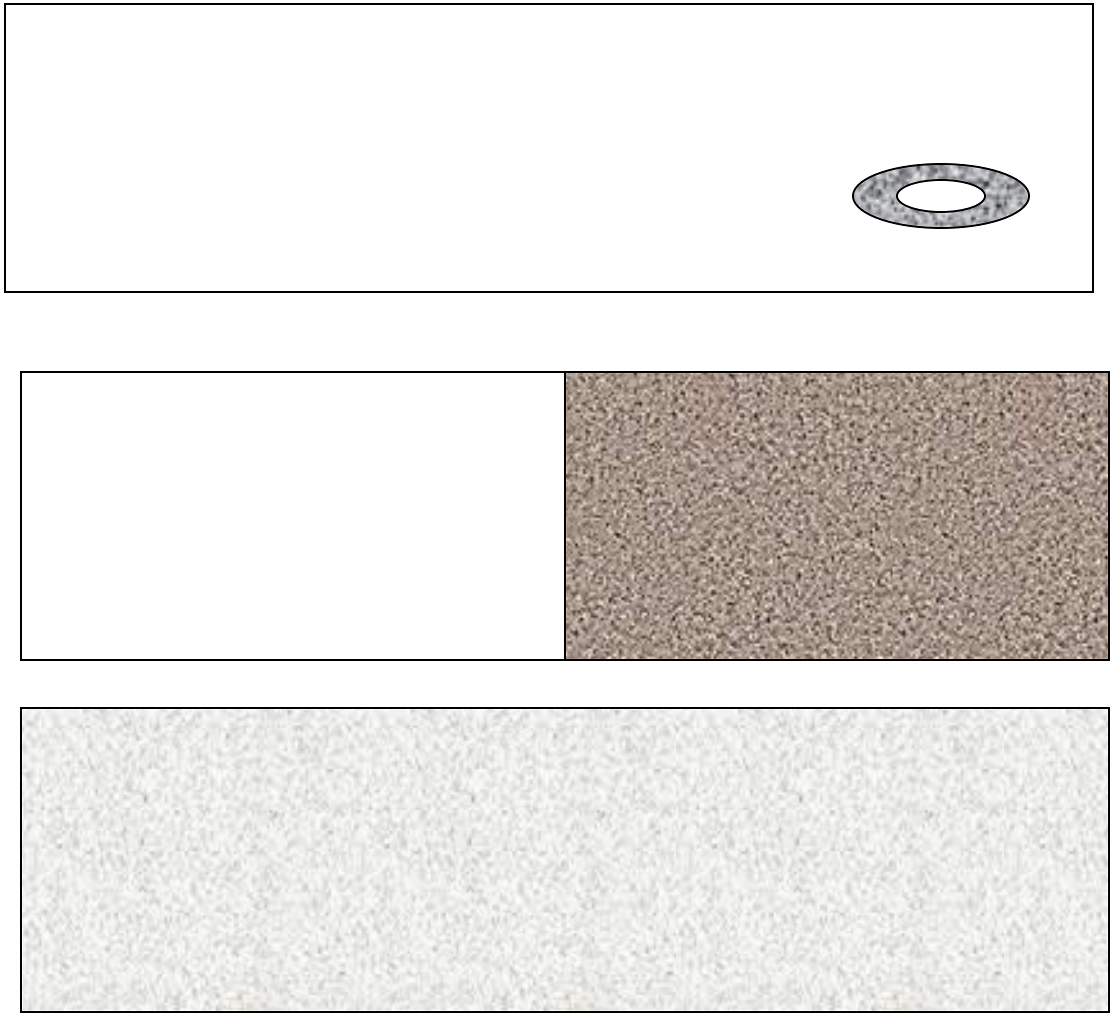
Microinfo vs Macroinfo



$\{ \mathbf{r}_i, \mathbf{p}_i, \mathbf{L}_i, \mathbf{S}_i, \mathbf{E}_i, \ldots\}$ $\quad i = 1,\ldots,$ hugen number

E_{tot}, P, V, T, N,…

Microstates vs Macrostate



Very few
microstates are
similar to this

Most
Probable
arrangement

Many microstates
are similar to this

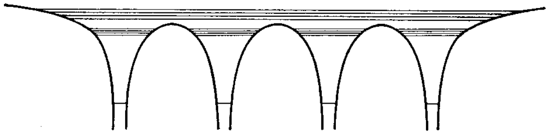
#

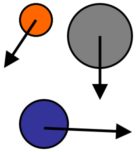
collection of most probable microstates should be described with macro-parameters

P, V, N, T, E_{tot},…

$S = k_B \ln W$

- Systems where microscopic approach is limited
  - Solids
  - 3-body problems in ‘planetary’ motion
  - Hartree-Fock Procedure
    - Multielectron atomic structure
    - Nuclear Structure
- e

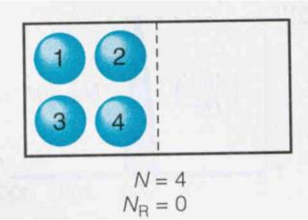


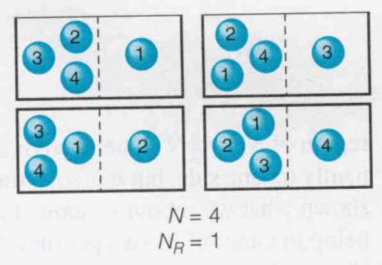


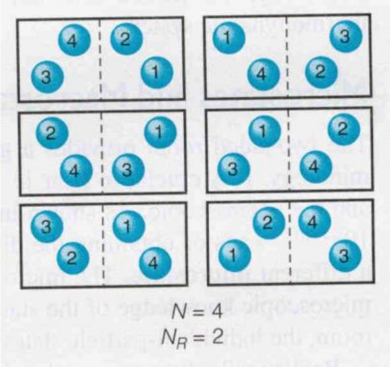
Each system has it’s own macroscopic parameters,
but the set always includes

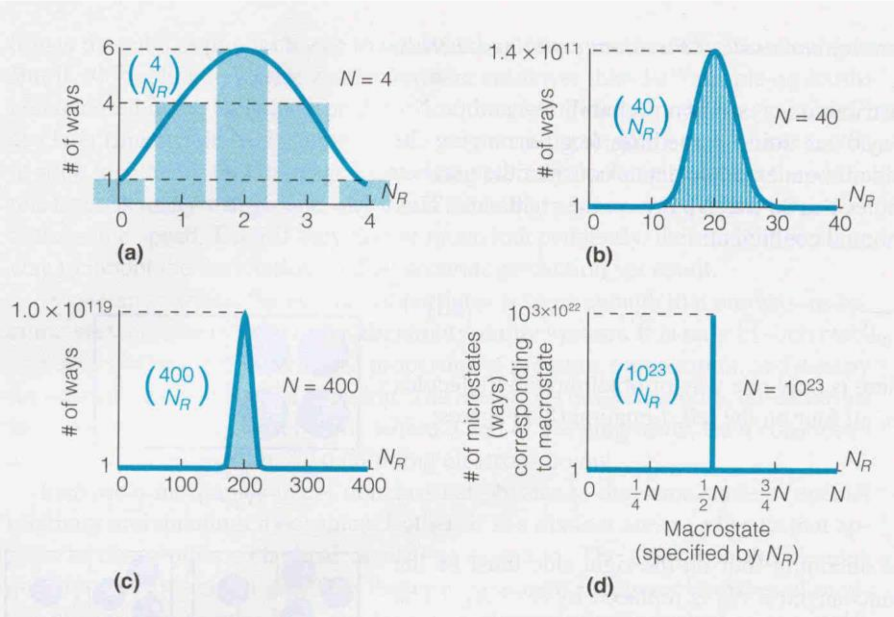
N_{tot} , E_{tot}, Ave Kinetic Energy (~T).

What is most likely arrangement of 4 balls in 2 bins?







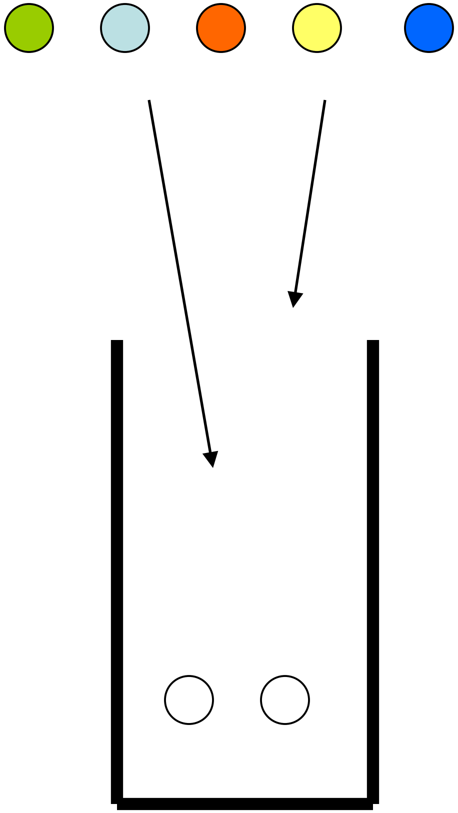


BACKGROUND PROBABILITY IDEAS

Given N=5 objects and p=1 bin;

How many ways can one put n=2 objects in the bin ?

(in a definite order)

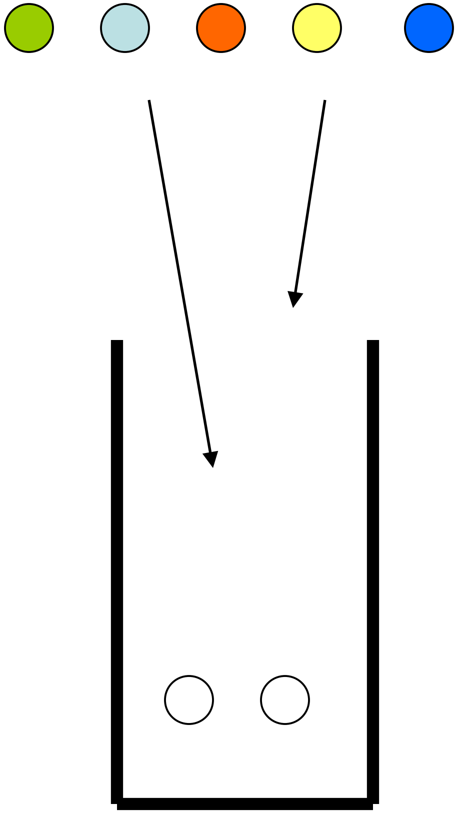


$$\frac{N!}{(N-n)!}$$

Given N=5 objects and p=1 bin;

How many ways can one put n=2 objects in the bin ?

(without regard to order)



$$\frac{N!}{(N-n)!\,n!}$$

Note that after filling this box, there are (N-n) objects unused.

Given N total objects and p total bins;

How many ways can one put

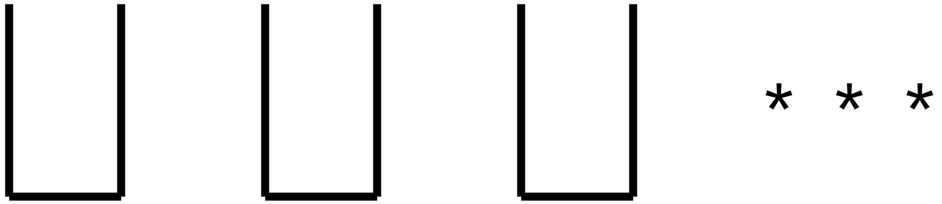
n_1 objects in bin #1

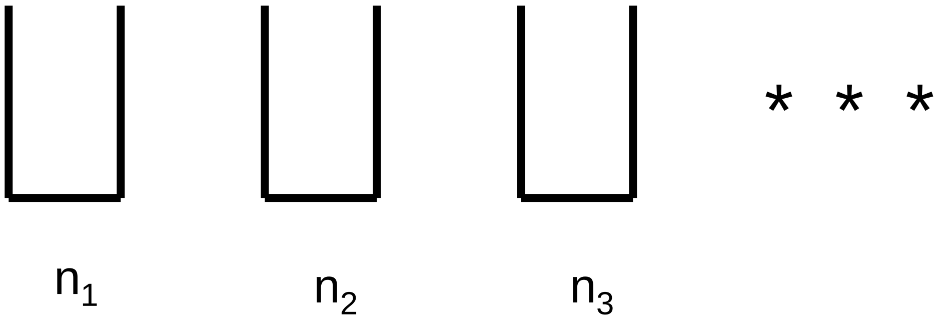
n_2 objects in bin #2

n_3 objects in bin #3

* * *

(without regard to order)

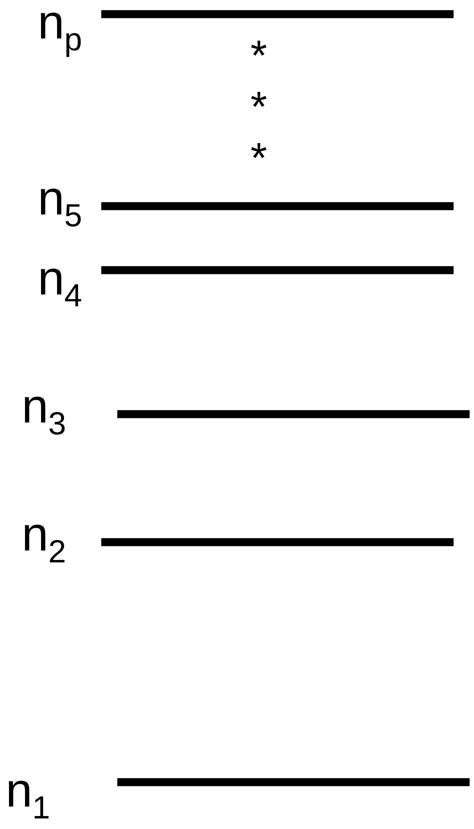



n_1
n_2
n_3
* * *

Probability of finding a particular arrangement:

Probability Summary

N total objects
p total states



n_p

*
*
*

n_5
n_4
n_3
n_2
n_1

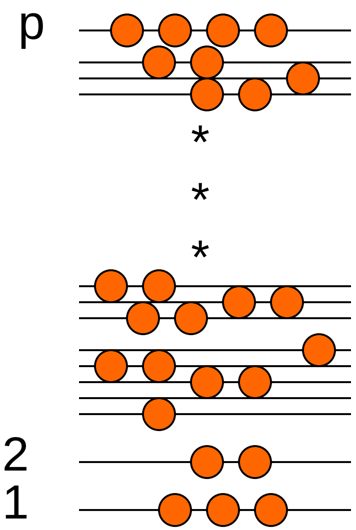
$$prob = \frac{N!}{n_1!\,n_2!\cdots n_p!} \begin{pmatrix} small \\ norm \\ const \end{pmatrix}$$

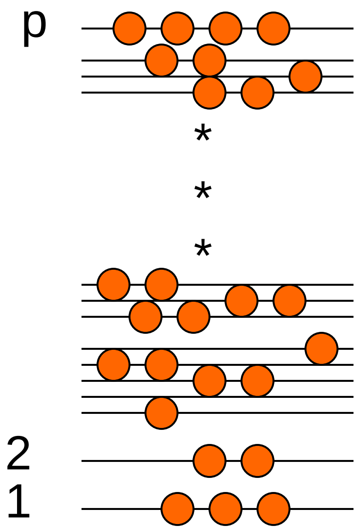
Harris 8.4
BOLTZMANN DISTRIBUTION

Probability of finding a particular energy ε

subject to the constraint that there are

N total particles and E_{tot} energy


p
*
*
*
2
1


p
*
*
*
2
1

Sterling’s Formula

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

$$\ln n! \approx \tfrac{1}{2}\ln 2\pi n + n\ln n - n$$

The second term is largest by at least a parsec

$$\ln n! \approx n \ln n$$

note: reset $1 + \alpha \rightarrow \alpha$

To discover the expression for the normalization constant (assume smooth spectrum)

OK, so what is β = ?

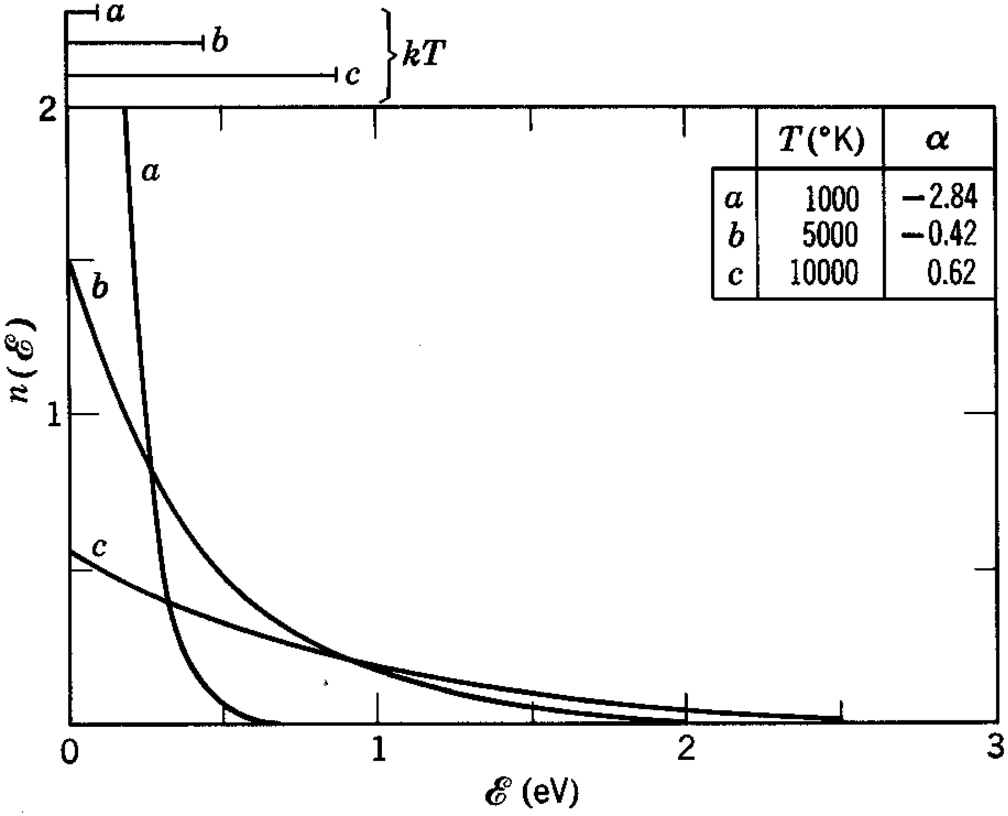
Temperature is defined in terms of the average kinetic energy

Boltzmann Distribution

Probability of finding a particular energy ε

subject to the constraints that there are

N total particles and fixed E_{tot}



	T(°K)	α
a	1000	−2.84
b	5000	−0.42
c	10000	0.62

$$\mathrm{Prob}(\varepsilon) = \frac{1}{kT} e^{-\varepsilon/kT}$$

$e^{\alpha} = 1/kT$

How to normalize the Boltzmann Distribution

and

Density of States

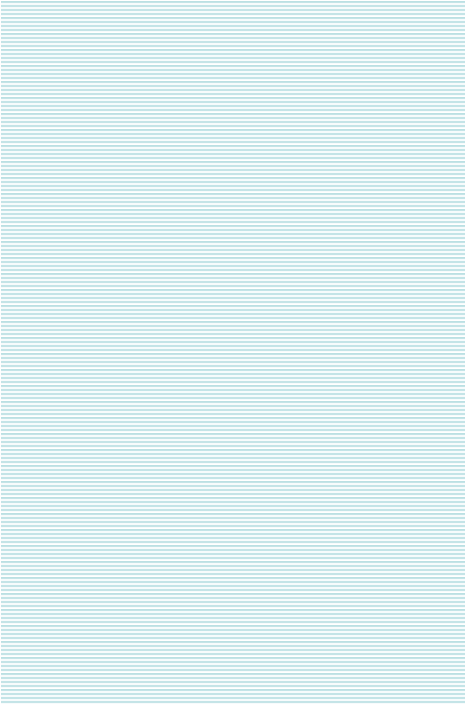
We normalized the Boltzmann distribution assuming all energies could occur

$$\text{Prob} = e^{-\alpha}\, e^{-E/kT} = A\, e^{-E/kT}$$

$$1 = \int_0^\infty A\, e^{-\varepsilon/kT}\, d\varepsilon$$

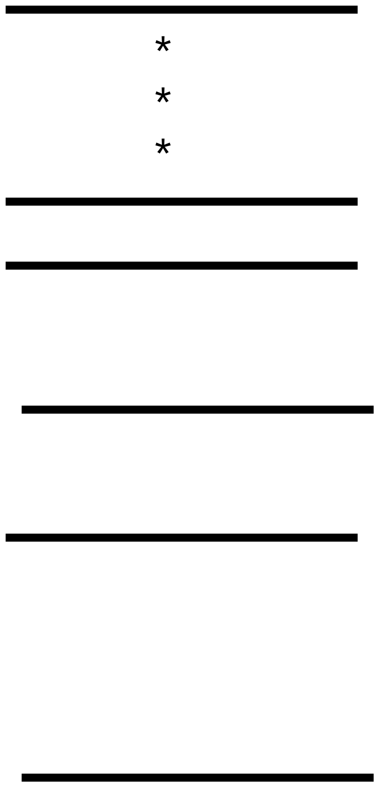
$$\Rightarrow \quad A = {}^{1}\!/_{kT}$$

Many, many possible states, closely spaced in energy

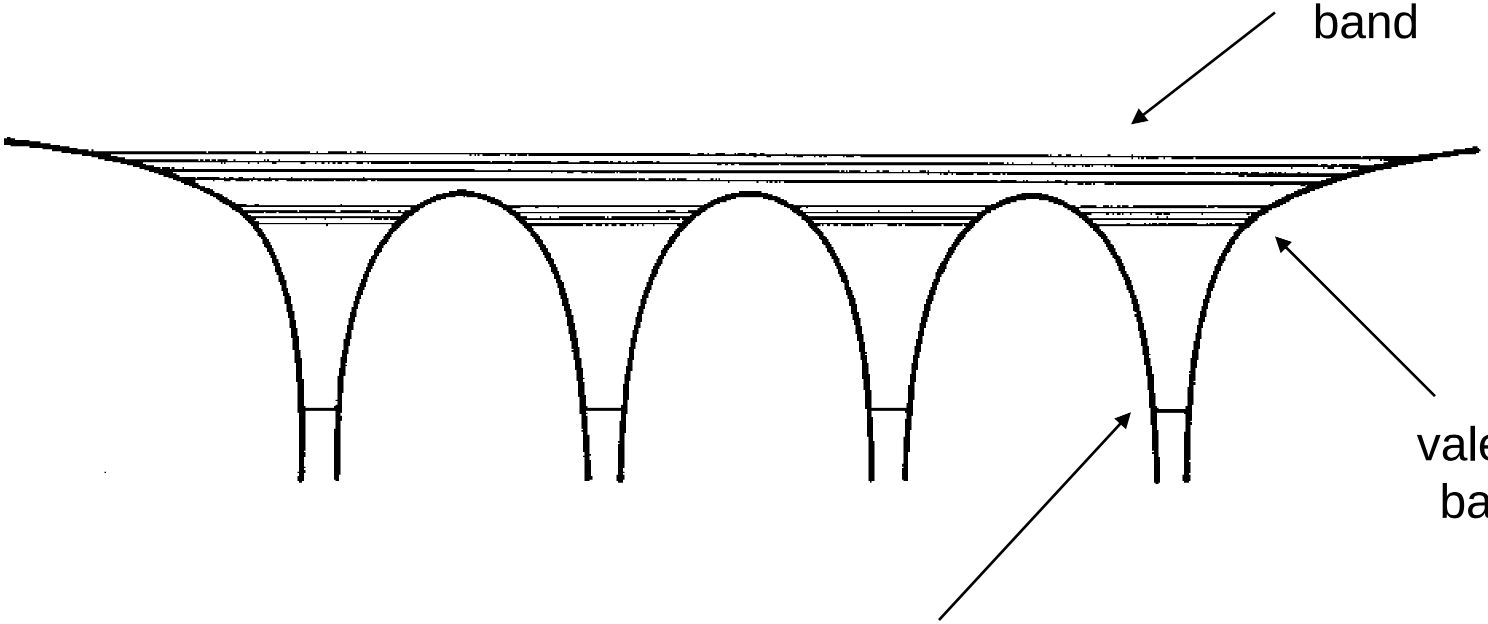


Just did this

Finite number of states, but no restriction on filling



Density of States

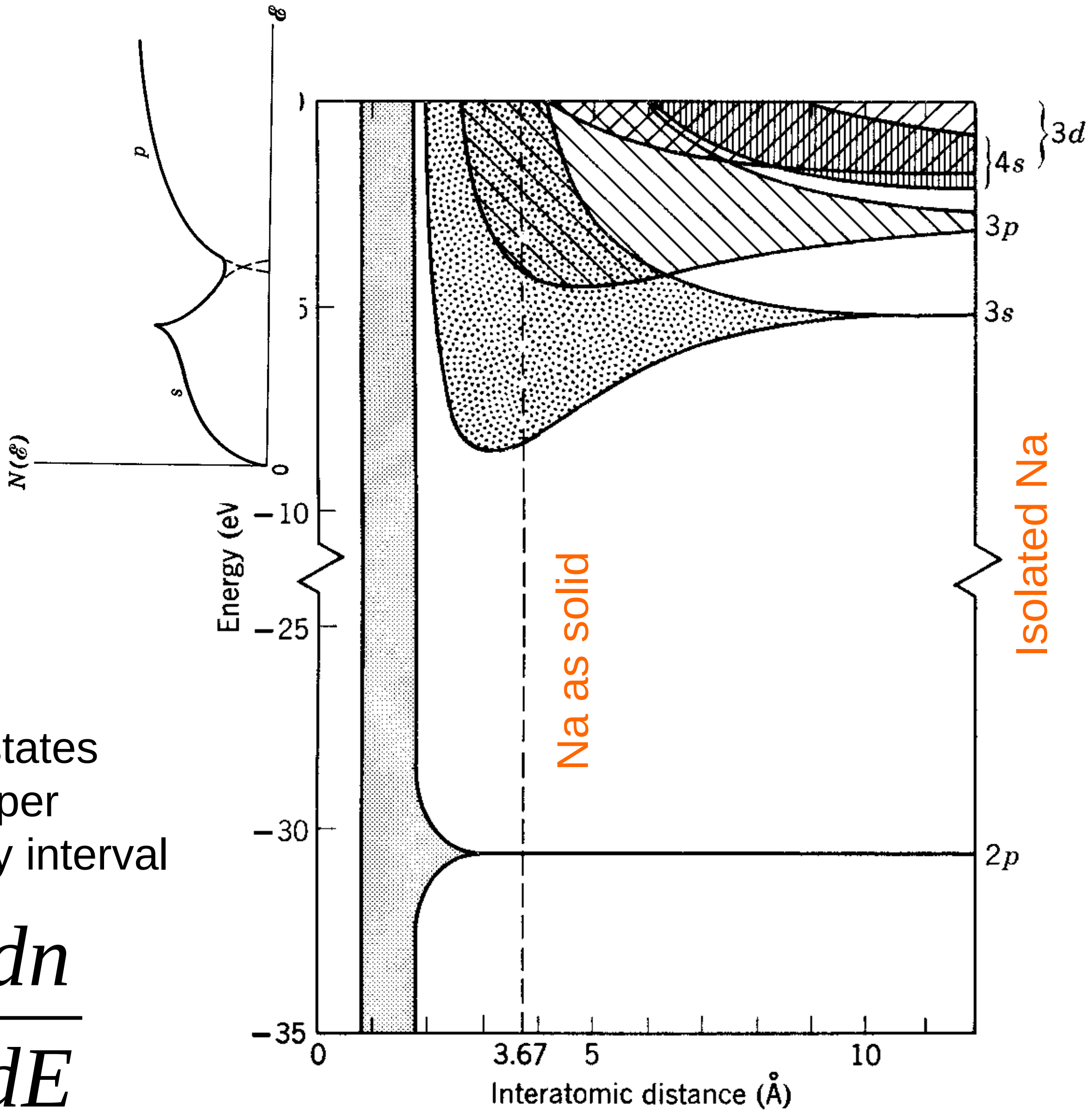


conduction
band

valence
band

core
electrons

Density of States



Density of states = # states per Energy interval

$$D(E) = \frac{dn}{dE}$$

Calculating Averages

$$\langle Q \rangle = \int Q(\varepsilon)\, N(\varepsilon)\, D(\varepsilon) d\varepsilon$$

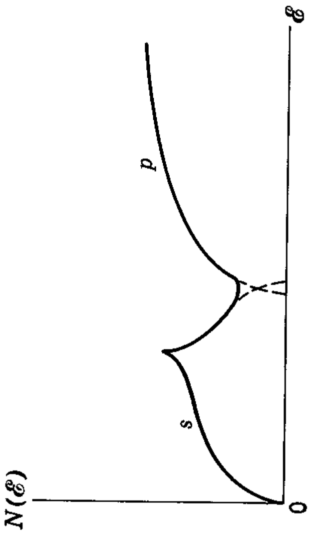
if were motivated enough to normalize ND before-hand

$$1 = \int N(\varepsilon)\, D(\varepsilon) d\varepsilon$$

$$\langle Q \rangle = \frac{\int Q(\varepsilon)\, N(\varepsilon)\, D(\varepsilon) d\varepsilon}{\int N(\varepsilon)\, D(\varepsilon) d\varepsilon}$$

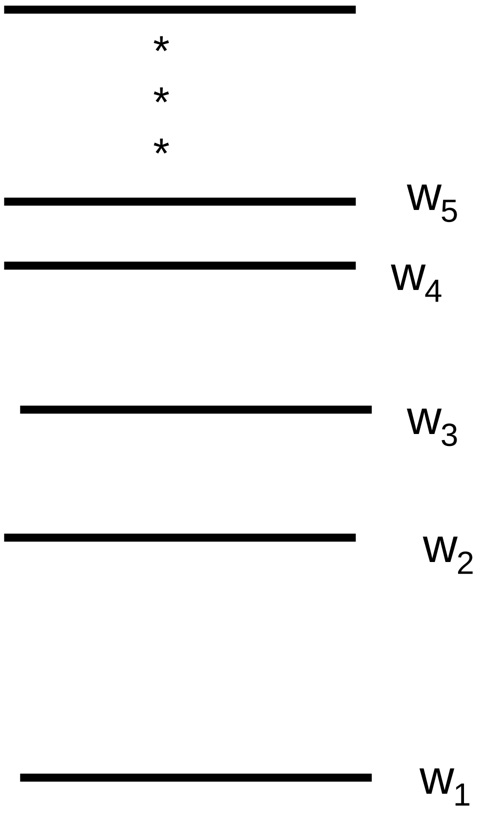
if decided to do it later

Many, many closely-spaced states, but with restriction on filling



Just did this

Finite number of states, but with restriction on filling



D(ε) is funky notation, so use w_i

Harris 8.2-8.3

Macroscopic Descriptions

Entropy & Flow of Time

James Sethna @ Cornell: Chapter 5
http://pages.physics.cornell.edu/sethna/StatMech/EntropyOrderParametersComplexity.pdf

http://www.tim-thompson.com/entropy1.html

http://en.wikipedia.org/wiki/Entropy_%28statistical_thermodynamics%29
http://en.wikipedia.org/wiki/Entropy
http://en.wikipedia.org/wiki/Ludwig_Boltzmann
http://en.wikipedia.org/wiki/Satyendra_Nath_Bose
http://en.wikipedia.org/wiki/Fermi_distribution

Types of Entropy

Entropy is what an equation defines it to be.

Wiki: Carnot

- Thermodynamic Entropy

$$dS = \frac{dQ}{T}$$

H (8-3)

- Statistical Mechanics Entropy

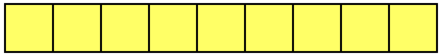
Wiki: boltz

$$S \quad = \quad k_B \ln(\# states) \quad or \quad -k_B \langle \ln\ p_i \rangle = -k_B \sum_i p_i \ln p_i$$

H (8-2)

- Information Entropy

$$S \quad = \quad \log_2(\# combinations) \quad or \quad \langle \log_2\ p_i \rangle = \sum_i p_i \log_2 p_i$$



http://en.wikipedia.org/wiki/Entropy_%28statistical_thermodynamics%29

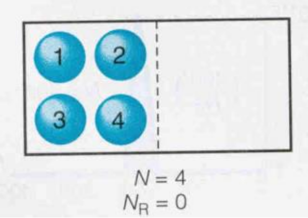
Shannon quote (1949):

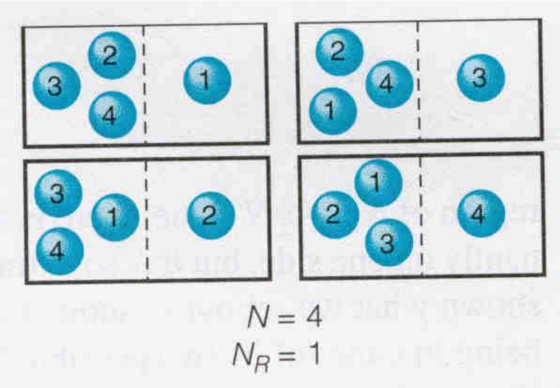
The theory was in excellent shape, except that he needed a good name for “missing information”. “Why don’t you call it entropy”, von Neumann suggested. “In the first place, a mathematical development very much like yours already exists in Boltzmann’s statistical mechanics, and in the second place, no one understands entropy very well, so in any discussion you will be in a position of advantage.

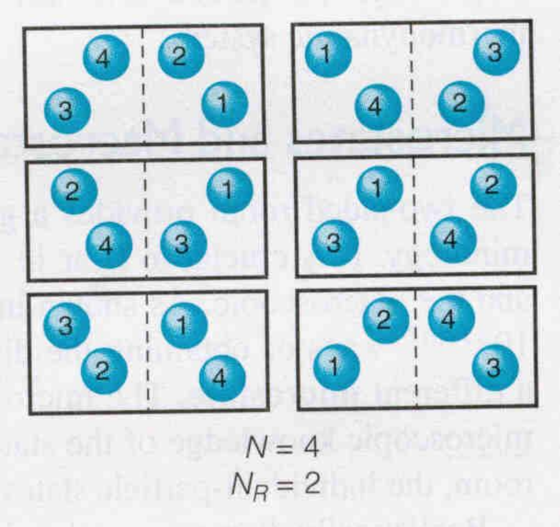
Wiki: History_of_Entropy

Stat Mech Example

$$S = k_B \ ln(\#microstates)$$







$S = k_B \ln(1)$

$S = k_B \ln(4)$

$S = k_B \ln(6)$

$S = 0$

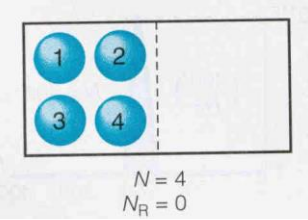
$S = 1.38\ k_B$

$S = 1.79\ k_B$

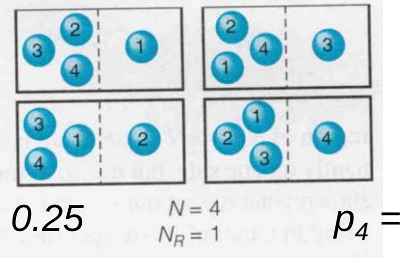
Stat Mech Example

$$S \quad = \quad -k_B \left\langle \ln\ p_i \right\rangle \quad = \quad -k_B \sum_i p_i \ln p_i$$

$p_i = 1$

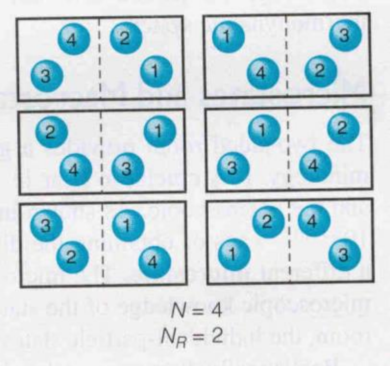


$p_1 = 0.25$ $p_3 = 0.25$



$p_2 = 0.25$ $p_4 = 0.25$

$p_i = 0.167$



$S = -k_B\ 1\ ln(1)$

$= 0$

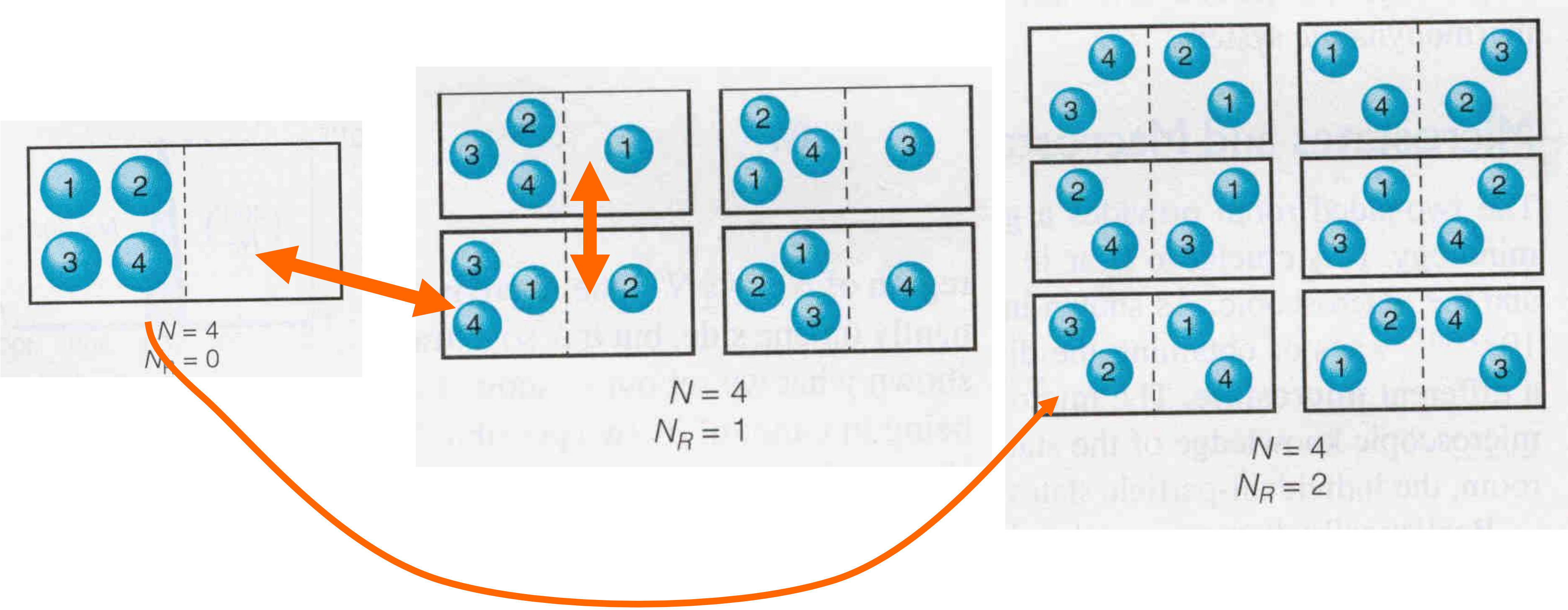
$$S = -k_B \left\{ \begin{matrix} 0.25\ln(0.25) \\ +0.25\ln(0.25) \\ +0.25\ln(0.25) \\ +0.25\ln(0.25) \end{matrix} \right\}$$

$S = 1.38\ k_B$

$$S = -k_B\ 6\ \{0.167\ln(0.167)\}$$

$S = 1.79\ k_B$

Flow of Time



Changes between microstates are generally easily reversible.

It is not necessarily likely that changes between macrostates can be reversed .

Harris 8.6
Back to Probability Distributions

COMPARING PROBABILITIES $\Psi^*\Psi$
for
Indistinguishable Boson/Fermion Particles
to those
without worrying about B/F requirements

OR

what do the B/F requirements

do to probabilities?

Distinguishable Particle Probabilities

One particle in a state β

$\Psi_{tot} = \Psi_\beta(1)$

Prob = $\Psi_{tot}{}^* \Psi_{tot} = \Psi_\beta(1)^* \Psi_\beta(1) = 1$

Two particles in a state β

$\Psi_{tot} = \Psi_\beta(1)\, \Psi_\beta(2)$

Prob = $\Psi_\beta(1)^* \Psi_\beta(1) \quad \Psi_\beta(2)^* \Psi_\beta(2) = 1$

Three particles in a state β

$\Psi_{tot} = \Psi_\beta(1)\, \Psi_\beta(2)\, \Psi_\beta(3)$

Prob = $\Psi_\beta(1)^* \Psi_\beta(1) \quad \Psi_\beta(2)^* \Psi_\beta(2) \quad \Psi_\beta(3)^* \Psi_\beta(3) = 1$

So what ? Nothing special happens here…..

Indistinguishable Boson Probabilities

One particle in a state β

$$\Psi_{tot} = \Psi_{\beta}(1)$$

$$\text{Prob} = \Psi_{tot}^{*}\,\Psi_{tot} = \Psi_{\beta}(1)^{*}\,\Psi_{\beta}(1) = 1$$

Two particles in a state β

$$\Psi_{tot} = \sqrt{\frac{1}{2}}\left[\Psi_{\beta}(1)\,\Psi_{\beta}(2) + \Psi_{\beta}(2)\,\Psi_{\beta}(1)\right] = 2\sqrt{\frac{1}{2}}\,\Psi_{\beta}(1)\,\Psi_{\beta}(2)$$

$$\text{Prob} = \left|\,2\sqrt{\frac{1}{2}}\,\Psi_{\beta}(1)\,\Psi_{\beta}(2)\,\right|^{2} = 2 = 2!$$

Three particles in a state β

$$\Psi_{tot} = \sqrt{\frac{1}{6}}\left[\,\Psi_{\beta}(1)\,\Psi_{\beta}(2)\,\Psi_{\beta}(3) + \ldots\,\right]$$

$$\text{Prob} = \left|\,6\sqrt{\frac{1}{6}}\,\Psi_{\beta}(1)\,\Psi_{\beta}(2)\,\Psi_{\beta}(3)\,\right|^{2} = 6 = 3!$$

If there are already n bosons in a state,
the probability of one more joining them is enhanced by (1+n)
than what the prob would be w/o indistinguishability requirements

Indistinguishable Fermion Probabilities

One particle in a state β

$$\Psi_{tot} = \Psi_\beta(1)$$

$$\text{Prob} = \Psi_{tot}^* \Psi_{tot} = \Psi_\beta(1)^* \Psi_\beta(1) = 1$$

Two particles in a state β

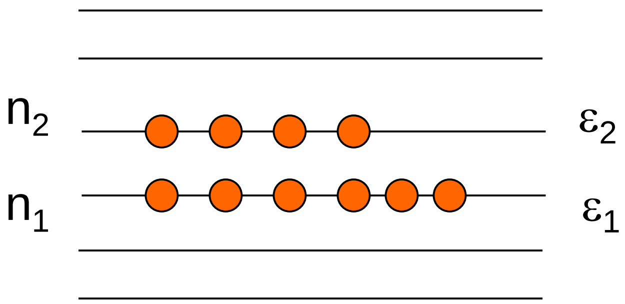
$$\Psi_{tot} = \sqrt{\tfrac{1}{2}}[\Psi_\beta(1)\,\Psi_\beta(2) - \Psi_\beta(2)\,\Psi_\beta(1)] = 0$$

$$\text{Prob} = 0$$

If there are already n fermions in a state,
the probability of one more joining them is enhanced by (1-n)
than what the prob would be w/o indistinguishability requirements

Principle of Detailed Balance

For two states of a system with fixed total energy,



Where the particles can jump between states by some unknown mechanism,

Rate of upward going transitions = Rate of downward going transitions

$$\mathbf{n_1\ Rate_{1\rightarrow 2} = n_2\ Rate_{2\rightarrow 1}}$$

transitions/sec
per
particle

$$\frac{n_1}{n_2} = \frac{R_{2\rightarrow 1}}{R_{1\rightarrow 2}}$$

Detailed Balance

distinguishable particles

(but with no other special requirements)

$$n_1 \, R_{1\to 2} \quad = \quad n_2 \, R_{2\to 1}$$

$$\frac{n_1}{n_2} = \frac{R_{2\to 1}}{R_{1\to 2}}$$

Since by the Boltzmann distribution $n \sim e^{-\varepsilon/kT}$

$$\frac{e^{-\varepsilon_1/kT}}{e^{-\varepsilon_2/kT}} = \frac{n_1}{n_2} = \frac{R_{2\to 1}}{R_{1\to 2}}$$

Gives us the ratio of the two transition rates

Detailed Balance

indistinguishable bosons

$$n_1 \; R_{1\to2}^{boson} \quad = \quad n_2 \; R_{2\to1}^{boson}$$

$$boson\,transition\;\;probabilities\,are\,enhanced \quad R_{1\to2}^{boson} = \left(1+n_2\right) R_{1\to2}$$

$$n_1 \left(1+n_2\right) R_{1\to2} \quad = \quad n_2 \left(1+n_1\right) R_{2\to1}$$

$$\frac{n_1\left(1+n_2\right)}{n_2\left(1+n_1\right)} \quad = \quad \frac{R_{2\to1}}{R_{1\to2}} \quad = \quad \frac{e^{-\varepsilon_1/kT}}{e^{-\varepsilon_2/kT}}$$

$$\frac{n_1}{1+n_1}\, e^{\varepsilon_1/kT} \quad = \quad \frac{n_2}{1+n_2}\, e^{\varepsilon_2/kT}$$

$$\frac{n_1}{1+n_1}\, e^{\varepsilon_1/kT} \quad = \quad \frac{n_2}{1+n_2}\, e^{\varepsilon_2/kT}$$

L & R sides are unrelated except for Temp

$$\frac{n_1}{1+n_1}\, e^{\varepsilon_1/kT} \quad = \quad some\,const \quad = \quad e^{-\alpha}$$

$$\frac{n_1}{1+n_1} \quad = \quad e^{-\alpha-\varepsilon_1/kT}$$

$$n_1 \quad = \quad \left(1+n_1\right) \quad e^{-\alpha-\varepsilon_1/kT}$$

$$n_1 = \left(1+n_1\right) \; e^{-\alpha - \varepsilon_1/kT}$$

$$n_1 = e^{-\alpha - \varepsilon_1/kT} \quad + \quad n_1\, e^{-\alpha - \varepsilon_1/kT}$$

$$n_1 \left(1 - e^{-\alpha - \varepsilon_1/kT}\right) = e^{-\alpha - \varepsilon_1/kT}$$

$$n_1 = \frac{e^{-\alpha - \varepsilon_1/kT}}{1 - e^{-\alpha - \varepsilon_1/kT}}$$

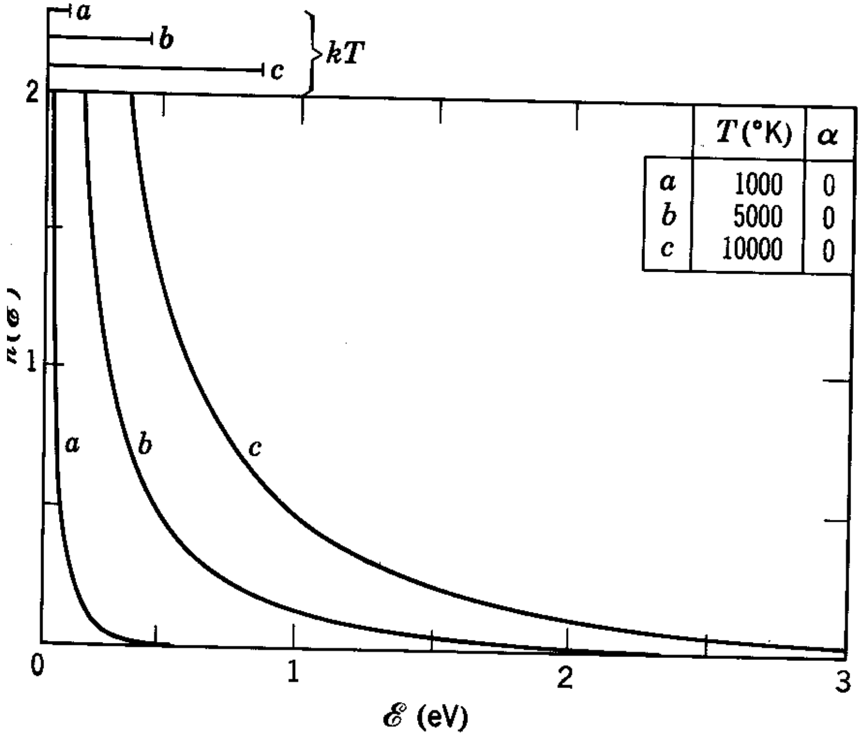
$$n_1 = \frac{1}{e^{\alpha + \varepsilon_1/kT} - 1}$$

!

Bose distribution function

Probable # bosons of an energy ε
in a system of fixed total energy at a temperature T

$$n(\varepsilon) = \frac{1}{e^{\alpha} e^{\varepsilon/kT} - 1}$$



Detailed Balance

indistinguishable fermions

(short derivation)

$$n_1 \, R_{1\to 2}^{fermion} \quad = \quad n_2 \, R_{2\to 1}^{fermion}$$

$fermion\ transition\ \ probabilities\ are\ de-enhanced \quad R_{1\to 2}^{fermion} = (1-n_2)\, R_{1\to 2}$

$$n_1 \,(1-n_2)\, R_{1\to 2} \quad = \quad n_2 \,(1-n_1)\, R_{2\to 1}$$

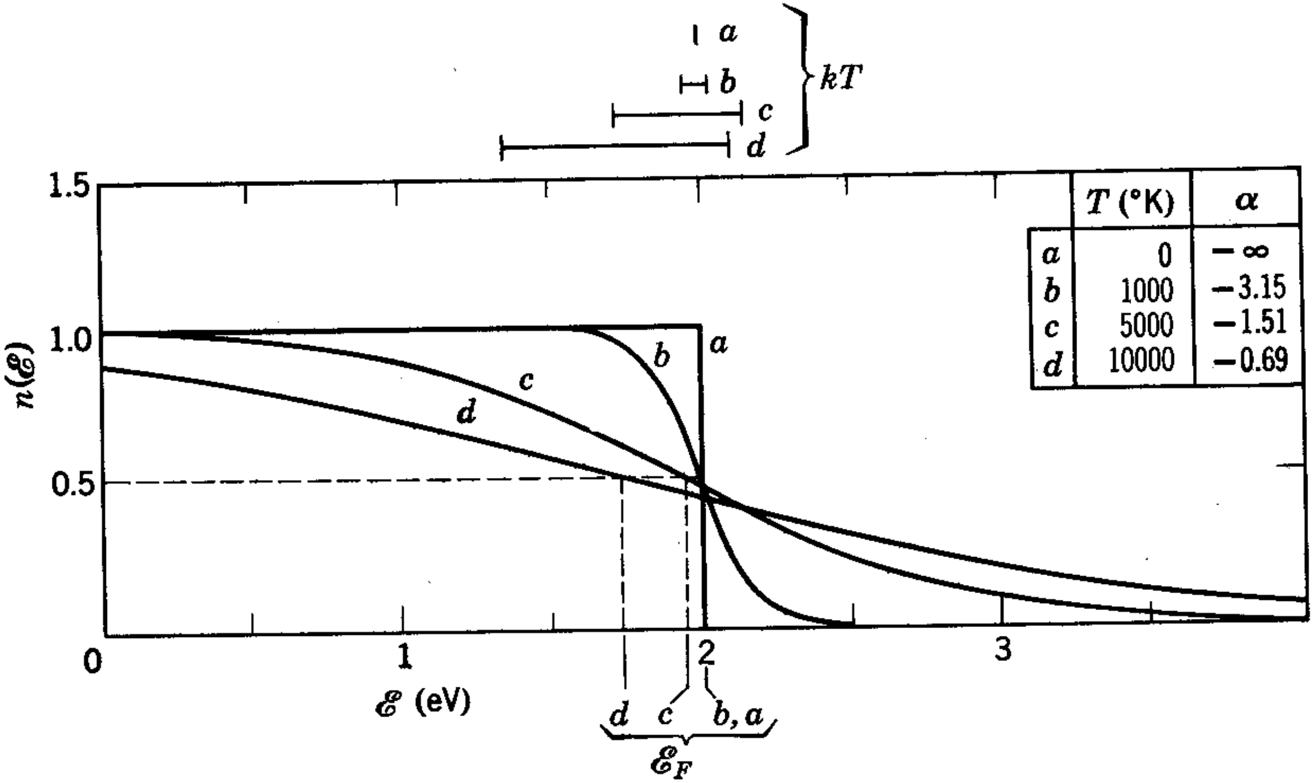
$$\frac{n_1}{1-n_1}\, e^{\varepsilon_1 / kT} \quad = \quad \frac{n_2}{1-n_2}\, e^{\varepsilon_2 / kT}$$

$$n_1 \quad = \quad \frac{1}{e^{\alpha + \varepsilon_1 / kT} + 1}$$

Fermi distribution function

Probable # fermions of an energy ε
in a system of fixed total energy at a temperature T

$$n(\varepsilon) = \frac{1}{e^{\alpha} e^{\varepsilon/kT} + 1}$$



SUMMARY
of
Distribution Functions

and

what is this α *thing?*

Collected Distribution Functions

Boltzmann	$n(\varepsilon) = \dfrac{1}{e^{\alpha} e^{\varepsilon / kT}}$
Bose	$n(\varepsilon) = \dfrac{1}{e^{\alpha} e^{\varepsilon / kT} - 1}$
Fermi	$n(\varepsilon) = \dfrac{1}{e^{\alpha} e^{\varepsilon / kT} + 1}$

Normalization Interpretation

$$\int_0^\infty n(\varepsilon)\, d\varepsilon \;=\; 1$$

Boltz	$n(\varepsilon) = \dfrac{1}{e^{\alpha} e^{\varepsilon/kT}}$	$e^{\alpha} = kT$
Bose	$n(\varepsilon) = \dfrac{1}{e^{\alpha} e^{\varepsilon/kT} - 1}$	α = a real mess $e^{-\alpha} \approx \dfrac{N_{tot}(2\pi\hbar)^3}{V(2\pi mkT)^{3/2}}$ *
Fermi	$n(\varepsilon) = \dfrac{1}{e^{\alpha} e^{\varepsilon/kT} + 1}$	α = a real mess $e^{-\alpha} \approx \dfrac{N_{tot}(2\pi\hbar)^3}{V(2\pi mkT)^{3/2}}$ *

This interpretation may not be so useful for Bose & Fermi distributions

* For N_{tot} free particles strictly confined to a 3-D region of space of volume V.

Chemical Potential Interpretation

$$\mu = -\alpha \; kT$$

Boltz	$n(\varepsilon) = \dfrac{1}{e^{(\varepsilon-\mu)/kT}}$	$e^{\alpha} = e^{-\mu/kT}$
Bose	$n(\varepsilon) = \dfrac{1}{e^{(\varepsilon-\mu)/kT} - 1}$	$e^{\alpha} = e^{-\mu/kT}$
Fermi	$n(\varepsilon) = \dfrac{1}{e^{(\varepsilon-\mu)/kT} + 1}$	$e^{\alpha} = e^{-\mu/kT}$

A uniform description for all three distributions.

Used for Bose distribution.

- Problem: chemical potential is not an easily measured or well understood quantity
(by most people)

  - Defn: How the total energy of a system changes as one changes the ***count*** of objects

  - How does the total NRG change if we replace a 10 eV photon with two 5 eV photons? Ans: it doesn't, μ=0
. *this system is called a photon/phonon gas*

  - How does the total NRG change if we replace a KE 10 eV proton with two 5 eV protons? Ans: some

  - How does the total NRG change if we replace a KE 10 eV H-atom with two 5 eV H-atoms? Ans: a v.s. amount

50% Probability Interpretation

At what energy is the probability 50% of it's maximum value?
(called the Fermi energy ε_f)

Boltz	*Not used*	
Bose	*Not used*	
Fermi	$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\varepsilon_f)/kT}+1}$	when $\varepsilon = \varepsilon_f$ $\frac{1}{e^{(0)/kT}+1} = \frac{1}{2}$

Used for Fermi distribution.

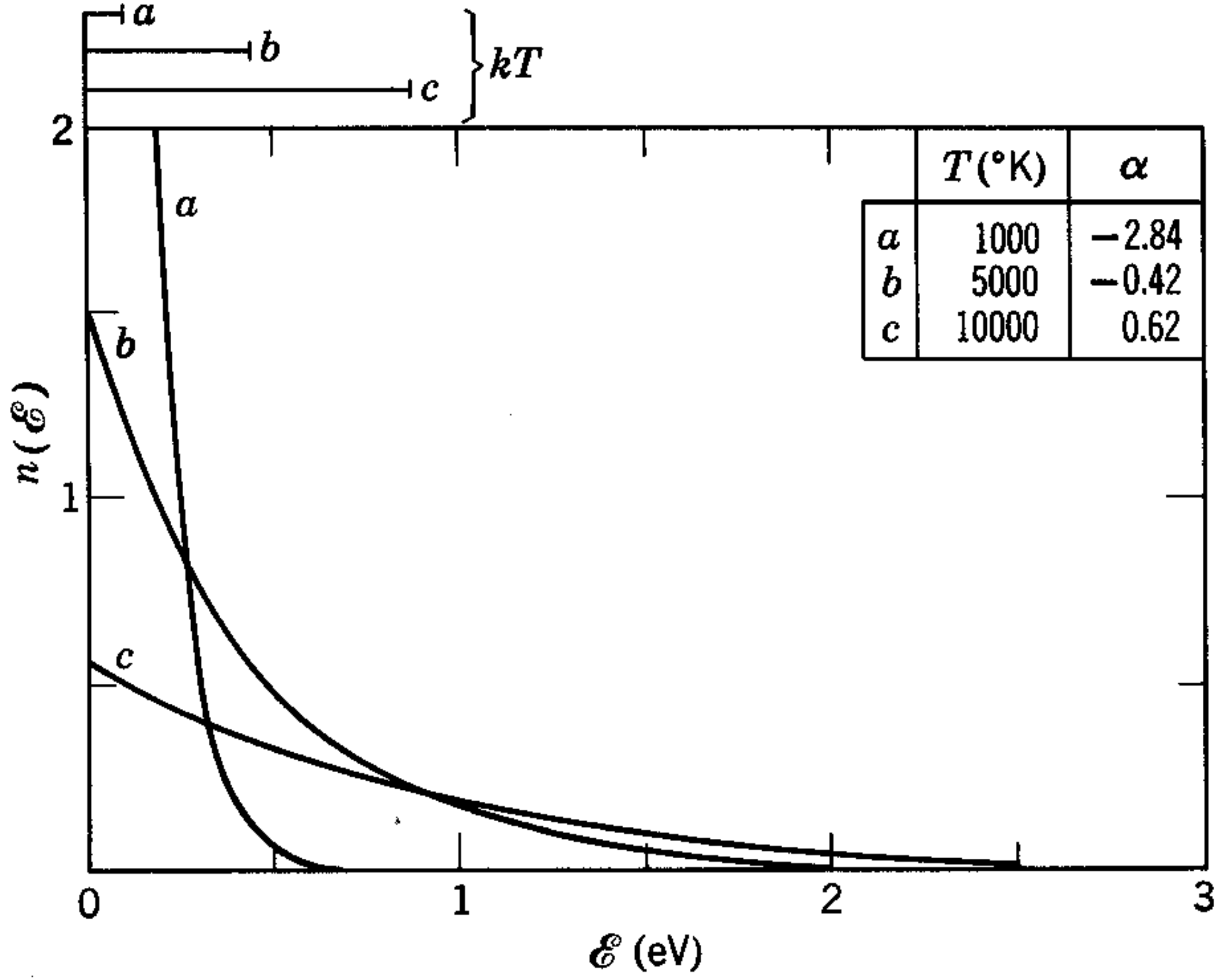
Summary of Common Usage

Boltz	$n(\varepsilon) = \frac{1}{e^{\alpha} e^{\varepsilon/kT}}$	Probability $e^{\alpha} = kT$
Bose	$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT} - 1}$	Chemical Potl μ
Fermi	$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\varepsilon_f)/kT} + 1}$	Fermi Energy ε_f

Boltzmann

normalization
interpretation

$e^{\alpha} = 1/kT$

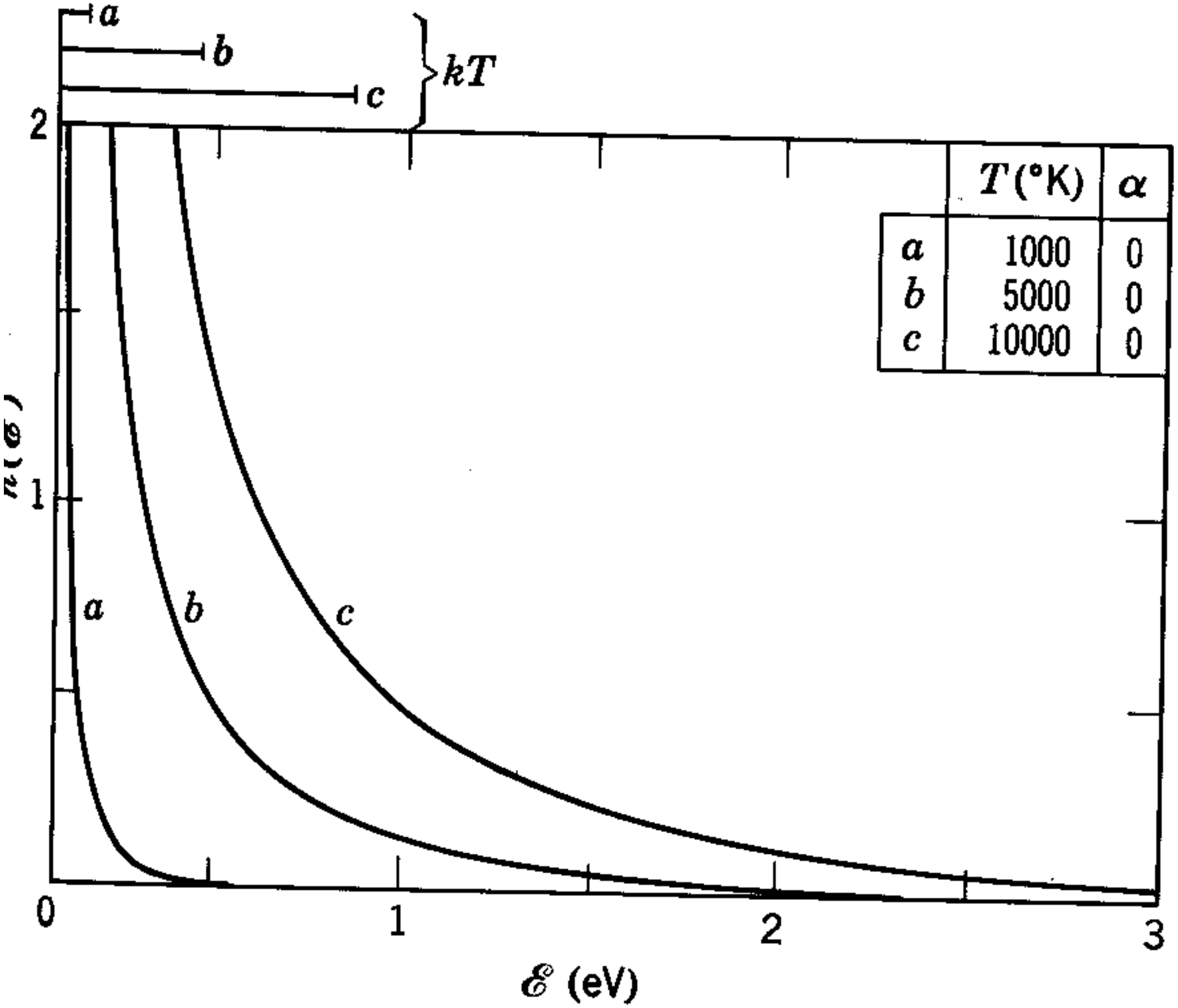


	T (°K)	α
a	1000	−2.84
b	5000	−0.42
c	10000	0.62

Bose for phonon gas

chemical
interpretation

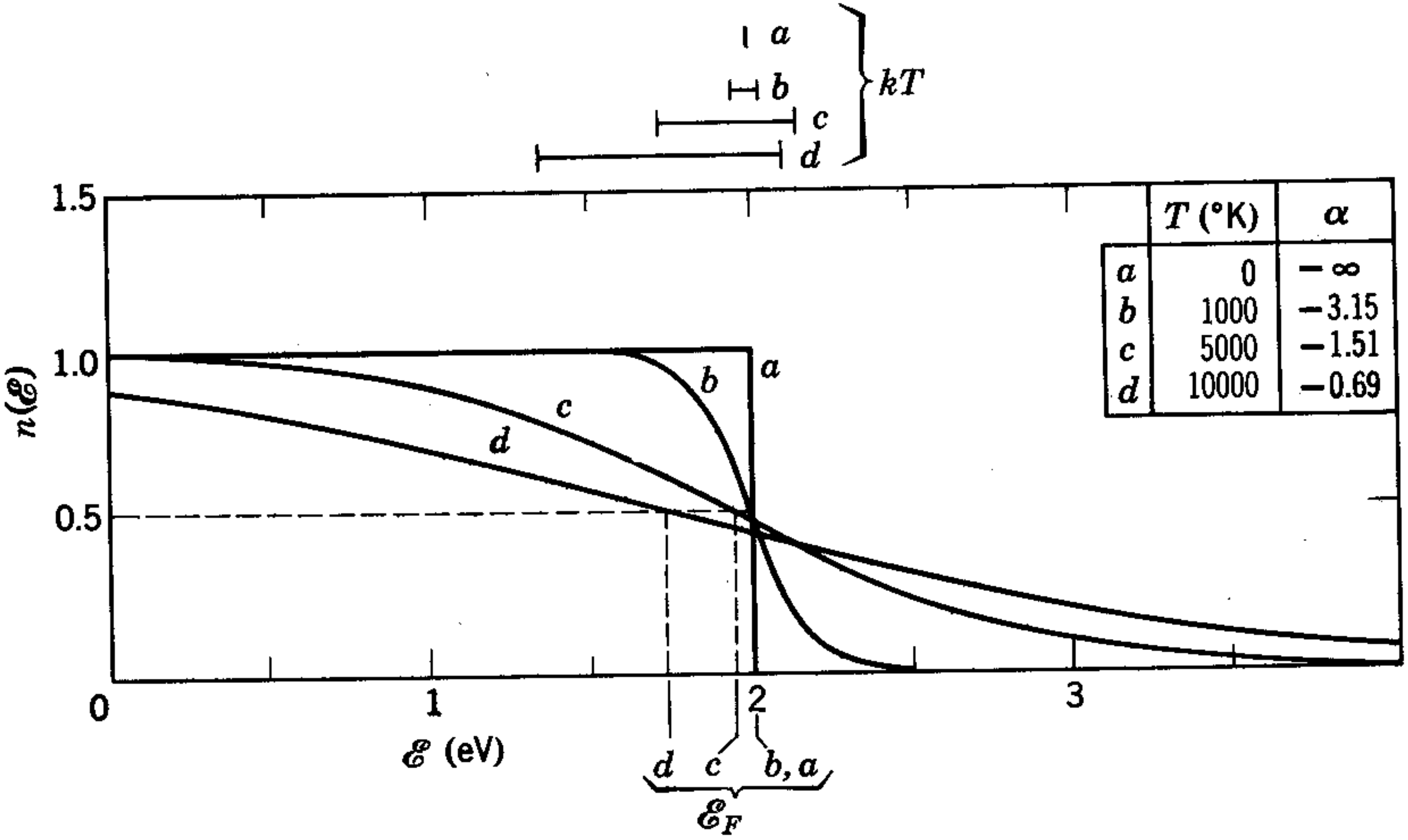
$\mu = 0$



Fermi

½ value interpretation

$\alpha = -\varepsilon_f / kT$



	T (°K)	α
a	0	−∞
b	1000	−3.15
c	5000	−1.51
d	10000	−0.69

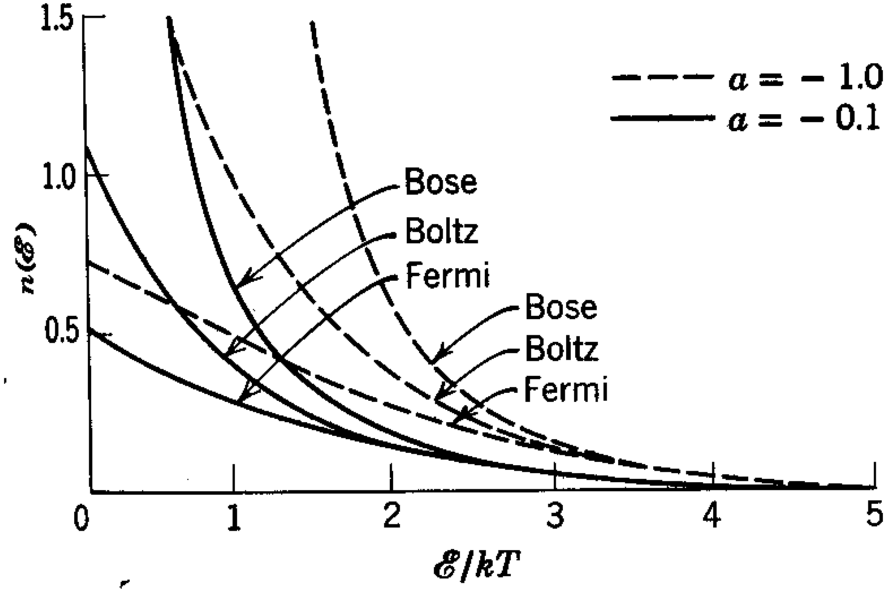


Figure 11-4 The Boltzmann, Bose, and Fermi distribution functions plotted versus $\mathscr{E}/kT$ for two different values of α, -0.1 and -1.0. It should be noted that the dashed curves, if moved to the left $(-0.1) - (-1.0) = 0.9$ units, would coincide exactly with the solid curves. This observation may provide some further insight into the physical interpretation of α.

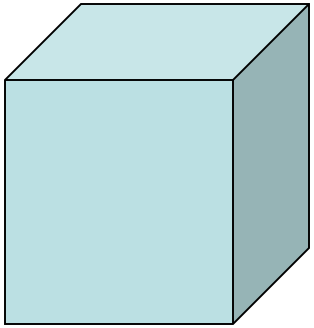
EXAMPLES OF QUANTUM GASES & FLUIDS

Harris 8.7-8.10

- Density of States in a 3D bound system (massive objects)
- Electron Gas: Conduction Electrons
- Photon Gas: Blackbody Spectrum
- Gas Laws: ‘PV=nRT’
- Bose Gases: 4He
- Bose-Einstein Condensates
- Specific Heat of Solids
- Laser Systems

Density of States
in 3D confined system

Harris 8.7



In a 3D slab of metal, e’s are free to move but must remain on the inside

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + 0\Psi \quad = \quad E\Psi$$

Solutions are of the form:

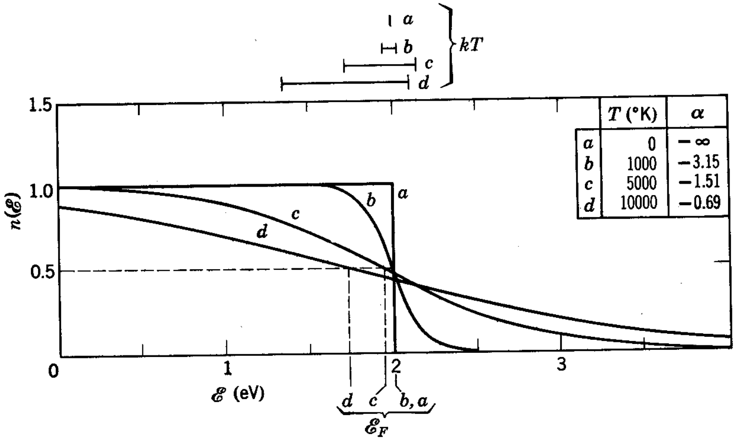
$$\Psi \quad = \quad \Psi(xyz) = \sqrt{\frac{8}{L^3}} \quad \sin k_x x \quad \sin k_y y \quad \sin k_z z$$

$$\frac{n_z \pi}{L}$$

With nrg’s:

$$\varepsilon \quad = \quad \frac{h^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

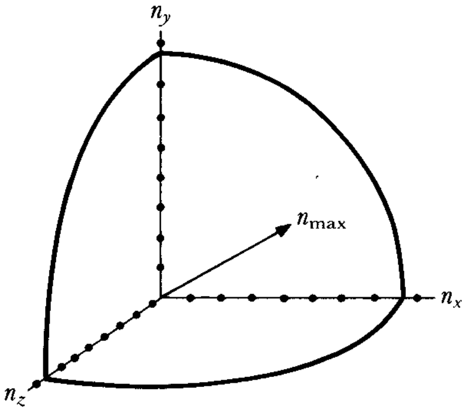
At T = 0, all states are filled up to the Fermi nrg



	T (°K)	α
a	0	−∞
b	1000	−3.15
c	5000	−1.51
d	10000	−0.69

$$\varepsilon_{fermi} = \frac{h^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)_{\max}$$

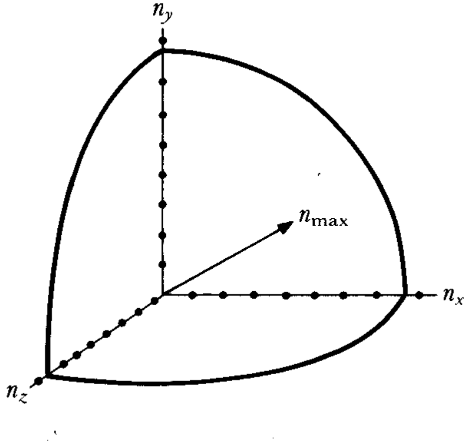
A useful way to keep track of the states that are filled is:



$$n_x^2 + n_y^2 + n_z^2 \equiv n^2{}_{\max}$$

$$\varepsilon_{fermi} = \frac{h^2}{8mL^2} \quad n^2_{\max}$$

total number of states up to an energy $\varepsilon_{\text{fermi}}$:



2s+1 → 2 spin states

$$\mathcal{N} = 2 \quad \frac{1}{8} \left(\begin{matrix} volume \\ of \\ sphere \end{matrix} \right) = 2 \, \frac{1}{8} \, \frac{4\pi n^3_{\max}}{3}$$

$$\varepsilon_{fermi} = \frac{h^2}{8m} \left(\frac{3N}{\pi V} \right)^{2/3} \rightarrow \frac{\pi^2 \hbar^2}{m} \left(\frac{3}{2\pi\sqrt{2}} \, \frac{N}{V} \right)^{2/3}$$

Harris (8-43)

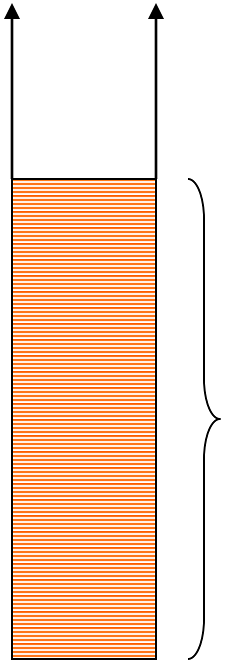
states/volume ~ # free e’s / volume

Sample Numerical Values for Copper slab

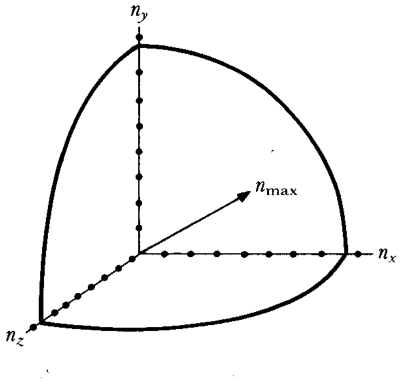
$$\frac{\mathcal{N}}{V} = 8.96\ \text{gm/cm}^3 \quad 1/63.6\ \text{amu} \quad 6\text{e}23 = 8.5\text{e}22\ \#/\text{cm}^3 = 8.5\text{e}28\ \#/\text{m}^3$$

$$\varepsilon_{fermi} = \frac{h^2}{8m}\left(\frac{3\,N}{\pi\,V}\right)^{2/3} \longrightarrow \varepsilon_{\text{fermi}} = 7\ \text{eV}$$

$$n_{\text{max}} = 4.3\ \text{e}\ 7$$



$\varepsilon_{\text{fermi}}$ = 7 eV



$$\overline{KE} = \frac{3}{2}kT \sim 0.04\, eV\ \ at\ 300K$$

Density of States

$$Tot\ KE = \int_0^\infty \varepsilon \ N(\varepsilon)\ D(\varepsilon)\, d\varepsilon$$

How many combinations of are there

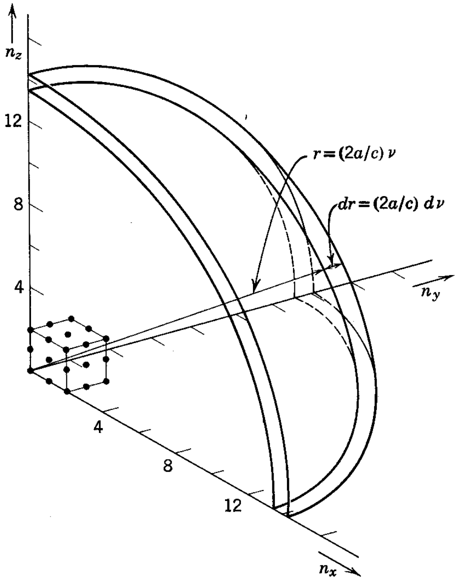
within an energy interval ε to ε + dε ?

$$\varepsilon_{fermi} = \frac{h^2}{8m}\left(\frac{3\,N}{\pi\,V}\right)^{2/3}$$

$$N = \left(\frac{\pi V}{3}\right)\left(\frac{8m\varepsilon}{h^2}\right)^{3/2}$$

$$dN = \left(\frac{\pi V}{3}\right)\ \frac{3}{2}\left(\frac{8m\varepsilon}{h^2}\right)^{1/2}\ \frac{8m}{h^2}\ d\varepsilon$$

$$\frac{dN}{d\varepsilon} = \frac{8\pi V}{h^3}\left(2m^3\right)^{1/2}\ \varepsilon^{1/2} \rightarrow \frac{2m^{3/2}V}{\pi^2\hbar^3\sqrt{2}}\,\varepsilon^{1/2}$$

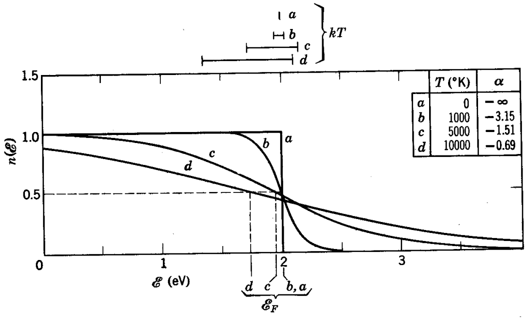


Harris
(8-40)

Electron Gas
Conduction Electrons

Harris 8.7

At $T \neq 0$ the electrons will be spread out among the allowed states



How many electrons are contained in a particular energy range?

$$N(\varepsilon) \qquad\qquad D(\varepsilon)$$

$$\left(\begin{array}{c} \textit{probability of} \\ \textit{this energy occuring} \end{array}\right) \left(\begin{array}{c} \textit{number of ways to have} \\ \textit{a particular energy} \end{array}\right)$$

$$\frac{1}{e^{(\varepsilon-\varepsilon_f)/kT}+1} \qquad \frac{8\pi V}{h^3}\left(2m^3\right)^{1/2} \quad \varepsilon^{1/2}$$

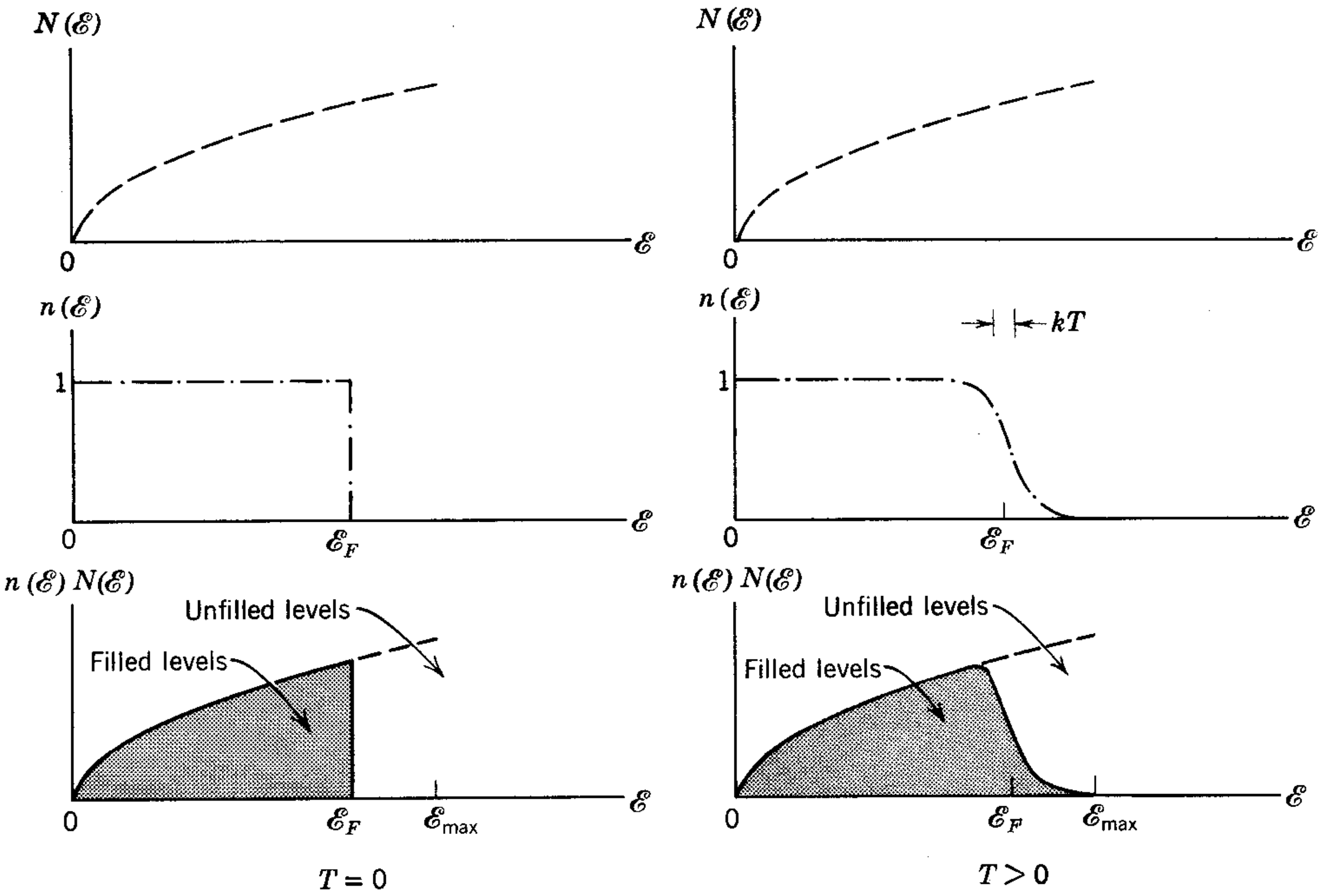
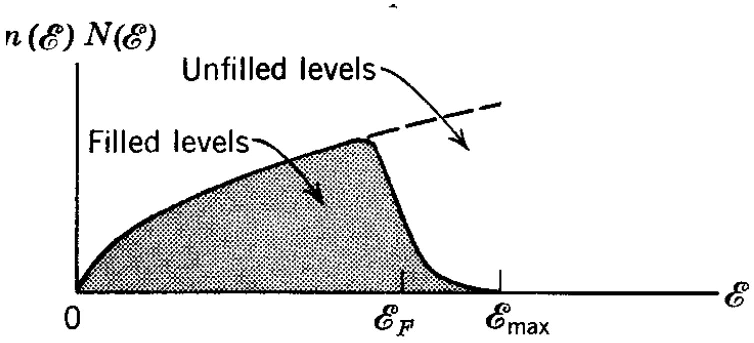


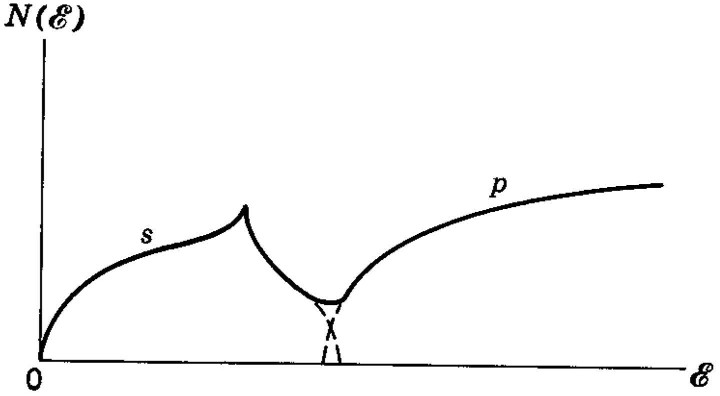
Figure 13-4 *Left:* The distribution with energy of conduction electrons in an unfilled band of width $\mathscr{E}_{\max}$ in a solid at $T = 0$, according to the free electron model. *Right:* The same at a higher temperature.

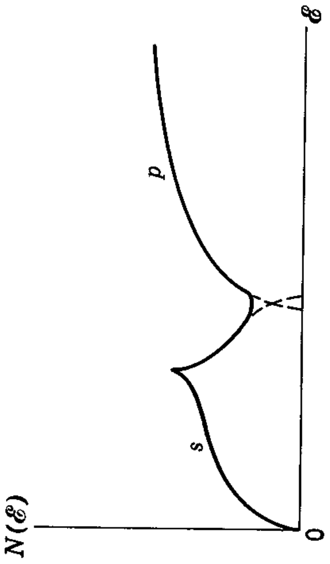
this assumes there are no other issues

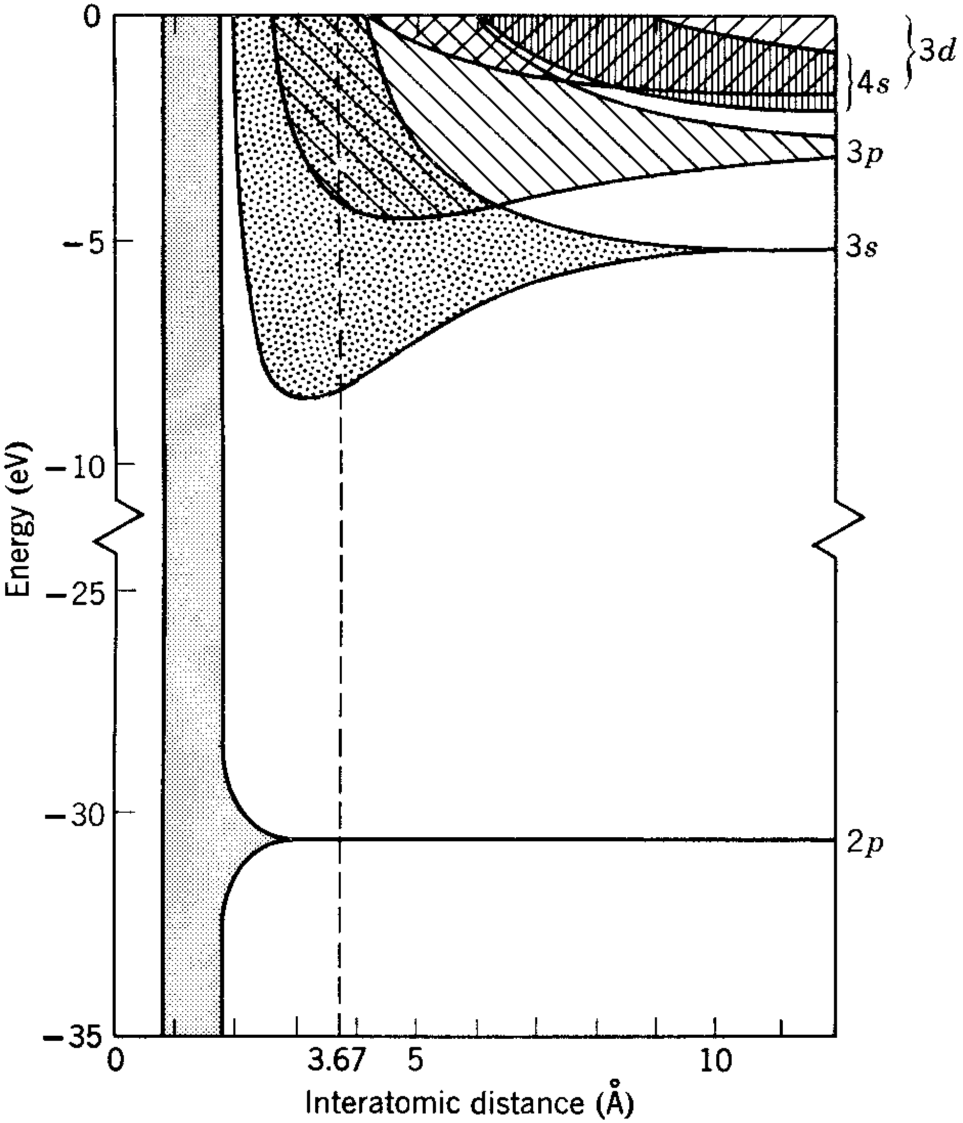
Distribution of States: Simple Free-Electron Model vs Reality



$T > 0$




ℰ
p
s
N(ℰ)
0


0
−5
−10
−25
−30
−35
Energy (eV)
3d
4s
3p
3s
2p
0
3.67
5
10
Interatomic distance (Å)

Photon Gas

Harris 8.8

Photon Gas -- Harris 8.8

$$Tot\ KE = \int_0^\infty \varepsilon\ N(\varepsilon)\ D(\varepsilon)\, d\varepsilon$$

distrib fn

Number of ways
to have a particular
energy

Photon Gas

$$Tot\ KE = \int_0^\infty \varepsilon\ N(\varepsilon)\ D(\varepsilon)\, d\varepsilon$$

Bose

$$N(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT} - 1}$$

$\mu = 0$

$$D(\varepsilon)\, d\varepsilon = \frac{8\pi V}{c^3}\frac{1}{h^3}\varepsilon^2\, d\varepsilon$$

$$\varepsilon = h\nu$$

$$D(\nu)\, d\nu = \frac{8\pi V}{c^3}\nu^2\, d\nu$$

1.

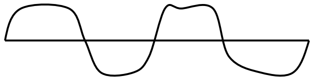
$$\frac{V}{(2\pi)^3}k^2\, dk\, d\Omega_k$$

1.

$$\varepsilon = h\nu = pc = \hbar kc = \frac{1}{2\pi}hkc$$

$$\int d\Omega = 4\pi$$

Factor of 2 for polarization states



Photon Gas

$$Tot\ KE = \int_0^\infty \varepsilon\ N(\varepsilon)\ D(\varepsilon)\, d\varepsilon$$

integrand is the

~ intensity
at an energy ε

$$\frac{8\pi\, \varepsilon^3\, d\varepsilon}{(2\pi\hbar c)^3 \left[e^{\varepsilon/kT} - 1\right]}$$

a.k.a. Planck’s Blackbody Spectrum

Photon Gas

$$Tot\ KE = \int_0^\infty \varepsilon\ N(\varepsilon)\ D(\varepsilon)\, d\varepsilon$$

$$\frac{8\pi\,\varepsilon^3\ d\varepsilon}{(2\pi\hbar c)^3\left[e^{\varepsilon/kT}-1\right]}$$

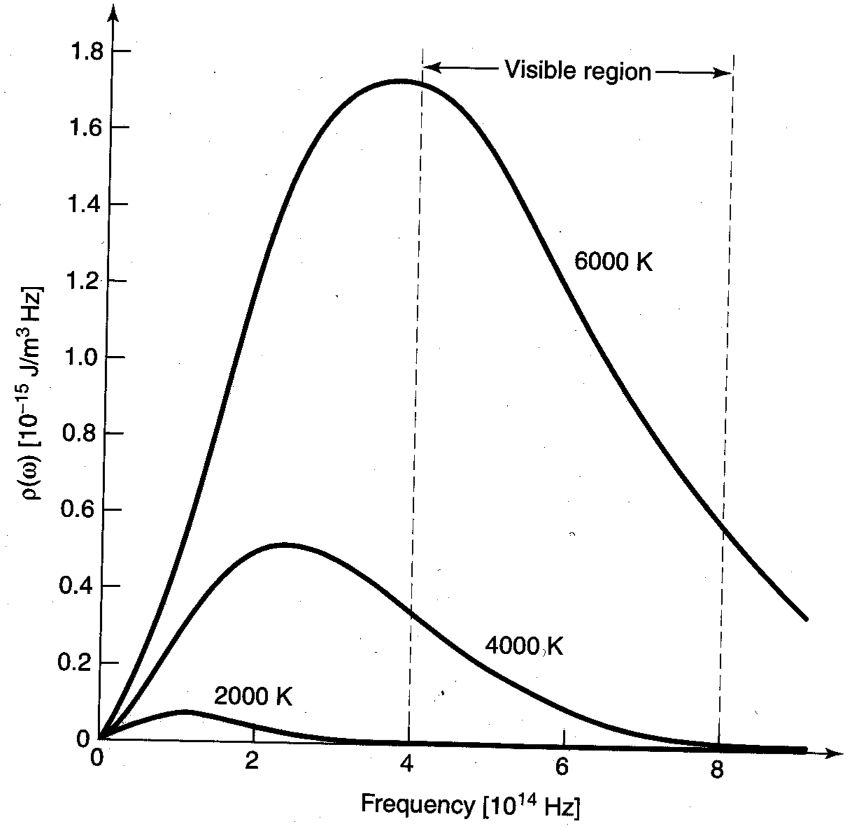


FIGURE 5.9: Planck's formula for the blackbody spectrum, Equation 5.113.

Stefan-Boltzmann Law

Radiated Intensity = $\sigma\, T^4$ W/m^2

σ = 5.67E-8

Wien Displacement Law

$\lambda_{max}T$ = 2.898E-3 m*K

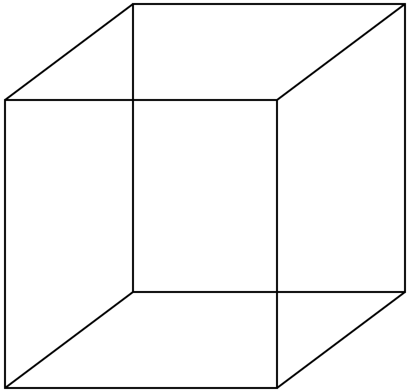
‘Ideal’ Gas Laws

GASES ‘PV=nRT’
Boson / Fermion / don’t care

$$Tot\ KE = \int_0^\infty \varepsilon\ N(\varepsilon)\ D(\varepsilon)\, d\varepsilon$$

distrib fn

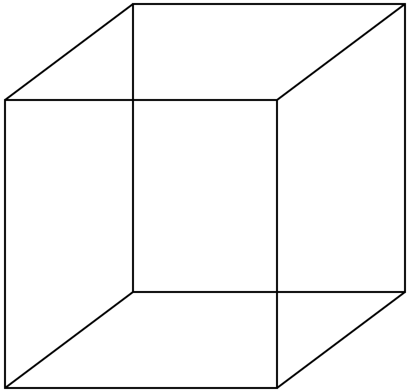
Number of ways to have a particular energy



$$\langle KE \rangle = \frac{Tot\ KE}{N_{tot}}$$

don’t care Gases

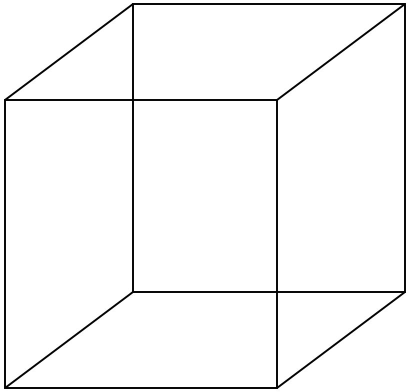
N(ε) = Boltzmann distrib



$$\langle KE \rangle = \frac{3}{2} k\, T$$

½ kT KE per degree of freedom

Boson Gases



Derivation assumes gas
lives in 3D box, infinite square well

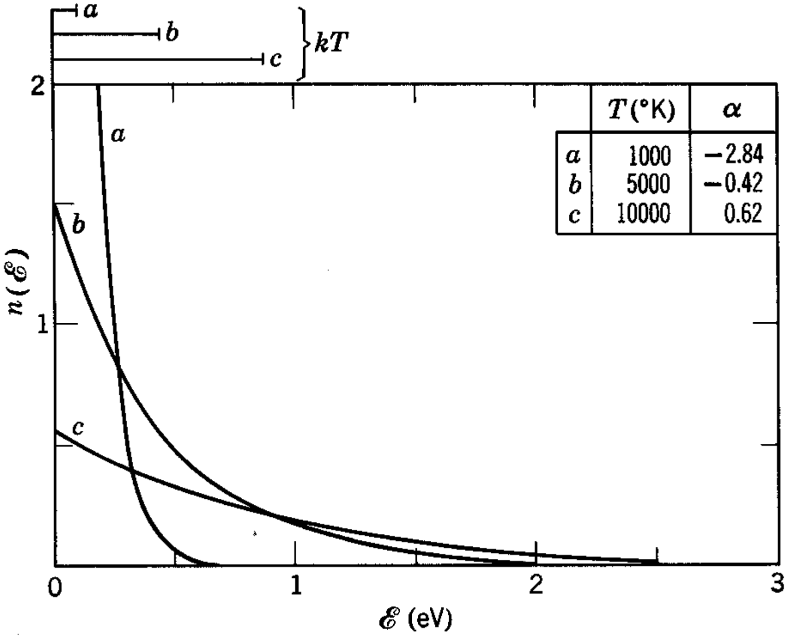
N(ε) = Bose distrib

Small 10^{-5} at STP

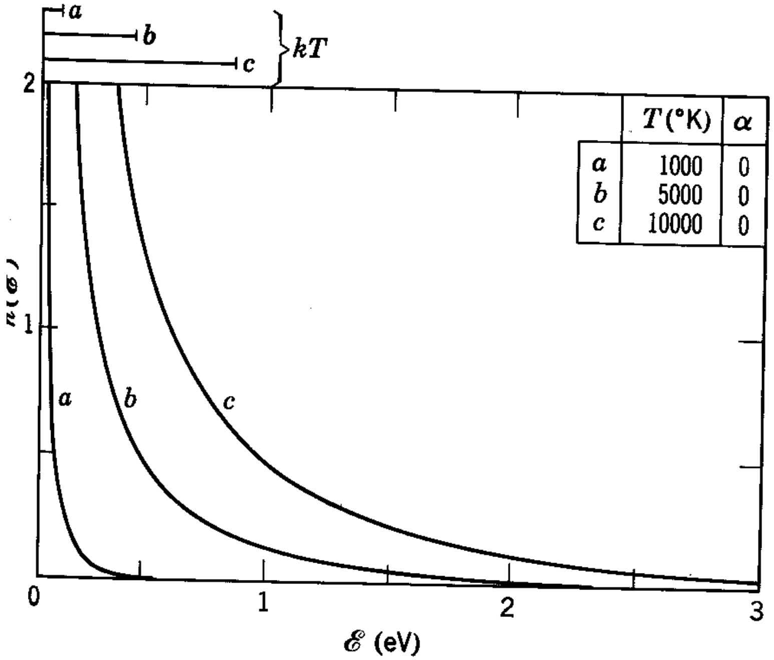
$$\langle KE \rangle = \frac{3}{2} k\,T \left[1 - \frac{1}{2^{5/2}} \frac{N_{tot} \left(2\pi\hbar\right)^3}{V \left(2\pi mkT\right)^{3/2}} \right]$$

Harris (8-42)

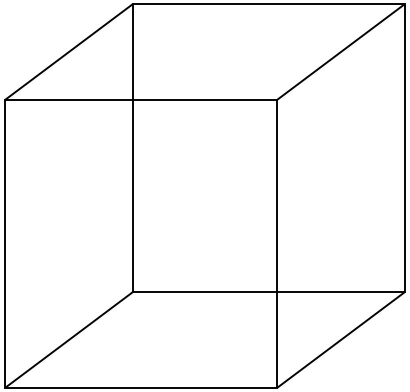
Boltz


a
b
c
kT
2
1
0
1
2
3
n(ℰ)
ℰ (eV)
a
b
c
T(°K) α
a 1000 −2.84
b 5000 −0.42
c 10000 0.62

Bose


a
b
c
kT
2
1
0
1
2
3
n(ℰ)
ℰ (eV)
a
b
c
T(°K) α
a 1000 0
b 5000 0
c 10000 0

Fermi Gases



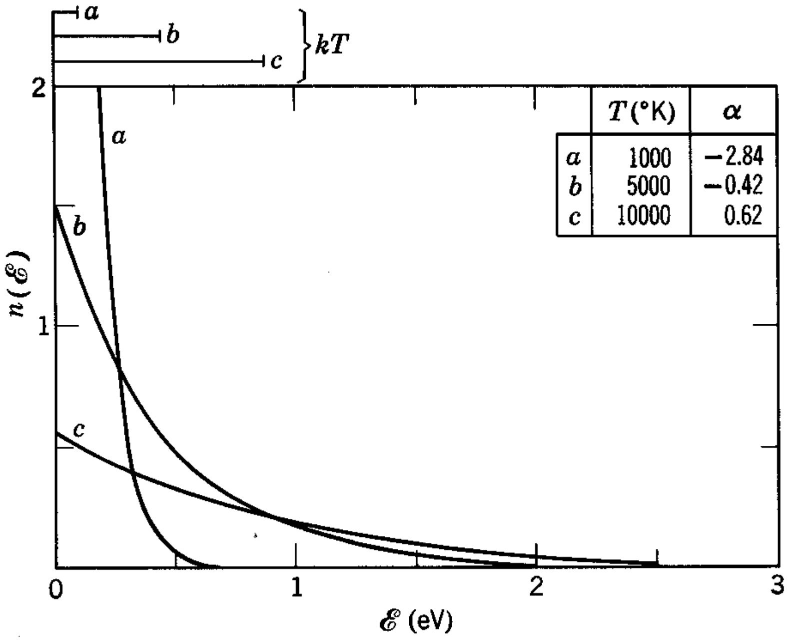
Derivation assumes gas
lives in 3D box, infinite square well

$N(\varepsilon)$ = Fermi distrib

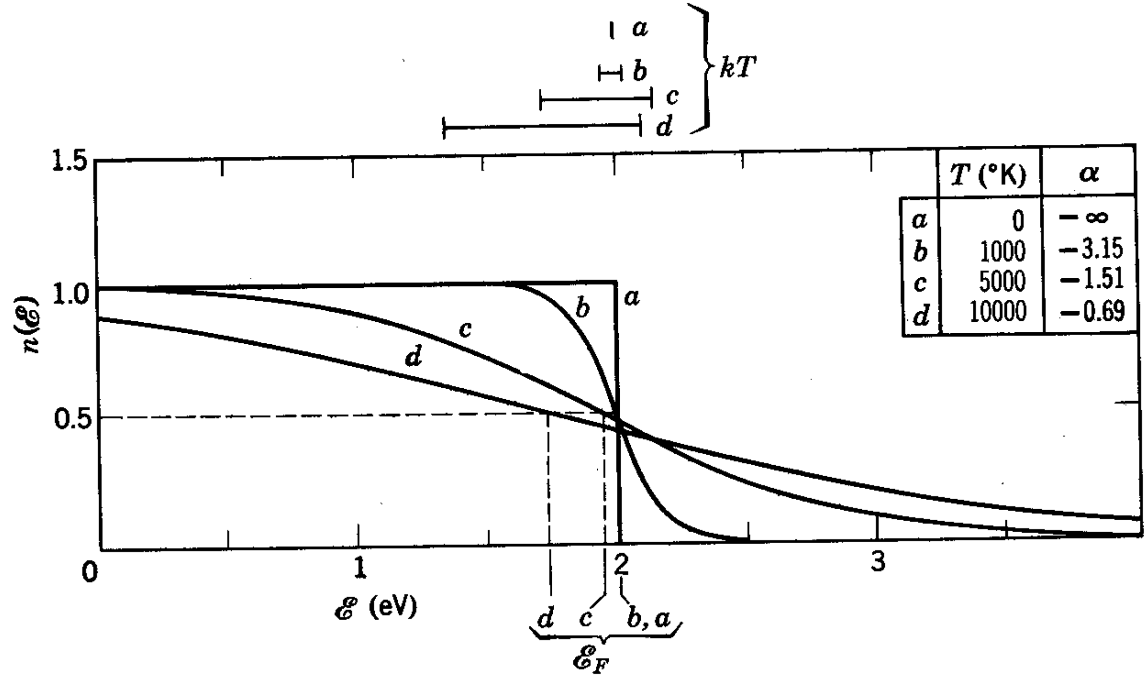
Small 10^{-5} at STP

$$\langle KE \rangle = \frac{3}{2} k\, T \left[1 + \frac{1}{2^{5/2}} \frac{N_{tot}\,(2\pi\hbar)^3}{V\,(2\pi mkT)^{3/2}} \right]$$

Boltz


a
b
c
kT
2
1
0
n(ℰ)
a
b
c
T(°K) | α
a 1000 −2.84
b 5000 −0.42
c 10000 0.62
0
1
2
3
ℰ (eV)

Fermi


a
b
c
d
kT
1.5
1.0
0.5
0
n(ℰ)
a
b
c
d
T (°K) | α
a 0 −∞
b 1000 −3.15
c 5000 −1.51
d 10000 −0.69
1
2
3
ℰ (eV)
d
c
b, a
ℰ_F

Can we find a gas that would exhibit Boson effects ?

$$\langle KE \rangle = \frac{3}{2} k\,T \left[1 - \frac{1}{2^{5/2}} \frac{N_{tot} (2\pi\hbar)^3}{V\,(2\pi mkT)^{3/2}} \right]$$

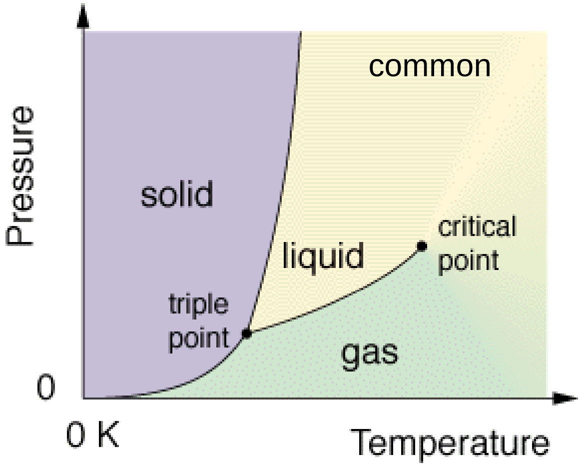
small mass m, low Temp, high density N_{tot} / V

H_2 at condensation point 20 K $e^{-\alpha} \sim 1/100$

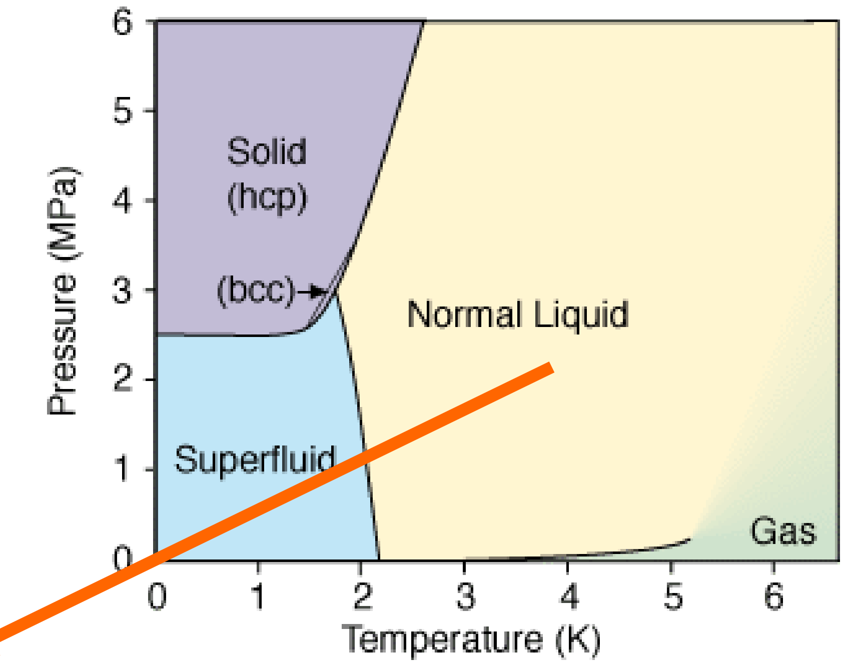
He at condensation point 4.2 K $e^{-\alpha} \sim 1/7$

Liquid He

Phonon gas – intra atomic interactions



helium



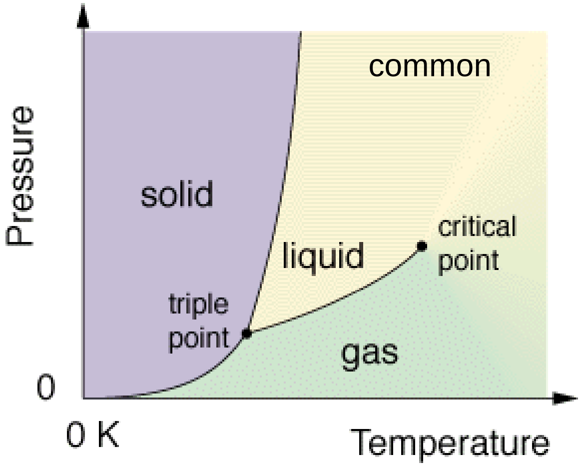
26 atm

- Very low viscosity
- Density = 0.125 g/cc (1/4 of what expected)
- nrg of thermal motion ~ nrg of inter-atomic effects

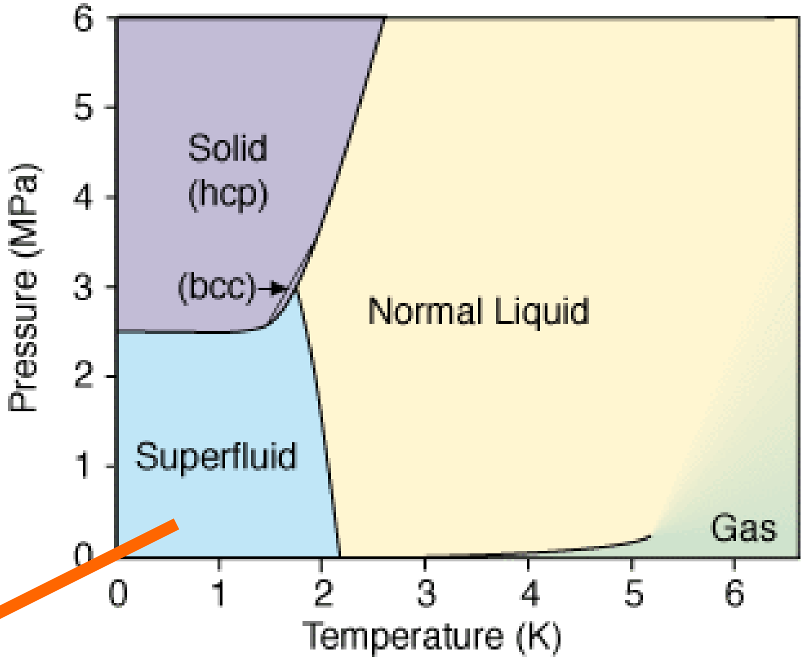
0.5 meV

Liquid He below T_λ

Not really a gas, but hey…

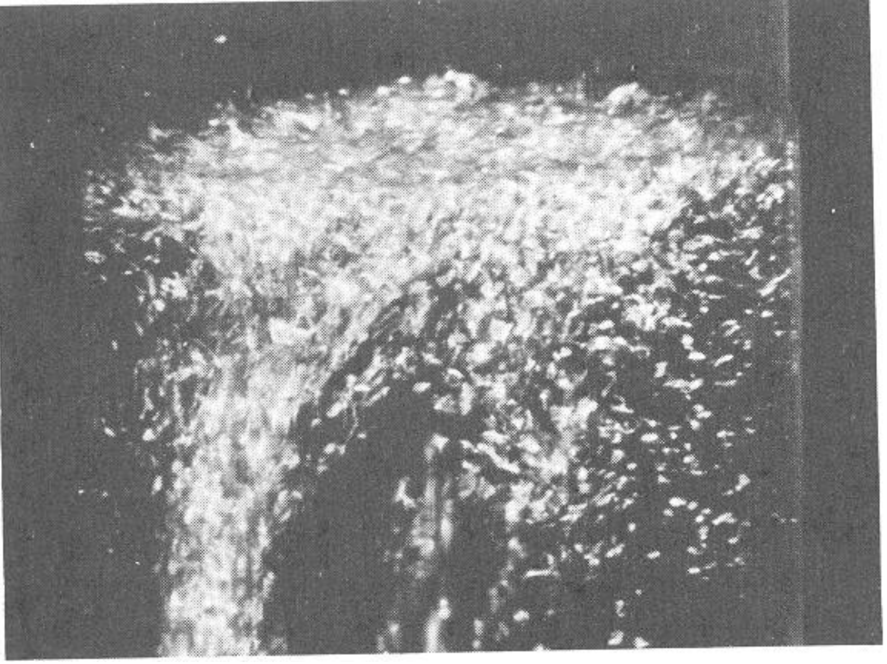


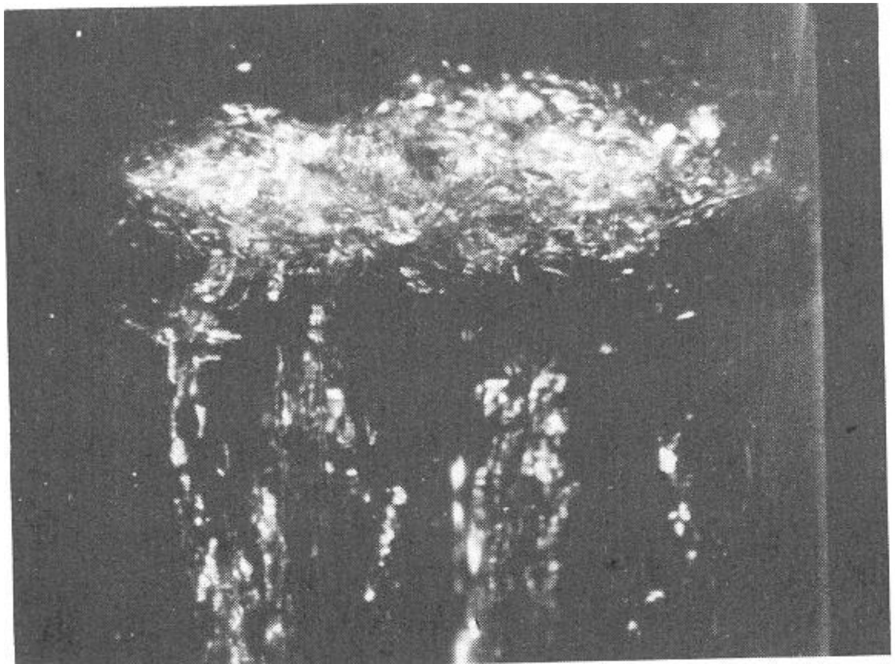
helium

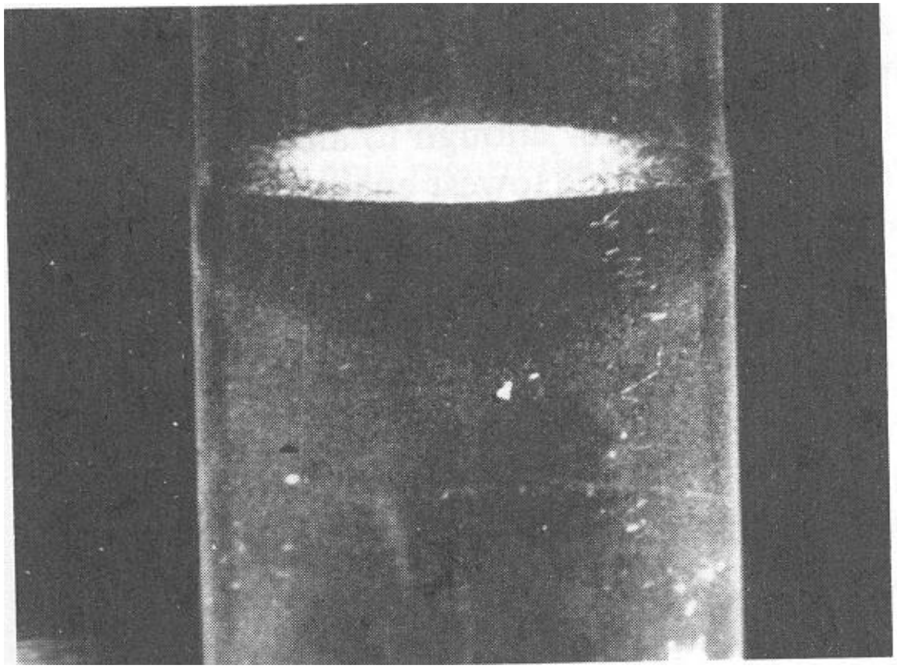


26 atm

- Heat is conducted through liquid w/o thermal resistance (drops by 10^6 at T_λ)
- Viscosity of fluid drops suddenly (drops by 10^6 at T_λ)
- Bulk ordered mass motion. Creep at ~ 30 cm/s







Below 4.2 K,
Heat is conducted without boiling.

Creep

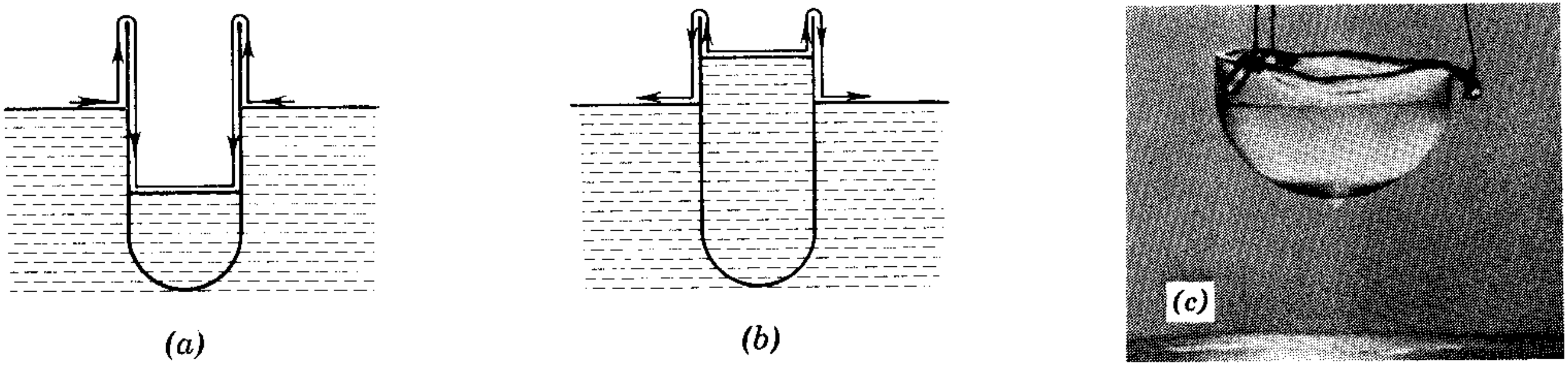


Figure 11-9 The creeping motion of a film of liquid He^4 below the transition temperature

K. Mendelssohn has written of the film flow as follows:

"If the beaker is withdrawn from the bath, the level will drop until it has reached the level of the bath. If the beaker is pulled out completely, the level will still drop, and one can see little drops of helium forming at the bottom of the beaker and falling back into the bath. This is the sort of thing that makes one look twice and rub his eyes and wonder whether it is quite true. I remember well the night when we first observed this film transfer. It was well after dinner, and we looked around the building and finally found two nuclear physicists still at work. When they, too, saw the drops, we were happier."

- Liquid Helium Film Creep
  - http://www.youtube.com/watch?v=fg1huRoaJdU
- Helium below λ-point
  - http://www.youtube.com/watch?v=TBi908sct_U
  - http://www.youtube.com/watch?v=YKjFPpuK-Jo
- s

wikipedia

Helium I has a gas-like index of refraction of 1.026 which makes its surface so hard to see that floats of Styrofoam are often used to show where the surface is.[5] This colorless liquid has a very low viscosity and a density 1/8th that of water, which is only 1/4th the value expected from classical physics.[5] Quantum mechanics is needed to explain this property and thus both types of liquid helium are called *quantum fluids*, meaning they display atomic properties on a macroscopic scale. This is probably due to its boiling point being so close to absolute zero, which prevents random molecular motion (heat) from masking the atomic properties.[5]

wikipedia

Boiling of helium II is not possible due to its high thermal conductivity; heat input instead causes evaporation of the liquid directly to gas.

Helium II is a superfluid, a quantum-mechanical state of matter with strange properties. For example, when it flows through even capillaries of 10-7 to 10-8 m width it has no measurable viscosity. However, when measurements were done between two moving discs, a viscosity comparable to that of gaseous helium was observed. Current theory explains this using the *two-fluid model* for Helium II. In this model, liquid helium below the lambda point is viewed as containing a proportion of helium atoms in a ground state, which are superfluid and flow with exactly zero viscosity, and a proportion of helium atoms in an excited state, which behave more like an ordinary fluid.[6]

A short explanation for the phenomenon would be that in this state, the temperature of the Helium is so low that almost all Helium atoms are in the lowest (quantum mechanical) energy state. Since energy can only be lost in discrete steps, and atoms in the lowest state cannot lose any energy, gravity and friction have no effect on single atoms.

Bose Condensates -- kinda Harris 8.7

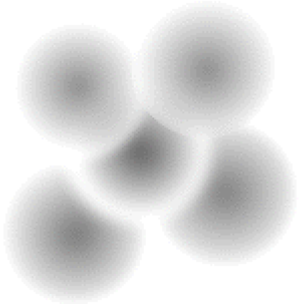
http://www.colorado.edu/physics/2000/bec

Java Applet: Thermal Box

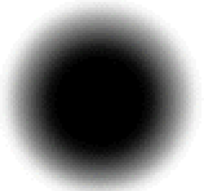
Java Applet: Thermal Quantum Well

Java Applet Evaporative Cooling

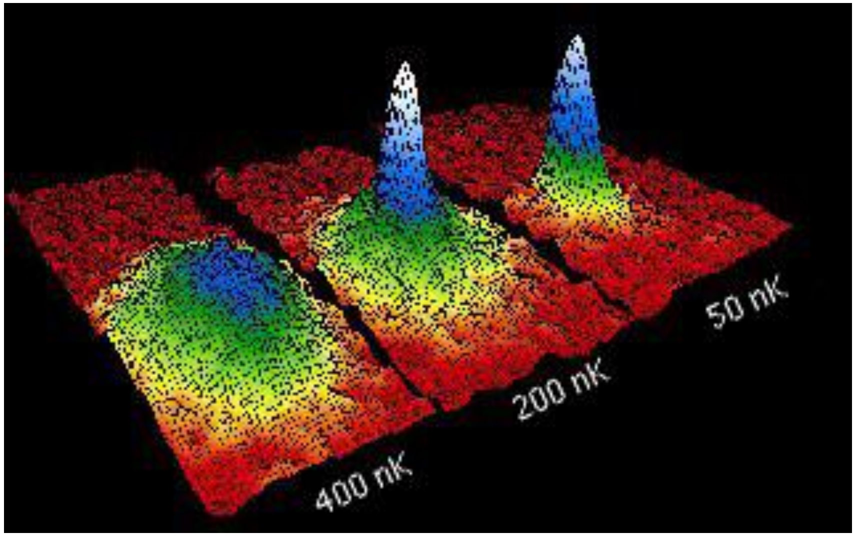
Animated gif of Condensation



Some very cold atoms



Some atoms in a BEC condensate

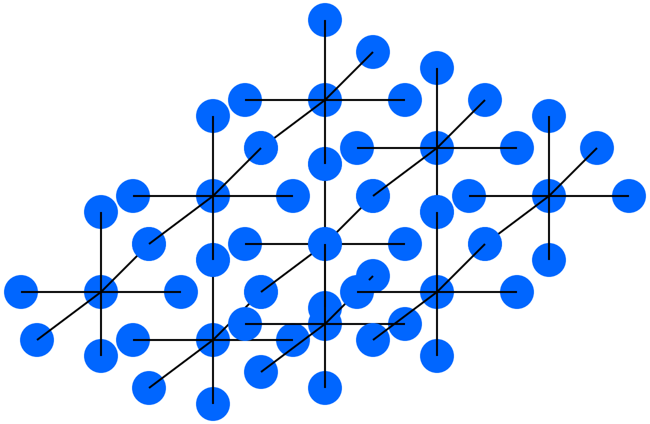


Interference of Two BEC
Manipulation of BEC by Optical Lattices
Quantum Computing
‘Slow Light’ 17 m/s

Specific Heats of Solids

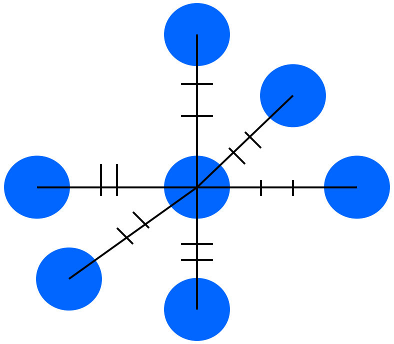
Harris 8.10

SPECIFIC HEAT of Solids at Normal Temps



kT of Tot E (=KE+U) per dof

$$\langle E_{tot}\rangle \quad = 3\left(kT\right)N \quad = 3NkT \quad = 3RT$$



Specific Heat

$$C_v \quad = \frac{d\langle E_{tot}\rangle}{dT} \quad = 3R$$

law of Dulong & Petit

Specific Heat of Solids at Lower Temps

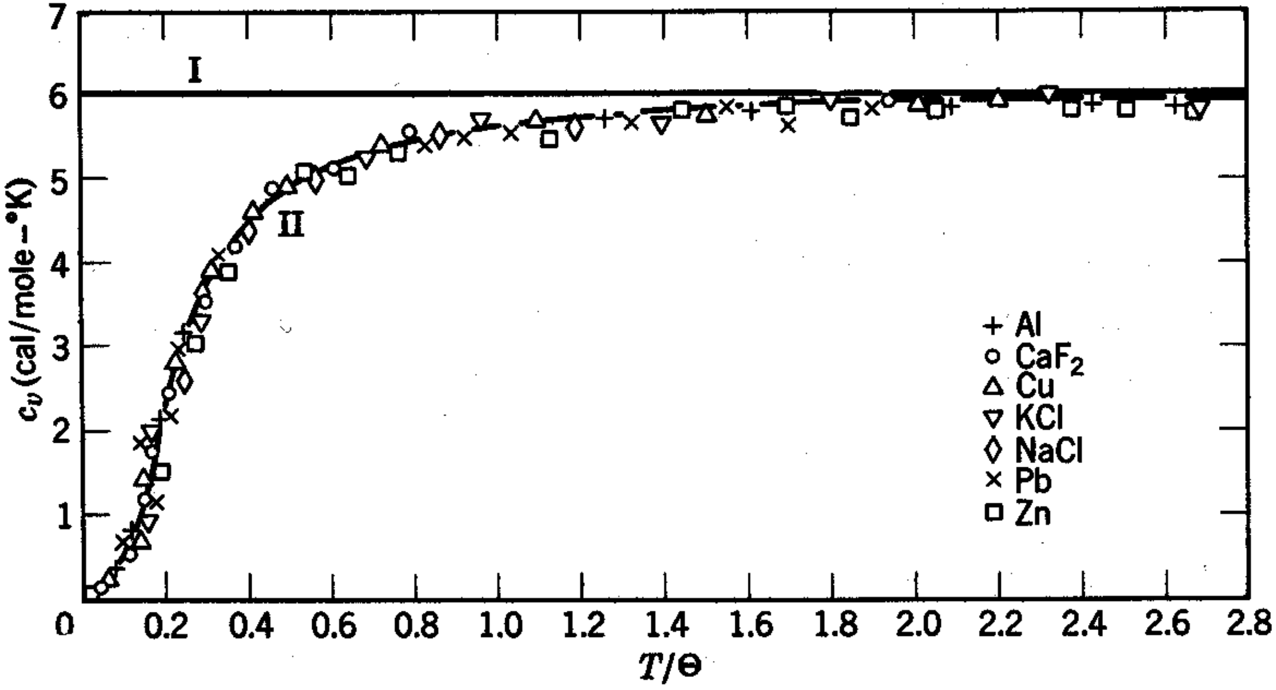


Figure 11-5 The measured specific heat at constant volume, as a function of temperature, for several materials. Horizontal line I represents the Dulong-Petit law, and curve II represents the predictions of the Debye theory.

1) Einstein treatment → incorrect T dependence
2) Debye treatment

- Fe Θ = 465 K
- Al Θ = 395 K
- Ag Θ = 210 K

Classical: Dulong & Petit

$$\left\langle E_{tot} \right\rangle \quad = 3\left(kT\right)N \quad = 3NkT \quad = 3RT$$

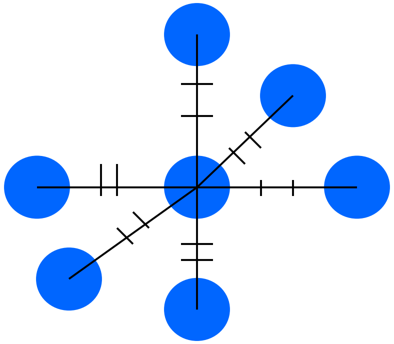
Einstein's approach: fudge it with Planck's bb distribution

$$kT \quad \rightarrow \quad \frac{h\nu}{e^{h\nu/kT} - 1}$$

But it didn't get the very low temp C_V correct

Peter Debye worked it out with the distribution functions

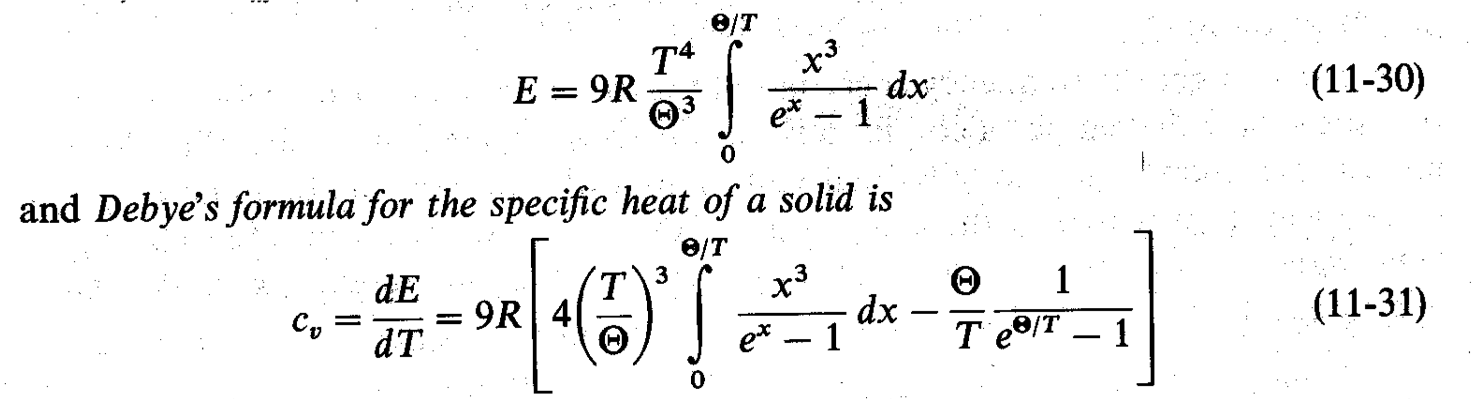
Specific Heat of Solids at Lower Temps



$$Tot\ KE = \int_0^{\varepsilon_{\max}} \varepsilon\ N(\varepsilon)\ \underline{D(\varepsilon)\, d\varepsilon}$$

Boltzmann
-- atom sites are distinguishable

number of states
of energy ε,
properly normalized
(Debye model)



$$E = 9R\frac{T^4}{\Theta^3}\int_0^{\Theta/T}\frac{x^3}{e^x-1}\,dx \tag{11-30}$$

and *Debye's formula for the specific heat of a solid is*

$$c_v = \frac{dE}{dT} = 9R\left[4\left(\frac{T}{\Theta}\right)^3\int_0^{\Theta/T}\frac{x^3}{e^x-1}\,dx - \frac{\Theta}{T}\frac{1}{e^{\Theta/T}-1}\right] \tag{11-31}$$

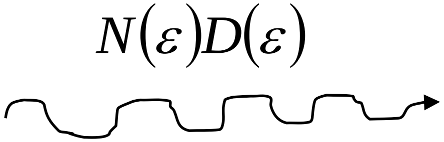
Laser Systems
Harris 8.9

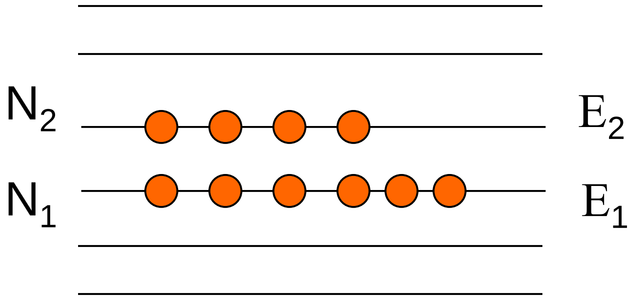
1. Two State System
2. Forcing a Population Inversion
3. Examples

Desired outcome:

Light Amplification by Stimulated Emission of Radiation

Two State Detailed Balance





$$\varepsilon = \Delta E = \varepsilon_2 - \varepsilon_1$$

$$Rate_{\downarrow} = A_{spon} N_2 + B_{stim} N_2 N(\varepsilon) D(\varepsilon)$$

$$Rate_{\uparrow} = B_{abs} N_1 N(\varepsilon) D(\varepsilon)$$

$$N(\varepsilon) D(\varepsilon) = \frac{1}{e^{\varepsilon/kT} - 1} \frac{8\pi V}{h^3 c^3} \varepsilon^2$$

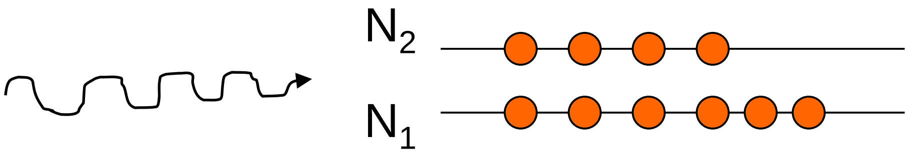
$$1 \quad = \quad \frac{Rate_{\downarrow}}{Rate_{\uparrow}} = \quad \frac{N_2}{N_1}\frac{A_{spon}}{B_{abs}\, N(\varepsilon)D(\varepsilon)} \quad + \quad \frac{N_2}{N_1}\frac{B_{stim}}{B_{abs}}$$

$$\frac{N_2}{N_1} = \frac{e^{-\varepsilon_2/kT}}{e^{-\varepsilon_1/kT}} \quad = e^{-(\varepsilon_2-\varepsilon_1)/kT} \quad = e^{-\varepsilon/kT}$$

$$\frac{1}{N(\varepsilon)D(\varepsilon)} \quad = \quad \left(e^{\varepsilon/kT}-1\right) \quad \frac{h^3c^3}{8\pi V}\frac{1}{\varepsilon^2}$$

$$1 = \frac{Rate_{\downarrow}}{Rate_{\uparrow}} = \frac{A_{spon}}{B_{abs}} \frac{h^3c^3}{8\pi V} \frac{1}{\varepsilon^2} \left(1 - e^{-\varepsilon/kT}\right) + \frac{B_{stim}}{B_{abs}} e^{-\varepsilon/kT}$$

$$\frac{A_{spon}}{B_{abs}} \frac{h^3c^3}{8\pi V} \frac{1}{\varepsilon^2} = 1$$



$$\frac{B_{stim}}{B_{abs}} = 1$$

Incoming photon just as likely to knock one down as knock one up
-- as long as system is in equilibrium.

Light Amplification by Stimulated Emission of Radiation

Back up to:

$$\frac{Rate_{\downarrow}}{Rate_{\uparrow}} = \frac{N_2}{N_1}\frac{A_{spon}}{\underbrace{B_{abs}\,N(\varepsilon)D(\varepsilon)}} + \frac{N_2}{N_1}\underbrace{\frac{B_{stim}}{B_{abs}}}_{1}$$

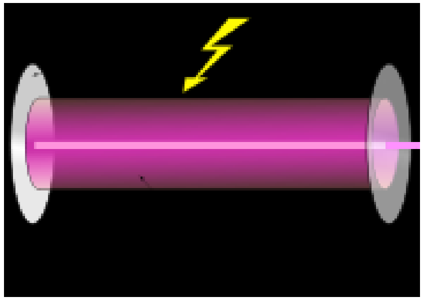
$$\frac{Rate_{\downarrow}}{Rate_{\uparrow}} = \frac{N_2}{N_1}\left(e^{\varepsilon/kT} - 1\right) + \frac{N_2}{N_1}$$

Light Amplification by Stimulated Emission of Radiation → $\frac{N_2}{N_1} >> 1$

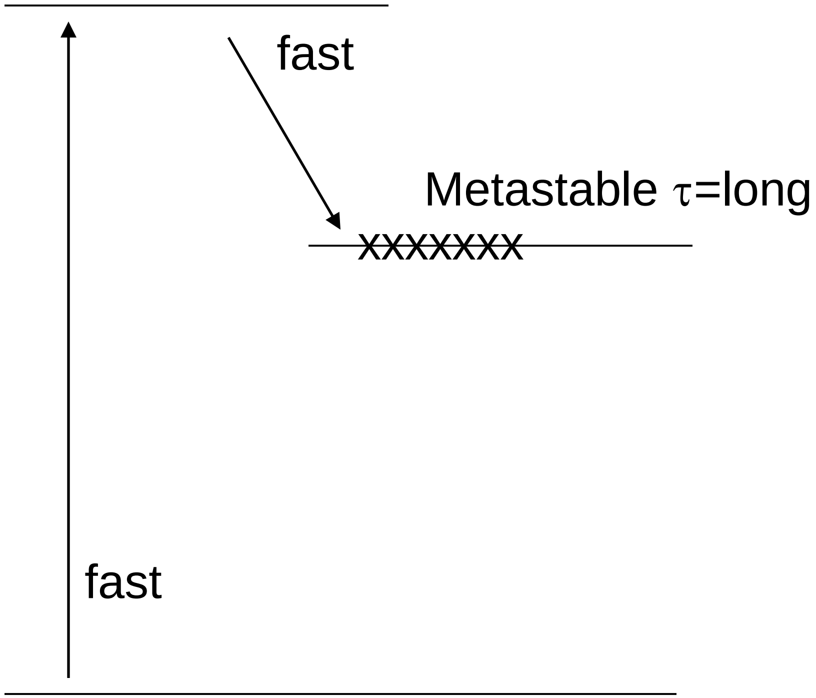
History of Light Amplification

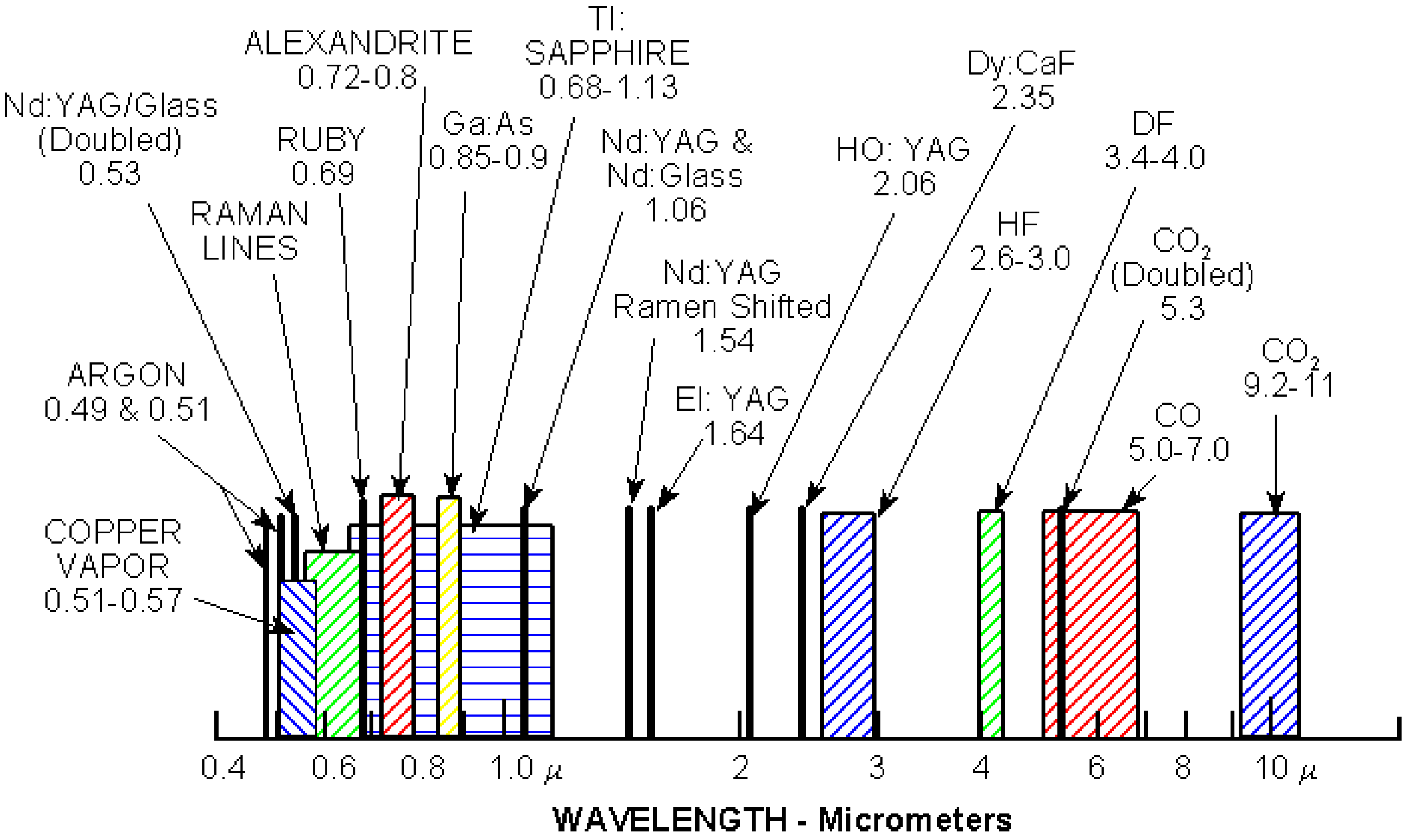
- 1953 Townes, Gordon, Zeiger: microwave amp
- 1955 Basov, Prokhov: 3 state
- 1957 Townes, Schawlow: change to optical
- 1957 Gould: design sketches
- 1959 Gould: “laser” and practical apps
- 1960 Maiman first working laser
- 1960-1987 Gould vs Townes court battles

Mechanisms for “pumping” a Population Inversion $N_2 >> N_1$



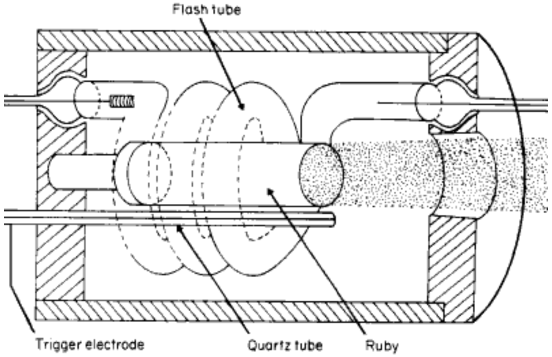
- Xe Flash lamp
- Electrical discharge
- Collisional excitation: HeNe
- Laser of another frequency
- Chemical Laser
- Excimer Laser
- Q-switching
- Solid State Semiconductor




Nd:YAG/Glass (Doubled) 0.53
RAMAN LINES
RUBY 0.69
ALEXANDRITE 0.72-0.8
Ga:As 0.85-0.9
TI: SAPPHIRE 0.68-1.13
Nd:YAG & Nd:Glass 1.06
Nd:YAG Ramen Shifted 1.54
El: YAG 1.64
HO: YAG 2.06
Dy:CaF 2.35
HF 2.6-3.0
DF 3.4-4.0
CO_2 (Doubled) 5.3
CO 5.0-7.0
CO_2 9.2-11
ARGON 0.49 & 0.51
COPPER VAPOR 0.51-0.57
0.4
0.6
0.8
1.0 μ
2
3
4
6
8
10 μ
WAVELENGTH - Micrometers

Ruby Laser

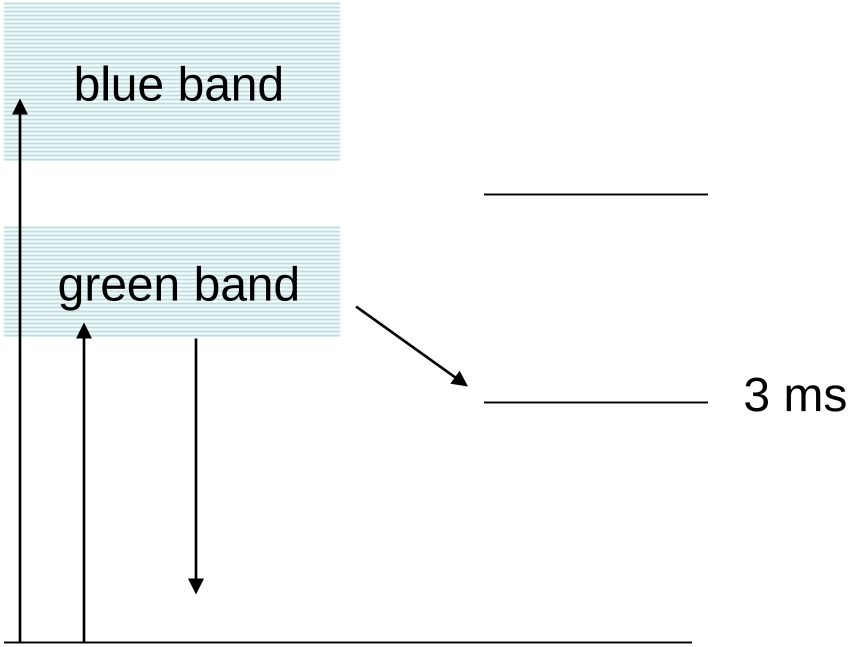
Theodore Maiman 1960



- Cr in Al_2O_3

- Ruby ends flat to 1/3 λ
- Ruby ends polished to form Fabry-Perot

- Xe flash lamp
- Cr^{+++} absorbs ~550 nm
- Cr^{+++} metastable ~3 ms



blue band

green band

3 ms

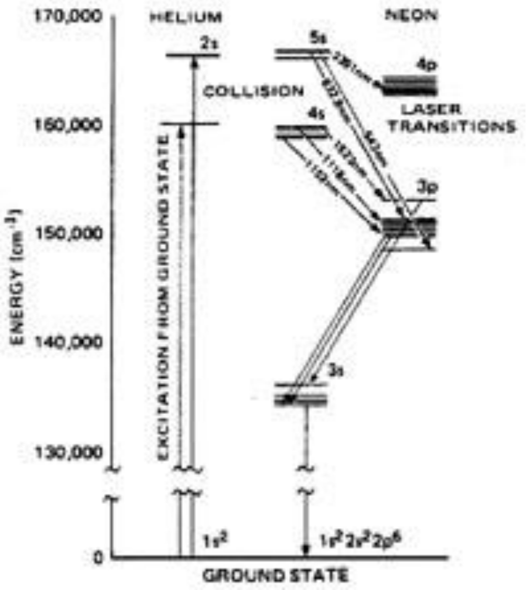
http://laserstars.org/history/ruby.html

HeNe

http://www.recycledgoods.com/item/18303.aspx

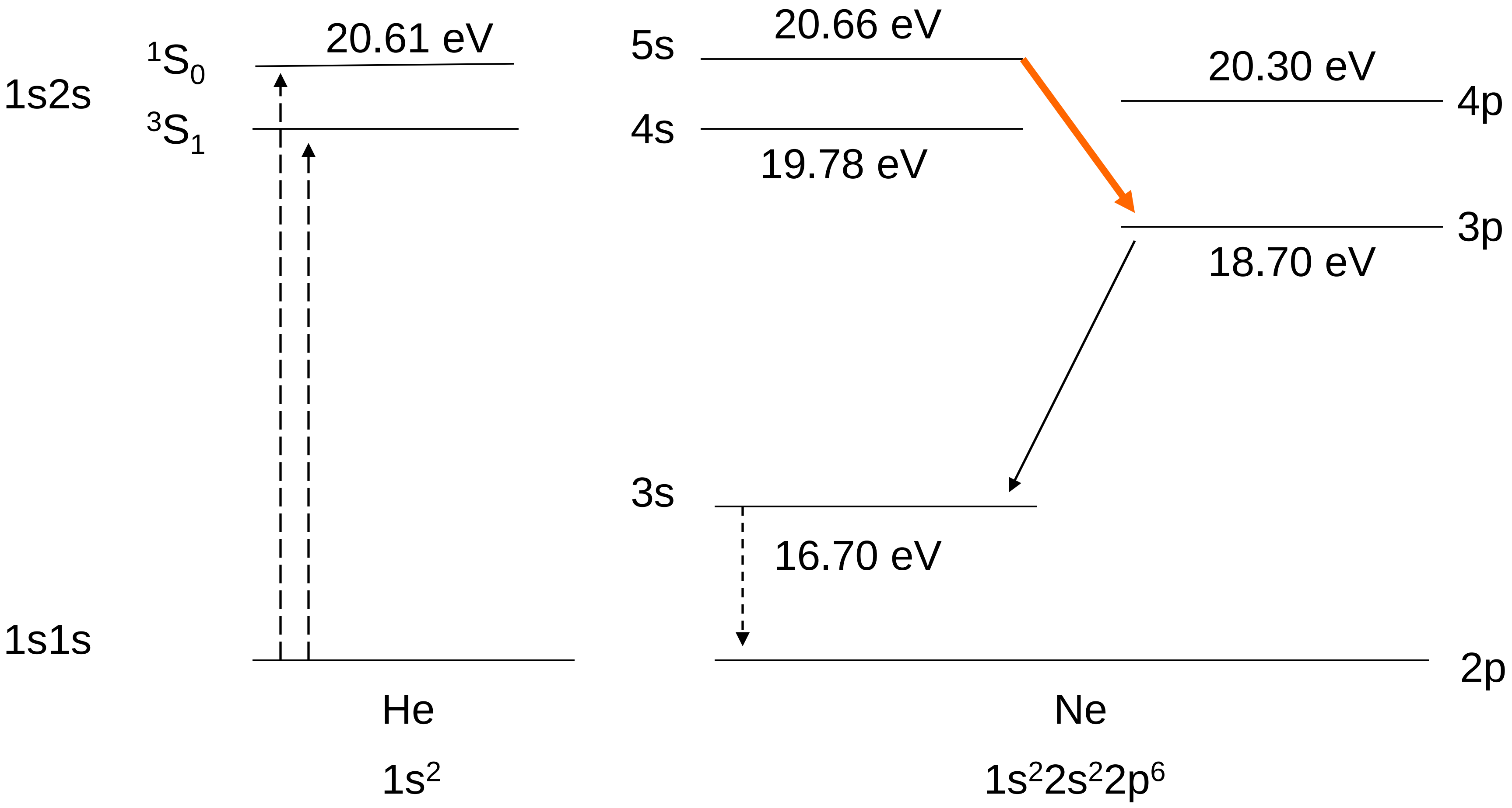
HeNe game http://phys.educ.ksu.edu/vqm/html/henelaser.html

http://www.shopeio.com/inventory/details.asp?id=953



HeNe

$$\overline{KE} = \frac{3}{2}kT \sim 0.04\, eV \;\; at\; 300K$$



http://repairfaq.ece.drexel.edu/sam/MEOS/EXP06.pdf good HeNe details, most of which are correct
http://technology.niagarac.on.ca/people/mcsele/lasers/LasersNeon.html

HeNe

5s

4s

3p

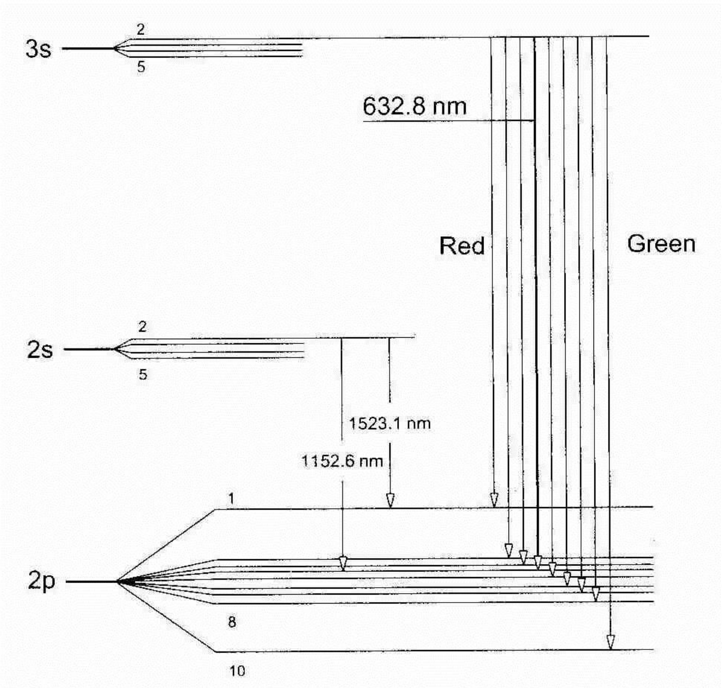
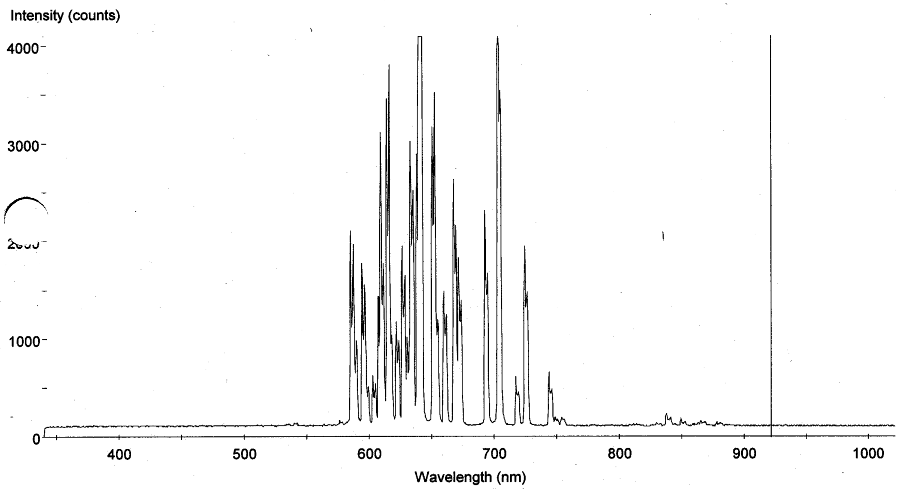


Fig. 3: The most important laser transitions in the neon system

Ocean Optics -- Neon



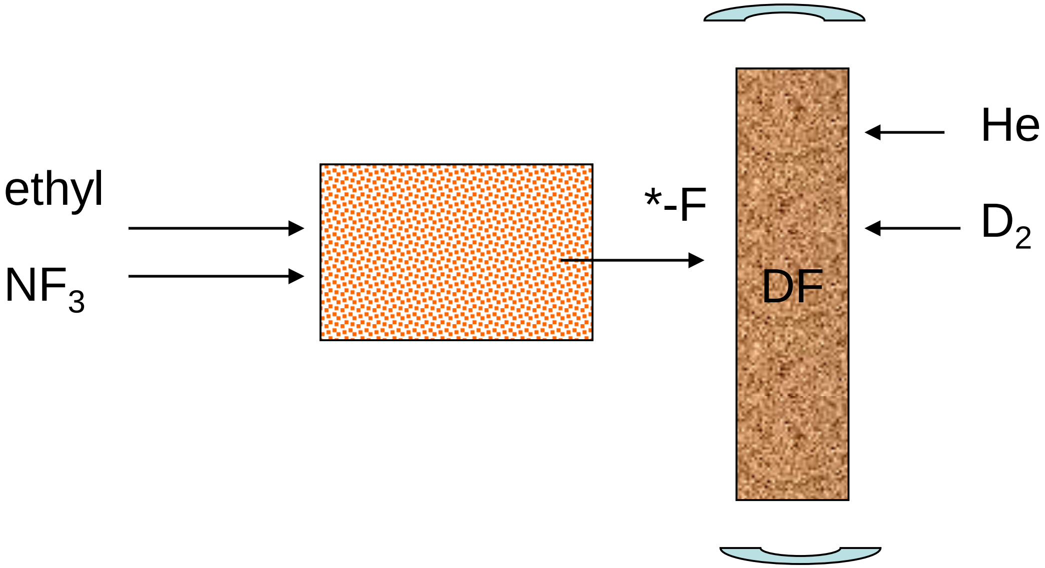
http://repairfaq.ece.drexel.edu/sam/MEOS/EXP06.pdf HeNe details

Chemical Lasers

‘HF’ 2.7-2.9 um

‘DF’ ~3.8 um

Mid-IR Advanced Chem Laser



Performance:
- 1980 ~MW for <70 sec
- 1997 USAF test against satellite @ 430 km
- 2006 pgm funding downgrade

MIRACL http://www.fas.org/spp/military/program/asat/miracl.htm

http://en.wikipedia.org/wiki/Boeing_YAL-1

The End