GCE 6A

We had $\langle N \rangle = \mathfrak{z}\, V/(\lambda_T)^3$

$$\mathfrak{z} = \lambda_T^3 \underbrace{\langle N \rangle / V}_{1/\ell^3}$$

ℓ = interparticle spacing

$$\lambda_T = h/(2\pi m k_B T)^{1/2}$$

$$= 6\cdot 10^{-34} / (2\pi\ \underbrace{32}_{O_2 \text{ molecules}}\ 1.67\cdot 10^{-27}\ 1.38\cdot 10^{-23}\ 300)^{1/2}$$

$$= 1.6\cdot 10^{-11}\ m$$

ℓ in solid $\sim 1\,\text{Å} = 10^{-10}\ m$

ℓ in air at STP $\sim 10\,\text{Å} \sim 10^{-9}\ m$

$\lambda_T/\ell \sim 10^{-2}$ $\Rightarrow$ μ is large and negative

$e^{\beta\mu} \sim 10^{-2}$

$E_i = p^2/2m \geq 0$

$\mu \sim -4.6\ k_B T$

Recall $\langle E \rangle = 3/2\ k_B T$

so $e^{\beta(\mu - E_i)} < 10^{-2}$

9CE6B

H_2O liquid

Solid $\rho \sim 1\ gm/cm^3$

$$\sim 1\ gm/cm^3\ \frac{6\cdot 10^{23}\ \text{atoms}}{18\ gm} = \frac{10^{23}}{3}\ \frac{\text{atoms}}{cm^3}$$

$$1/\ell^3 \sim 10^{24}/30 \qquad 1/\ell \sim 10^8/3\ \ 1/cm$$

$$1/\ell \sim 10^{10}/3\ \ 1/m$$

$\ell \sim 3\cdot 10^{-10}\ m$ for H_2O liquid

gas $PV = N k_B T$

$$10^5/(1.38\cdot 10^{-23})(300) = \frac{N}{V}$$

$1\,atm = 10^5 \frac{N}{m^2}$

$$\frac{10^{26}}{4} \sim \frac{N}{V} \sim \frac{10^{27}}{40} \qquad \frac{1}{\ell} \sim \frac{10^9}{3}$$

$\ell \sim 3\cdot 10^{-9}\ m$

Discrete Energy levels $E_1, E_2, \ldots$

<u>Classically</u>

N	Z_N	$e^{+\beta\mu N}$	$1/N!$
0	1	1	1
1	$(e^{-\beta E_1} + e^{-\beta E_2} + \ldots)$	$e^{+\beta\mu}$	1
2	$(\quad\downarrow\quad)^2$	$e^{2\beta\mu}$	$1/2!$

$$Q = \sum_{N=0}^{\infty} \xi^N (Z_1)^N \, 1/N! = e^{\xi Z_1}$$

with fugacity $\xi \equiv e^{\beta\mu}$

$$Z_1 \equiv \sum_i e^{-\beta E_i}$$

$$\Omega = -1/\beta \ln Q = -1/\beta \, \xi Z_1 = -1/\beta \sum_i e^{\beta(\mu - E_i)}$$

$$\langle N \rangle = 1/\beta \, \partial/\partial\mu \ln Q = -\partial\Omega/\partial\mu$$

$$= \sum_i e^{\beta(\mu - E_i)} = \sum n_i$$

small for classical system

GCE 8

GCE fermions

N	Z_N	$e^{\beta\mu N}$ $\cancel{1/N!}$ → No!
0	1	1
1	$e^{-\beta E_1} + e^{-\beta E_2} + \ldots$	$e^{\beta\mu}$
2	$e^{-\beta(E_1+E_2)} + e^{-\beta(E_1+E_3)} + \ldots$	$e^{2\beta\mu}$

$$Q = 1 + e^{\beta(\mu-E_1)} + e^{\beta(\mu-E_2)} + e^{\beta[(\mu-E_1)+\mu-E_2]} + \ldots$$

$$= \left(1+e^{\beta(\mu-E_1)}\right)\left(1+e^{\beta(\mu-E_2)}\right)\ldots = \prod_i \left(1+e^{\beta(\mu-E_i)}\right)$$

Clearly each E_i can appear only 1 time in product.

$$\Omega = -1/\beta \ln Q = -k_B T \sum_i \ln\left(1+e^{\beta(\mu-E_i)}\right)$$

$$\langle N \rangle = -\frac{\partial\Omega}{\partial\mu} = \sum_i \left(1+e^{\beta(\mu-E_i)}\right)^{-1} e^{\beta(\mu-E_i)}$$

IMPT: Indep sum!

$$= \sum_i \frac{1}{e^{\beta(E_i-\mu)}+1}$$

n_i Fermi-Dirac Distribution!

GCE 9

GCE BOSONS

N	Z_N	$e^{\beta\mu N}$	~~$1/N!$~~ NO!
0	1	1	
1	$e^{-\beta E_1} + e^{-\beta E_2} + \ldots$	$e^{\beta\mu}$	
2	$e^{-2\beta E_1} + e^{-\beta(E_1+E_2)} + e^{-2\beta E_2} + \ldots$	$e^{2\beta\mu}$	

$$Q = \left(1 + e^{\beta(\mu-E_1)} + e^{2\beta(\mu-E_1)} + \ldots\right)$$

$$\left(1 + e^{\beta(\mu-E_2)} + e^{2\beta(\mu-E_2)} + \ldots\right) \ldots$$

$$= \prod_i \left(1 - e^{\beta(\mu-E_i)}\right)^{-1}$$

Signs differ from FERMIONS

$$\Omega = -\frac{1}{\beta}\ln Q = +k_BT \sum_i \ln\left(1 - e^{\beta(\mu-E_i)}\right)$$

Signs differ from FERMIONS

$$\langle N \rangle = -\frac{\partial\Omega}{\partial\mu} = \sum_i \frac{e^{\beta(\mu-E_i)}}{1-e^{\beta(\mu-E_i)}} = \sum_i \frac{1}{e^{\beta(E_i-\mu)}-1}$$

Bose Einstein distribution

Anyons, Spin-charge Separation, Topological Excitations

FD: $$Q = \prod_i \left(1+e^{\beta(\mu+E_i)}\right)$$

BE: $$Q = \prod_i \left(1-e^{\beta(\mu-E_i)}\right)^{-1}$$

Natural generalization

$$Q = \prod_i \left(1+e^{i\phi}e^{\beta(\mu-E_i)}\right)^{e^{i\phi}}$$

Fermions $\phi = 0$ $e^{i\phi} = +1$

Bosons $\phi = \pi$ $e^{i\phi} = -1$

Anyons general ϕ

Actually such "complex generalizations" occur in various contexts in stat mech

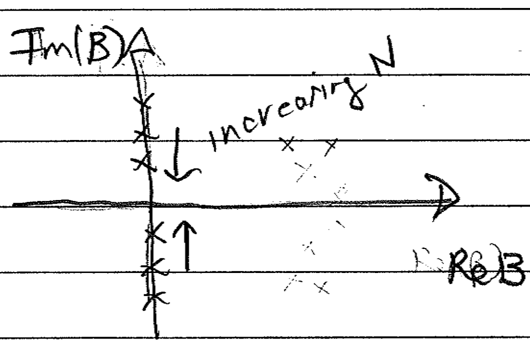
$$H = -J\sum s_i s_j - B\sum s_i$$

$$Z = \sum_{\{s\}} e^{-\beta H(\{s\})}$$

Ising model: Allow B to be a complex # and look for poles of Z in complex plane, eg on finite lattice sizes N

"Lee Yang theorem": poles of Z only for imaginary B

"Lee-Yang zeroes"

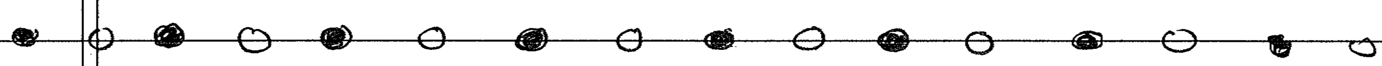


As N increases poles pinch down towards B=0 signalling the phase transition

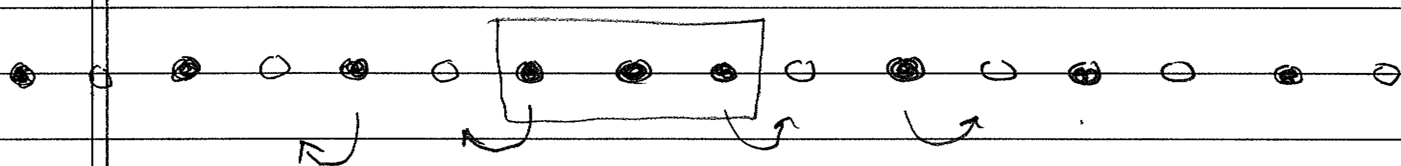
A-2

Tied to some of most interesting issues in modern CMP. Eg "spin-charge separation".

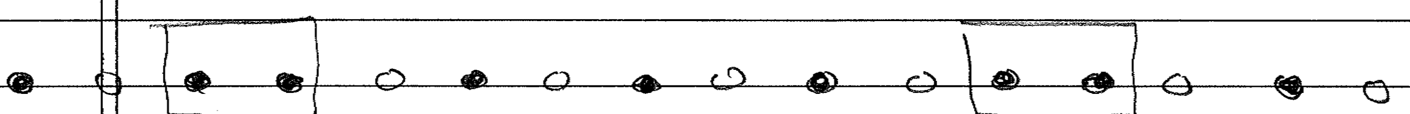
How a single added particle can split into two separate excitations: Spinless fermions with nn repulsion



ADD PARTICLE

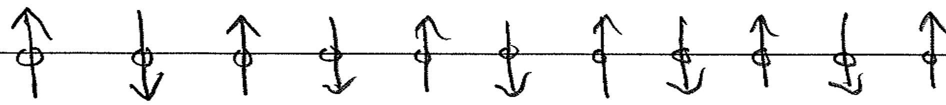


ALLOW TO MOVE

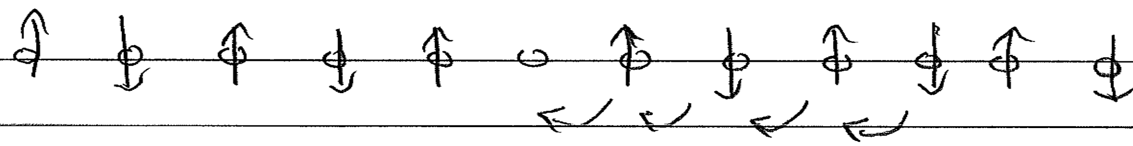


More interesting if spin involved

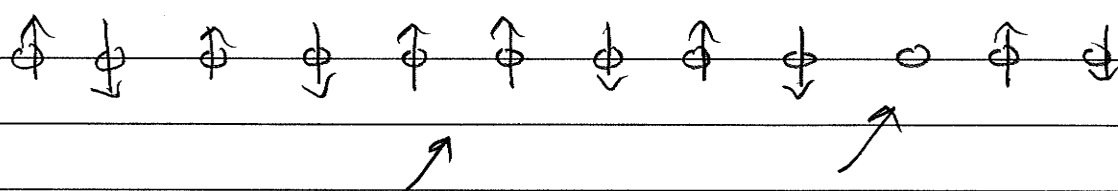
Antiferromagnet



photon knocks one e^- out



Again, allow time to pass create hole spin ½ charge 1 } missing e^- of spin ↓



"spinon"	"holon"
spin ½	spin ϕ
charge ϕ	charge 1

We emphasized GCE as easier computationally especially for quantum systems. Another motivation is that it is the correct way to do things if there really are # fluctuations, eg with 2 systems in contact

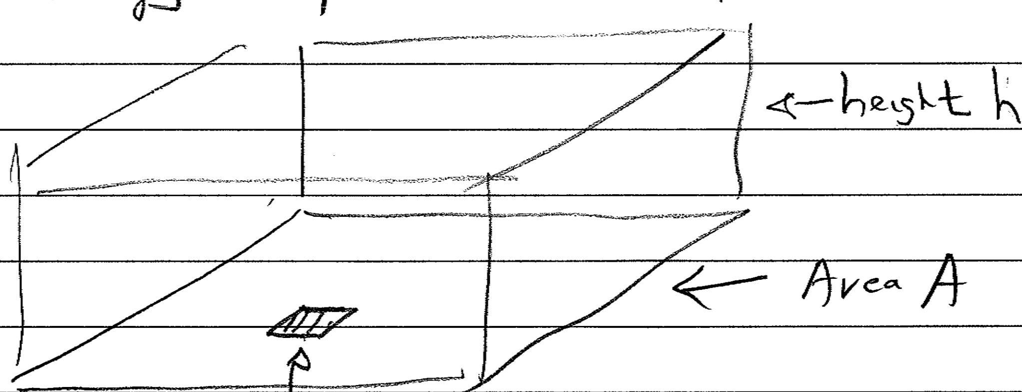
Just as $T_1 = T_2$ thermal equilibrium

$\mu_1 = \mu_2$ "chemical equilibrium"

Indeed exact same proof as before(!) for $T_1 = T_2$.

~~You have HW problem on this~~

Example: Classical 3D Ideal gas at pressure P, T above a surface in which there are bound states of energy $-E_1$. Q: How many surface states are occupied?



each area a_0 contains bound state

$N_0 = A/a_0$ = # bound states

GCE11

Stat mech of surface states

Two ways give $\boxed{\text{same}}$ answer

Method #1

N	3^N	E		$1/N!$
0	1	0		1
1	3	$-E_1$	← N_0 of these	$1/1!$
2	3^2	$-2E_1$	$N_0(N_0-1)$ of these	$1/2!$

$$Q_s = \sum_{N=0}^{N_0} 3^N e^{+N\beta E_1} \underbrace{\frac{N_0!}{(N_0-N)!}}_{} \frac{1}{N!}$$

Z_N because all states have same $E = -NE_1$ and there are $N_0!/(N_0-N)!$ of them

$$= \sum_{N=0}^{N_0} e^{\beta(\mu+E_1)N} \binom{N_0}{N}$$

$$= \left\{1 + e^{\beta(\mu+E_1)}\right\}^{N_0}$$

GCE 12

Alternately have N_0 systems each with GCE

$$1 + e^{\beta(\mu + E_1)}$$

so $$Q_S = \left(1 + e^{\beta(\mu+E_1)}\right)^{N_0}$$ $$\Omega_S = -k_BT \ln Q_S = -N_0 k_B T \ln\left(1 + e^{\beta(\mu+E_1)}\right)$$

For ideal gas above the surface

$$Q_V = e^{V/\lambda_T^3 \, z}$$

$$\Omega_V = -k_BT \, V z / \lambda_T^3$$

$$P = -\frac{\partial \Omega_V}{\partial V} = k_BT z / \lambda_T^3$$

same μ, T in these analyses

Surface

$$\langle N \rangle_S = -\frac{\partial \Omega_S}{\partial \mu} = N_0 \frac{1}{1 + e^{\beta(\mu+E_1)}} e^{\beta(\mu+E_1)}$$

$$= N_0 \frac{1}{e^{-\beta(\mu+E_1)} + 1}$$

$$e^{-\beta\mu} = \frac{1}{z} = \frac{k_BT}{P\lambda_T^3}$$

$$\langle N \rangle_S = N_0 \frac{1}{\frac{k_BT}{P\lambda_T^3} e^{-\beta E_1} + 1}$$

Think about structure of this result.

What do you expect for $E_1 \to \infty$ (very tightly bound state $-E_1$)?

$\langle N_s \rangle \to N_0$ as expected

What about high pressure P?

$\langle N_s \rangle \to N_0$ as expected at high P

$\to 0$ at low P (as expected)

Temperature dependence is less obvious?

$T \to \infty \quad \beta \to 0 \quad e^{-\beta E_1} \to 1$

$$\frac{k_B T}{\left(h / (2\pi m k_B T)^{1/2} \right)^3} \sim T^{5/2}$$

High T $\quad \langle N \rangle_s \to 0$ "desorption"

Two effects E_1 becomes less effective at binding atoms

$e^{-\beta E_1} \to 1$ but also more "phase space" for 3D gas above surface.

GCE-14

Application of GCE formalism to fermions

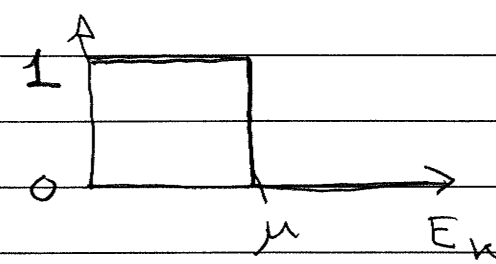
Fermi gas @ temperature T $\qquad E_k = \hbar^2 k^2 / 2m$

$$N = 2 \sum_k \frac{1}{e^{\beta(E_k - \mu)} + 1}$$

for spin

$$N = 2 \frac{V}{(2\pi)^3} \int d^3k \, \frac{1}{e^{\beta(E_k - \mu)} + 1}$$

If $\beta \to \infty$ $\quad (T \to 0)$



$$N = 2 \frac{V}{(2\pi)^3} \frac{4}{3} \pi k_F^3$$

where k_F is largest k which is occupied

$\mu = E_F = \hbar^2 k_F^2 / 2m$

$$n = \frac{N}{V} = k_F^3 / 3\pi^2$$

e^- density.

GCE-15

Take a typical metal like sodium

$$n = \frac{N}{V} = \frac{6 \cdot 10^{23}}{23 \cdot 10^{-6}\,m^3}$$

← mole

← density of sodium is $\sim 1\,{}^{gm}/_{cm^3}$ so 23g of sodium (1 mole) occupy $23\,cm^3$

$$k_F^3 = 3\pi^2 \frac{6}{23} \cdot 10^{29}$$

$$= 0.77 \cdot 10^{30}$$

$$k_F = 0.92 \cdot 10^{10}\ m$$

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{(1 \cdot 10^{-34})^2 (10^{10})^2}{2(9 \cdot 10^{-31})} = \frac{1}{2}\ 10^{-68+20+30} = \frac{1}{2} \cdot 10^{-18}$$

$$1\ eV = 1.6 \cdot 10^{-19}\ J$$

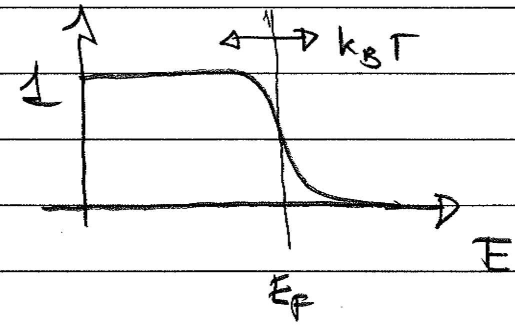
$$E_F = 3\ eV \sim 36000\ {}^\circ K$$

or $$\frac{E_F}{k_B} = \frac{1/2 \cdot 10^{-18}}{1.38 \cdot 10^{-23}} \sim \frac{1}{3} \cdot 10^{5}\ {}^\circ K$$

Anyway, the point is electrons have a huge kinetic energy. This is why treating metals as a free electron gas (ignoring interactions) is a good starting point.

In a CMP course you will learn how to

handle finite T



The method is called the "Sommerfeld Expansion"

and is an expansion in $k_B T / E_F$ which we

just saw is a very small #

Basic identity (see CMP text for derivation)

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\mu} H(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \ldots$$

Fermi function

Can use this to show $C \sim T$ for a gas of electrons.

Impt also to astrophysics: Very high KE of neutrons in collapsed neutron star prevents further gravitational collapse.

"degeneracy pressure"

GCE-17

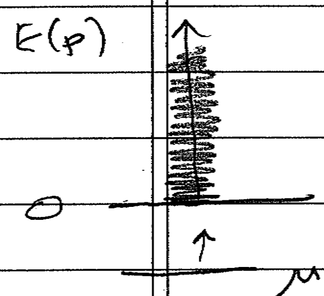
Bose Einstein Condensation

$$N = \sum_p n_{BE}(p) \qquad E_p = p^2/2m$$

$$= \sum_p 1/e^{\beta(E_p-\mu)} - 1$$

$$= \frac{V}{(2\pi)^3}\frac{1}{\hbar^3}\int d^3p \; 1/e^{\beta(E_p-\mu)} - 1$$

In order to increase N we move μ up towards lowest energy state $E = 0$.



$$\frac{N}{V} = \frac{4\pi}{h^3}\int_0^\infty p^2\,dp \,\frac{1}{e^{\beta(p^2/2m-\mu)}-1}$$