Lecture

Fermi gas

At the end of the Lecture: Perfect Gas part II, the BOSE and FERMI GASES were described. Namely, we need to find $\mu(T,V,N)$ from

$$N = \int_0^\infty d\epsilon\, g(\epsilon) \frac{1}{e^{-\beta\mu+\beta\epsilon} \mp 1} + \text{other terms if necessary}$$

and then substitute this $\mu(T,V,N)$ into

$$\frac{pV}{kT} = \mp \int_0^\infty d\epsilon\, g(\epsilon) \ln\left(1 \mp e^{\beta\mu-\beta\epsilon}\right) + \text{other terms if necessary}$$

the $-$ sign was for bosons and $+$ for fermions.

For fermions, we showed that the chemical potential μ is not restricted (for bosons $-\infty < \mu \leq 0$).

$$-\infty < \mu < +\infty \quad \text{for fermions.}$$

the fugacity

$$z = e^{\beta\mu}$$

can take any positive value

$$0 \leq z < +\infty$$

Moreover, because fermions cannot be crowded in a single state, the integral is a good approximation. We conclude that for fermions

$$N = \int_0^\infty d\epsilon\, g(\epsilon) \frac{1}{e^{-\beta\mu+\beta\epsilon}+1}$$

No need for additional terms

$$\frac{pV}{kT} = \int_0^\infty d\epsilon\, g(\epsilon) \ln\left(1 \mp e^{\beta\mu-\beta\epsilon}\right)$$

Following the same mathematical technique as for the Bose gas we arrive at

$$\frac{N}{V} = \frac{1}{\lambda^3} f_{\frac{3}{2}}(z) \qquad (1)$$

$$\frac{pV}{kT} = \frac{1}{\lambda^3} f_{\frac{5}{2}}(z) \qquad (2)$$

with the thermal wavelength

$$\lambda = \frac{h}{\sqrt{2\pi m kT}}$$

and $f_\nu(z)$ the Fermi-Dirac functions

$$f_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{z^{-1} e^x + 1} dx \quad , \quad \nu \text{ real number}$$

this function, for small z, can be expanded as

$$f_\nu(z) = z - \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} - \dots$$

The formulas (1) and (2) above were determined using for the density of states

$$g(\epsilon) = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} \epsilon^{\frac{1}{2}}$$

which was a consequence of the energy spectrum

$$\epsilon_{j_1 j_2 j_3} = \frac{h^2}{2mL^2} (j_1^2 + j_2^2 + j_3^2).$$

This spectrum reflects the translational motion of the particle. If the particle has an <u>internal</u> structure (like a quantum spin) then the energy spectrum will acquire an additional index

$$\epsilon_{j_1 j_2 j_3 s} = \frac{h^2}{2mL^2} (j_1^2 + j_2^2 + j_3^2)$$

spin index

The spin index will take g discrete values

$$s = s_1, s_2, \ldots, s_g$$

g the number of the discrete values of the "internal" structure.

Notice that the formula for the energy spectrum is the same as before; only the number of states increased g times. The mathematical computation is the same as before, with the result that (1) and (2) become

$$\frac{N}{V} = \frac{g}{\lambda^3} f_{\frac{3}{2}}(z) \qquad (3)$$

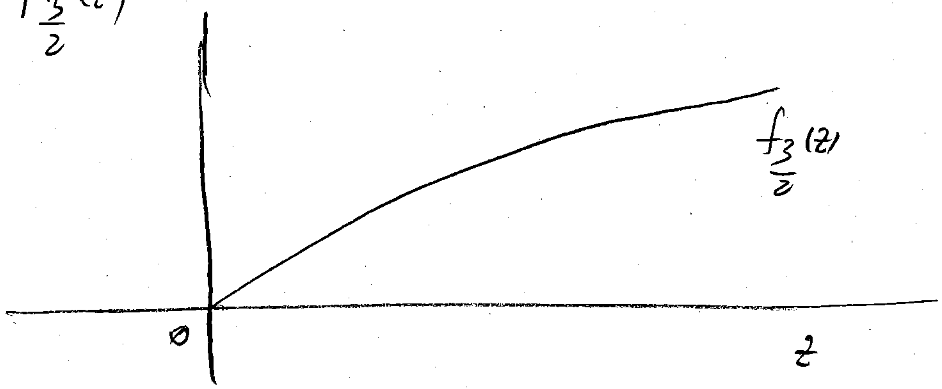
$$\frac{pV}{kT} = \frac{g}{\lambda^3} f_{\frac{5}{2}}(z) \qquad (4)$$

The logic is as before: find z in terms of $\frac{N}{V} \cdot \frac{\lambda^3}{g}$ from (3) and insert it in (4). When the density of the gas is very low and/or its temperature is very high, the parameter

$$\frac{N}{V} \frac{\lambda^3}{g}$$

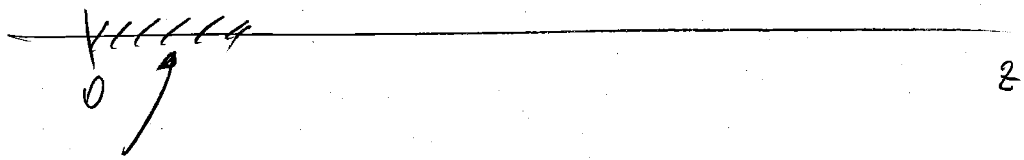
is small, the fugacity z is small also because from $\frac{N}{V}\frac{\lambda^3}{g} = f_{\frac{3}{2}}(z)$

we find that $f_{\frac{3}{2}}(z)$ is small. From the graph of $f_{\frac{3}{2}}(z)$



we see that $f_{\frac{3}{2}}(z)$ small implies z small.

The physical region of small fugacity, $z \approx 0$, like in the Bose gas, corresponds to a normal behaviour of that gas.



jargon: NONDEGENERATE FERMI GAS

The thermodynamic equation of state for a nondegenerate Fermi gas can be obtained in exactelly the same manner as for the Bose gas, we obtaine

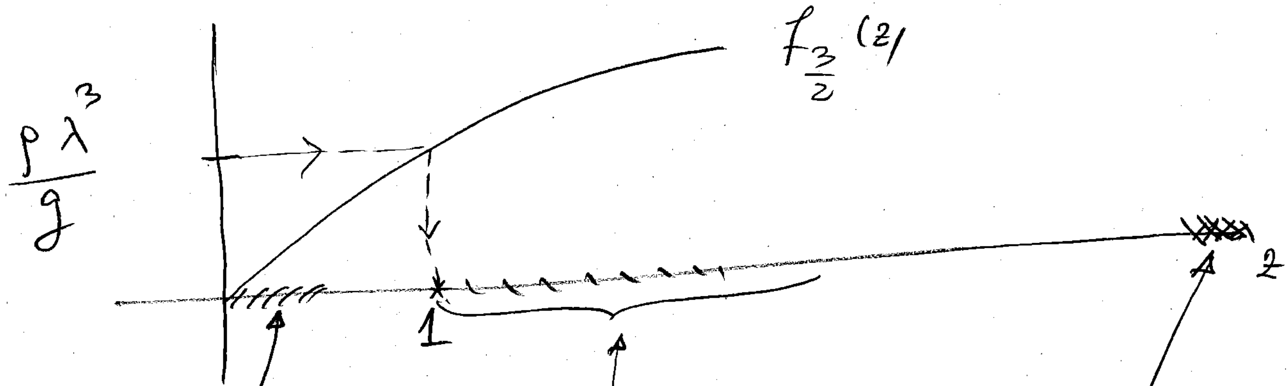
$$\text{FERMI}: \quad \frac{pV}{kT} = 1 + 0.17678\,\frac{\rho\lambda^3}{g} - 0.00330\left(\frac{\rho\lambda^3}{g}\right)^2 + 0{,}00011\left(\frac{\rho\lambda^3}{g}\right)^3 \cdots$$

To constrast it with BOSE gas, we write the previous formula (with g inserted to consider the spin index)

$$\text{BOSE}: \quad \frac{pV}{kT} = 1 - 0{,}17678\,\frac{\rho\lambda^3}{g} - 0{,}00330\left(\frac{\rho\lambda^3}{g}\right)^2 - 0{,}00011\left(\frac{\rho\lambda^3}{g}\right)^3 \cdots$$

We observe that the first quantum term $0{,}17678\,\frac{\rho\lambda^3}{g}$ is POSITIVE for FERMIONS and NEGATIVE for BOSONS. thus the pressure p is <u>increased</u> by the quantum effect for fermions and <u>decreased</u> for bosons. Femions exclude each other, a quantum phenomena that appears as an increase of the macroscopic parameter pressure. Contrarry, the Bose particles can accumulate indefinetly on a quantum state, a phenomena perceived at the thermodynamic level as a decrease in pressure.

If $\frac{\rho \lambda^3}{g}$ is not small, the fugacity z will move away from zero



NONDEGENERATE FERMI GAS

mathematical technique to study this region: expansion in powers of z, because $z \approx 0$

DEGENERATE FERMI GAS

mathematical techniques to study this region: NUMERICAL ALGORITHMS, ASYMPTOTIC EXPANSIONS IN powers of $(\ln z)^{-1}$

For very high values of z, COMPLETE DEGENERATE FERMI GAS

mathematical technique to study this region: take the limit $\frac{\rho \lambda^3}{g} \to \infty$

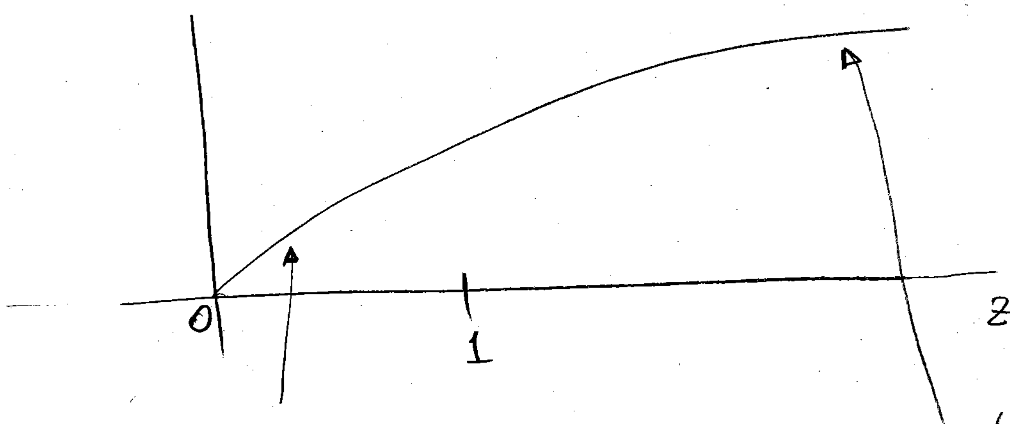
Complete degenerate Fermi gas

To achive high values of $\frac{\rho\lambda^3}{g}$ we will consider a Fermi gas with N particles and at $T \simeq 0$.

then

$$\frac{\rho\lambda^3}{g} = \frac{N}{V}\frac{1}{g}\left(\frac{h}{\sqrt{2\pi m kT}}\right)^3 \to \infty$$

The behavior of the Fermi - Dirac functions for high values of z was discovered by Sommerfeld in 1928



$f_\nu(z) \approx z$ for $z \ll 1$

$$f_\nu(z) \simeq \frac{(\ln z)^\nu}{\Gamma(\nu+1)}$$

for $z \gg 1$

So

$$\begin{cases} \dfrac{N}{V} \simeq \dfrac{g}{\lambda^3}\dfrac{\left(\ln e^{\beta\mu}\right)^{\frac{3}{2}}}{\Gamma\left(\frac{3}{2}+1\right)} \\[2ex] \dfrac{pV}{kT} \simeq \dfrac{g}{\lambda^3}\dfrac{\left(\ln e^{\beta\mu}\right)^{\frac{5}{2}}}{\Gamma\left(\frac{5}{2}+1\right)} \end{cases}$$

Remember that $z = e^{\beta\mu}$

$$\frac{N}{V} = \frac{g}{\lambda^3}\frac{(\beta\mu)^{\frac{3}{2}}}{\Gamma(\frac{5}{2})} = g\Bigg(\underbrace{\frac{\sqrt{2\pi m kT}}{h}}_{\frac{1}{\lambda}}\Bigg)^3 \Bigg(\underbrace{\frac{\mu}{kT}}_{\beta\mu}\Bigg)^{\frac{3}{2}} \cdot \frac{1}{\underbrace{\frac{4}{3}\sqrt{\pi}}_{\Gamma(\frac{5}{2})}} =$$

$$= g\left(\frac{2\pi m}{h^2}\right)^{\frac{3}{2}} \mu^{\frac{3}{2}} \frac{4}{3\sqrt{\pi}}$$

Notice that the temperature T dropped out! the chemical potential obtained as a solution of the above equation is <u>independent</u> of the temperature.

$$\boxed{\mu = \left(\frac{3N}{4\pi g V}\right)^{\frac{2}{3}} \frac{h^2}{2m}} \qquad (5)$$

From a general perspective, we expect μ to be a function of T, N, V. However T is not present. We will discuss the physical meaning of this fact later. Now we follow the method, and insert (5) into the pressure formula

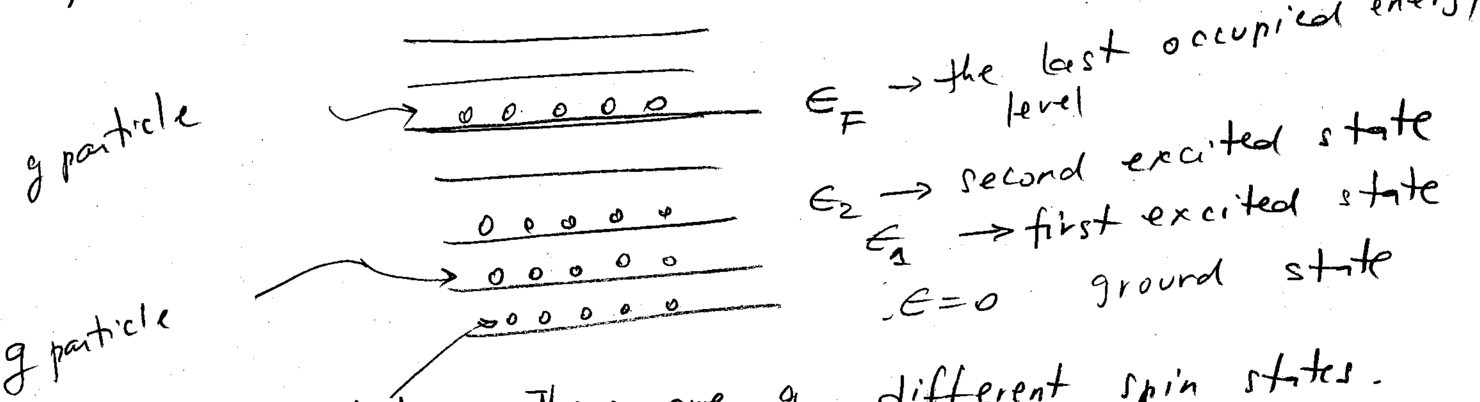
$$\frac{pV}{kT} = \frac{g}{\lambda^3}\frac{(\beta\mu)^{\frac{5}{2}}}{\Gamma(\frac{7}{2})} = \frac{g}{\lambda^3}\left(\frac{1}{kT}\right)^{\frac{5}{2}} \cdot \left[\left(\frac{3N}{4\pi g V}\right)^{\frac{2}{3}} \frac{h^2}{2m}\right]^{\frac{5}{2}} \frac{1}{\Gamma(\frac{7}{2})}$$

$$\frac{pV}{kT} = g\left(\frac{\sqrt{2\pi m kT}}{h}\right)^{3}\left(\frac{1}{kT}\right)^{\frac{5}{2}}\left[\left(\frac{3N}{4\pi g V}\right)^{\frac{2}{3}}\frac{h^{2}}{2m}\right]^{\frac{5}{2}}\cdot\underbrace{\frac{8}{15\sqrt{\pi}}}_{\frac{1}{\Gamma\left(\frac{7}{2}\right)}}$$

we get for COMPLETELY DEGENERATE FERMI GAS

$$p = \left(\frac{6\pi^{2}}{g}\right)^{\frac{2}{3}}\frac{h^{2}}{5m}\left(\frac{N}{V}\right)^{\frac{5}{3}}$$

the pressure is also independent of temperature and is <u>NOT ZERO</u> even if $T \to 0$. This is a quantum effect arising from PAULI EXCLUSION PRINCIPLE, the particles cannot settle down in a ground state (like bosons).



g particle. There are g different spin states.

Each 1-particle state is occupied by <u>ONE</u> fermion.

At $T=0$, the Fermi particles will occupy ALL 1-particle states up to a maximum 1-particle energy ϵ_F. There is only one N-particle state

COMPLETELY DEGENERATE N-particle state [ONLY ONE!]

$$(1, 1, 1, 1, \ldots, 1, 0, 0, 0, 0, \ldots 0)$$

occupation number description

$$N\text{-particle state in general} = (n_1, n_2, n_3, \ldots)$$

$1, 2, 3 \ldots$ = 1-particle states

n_1 = # of particles in 1-particle state 1

n_2 = # of particles in 1-particle state 2

n_3 = # of particles in 1-particle state 3

⋮

The 1-particle states are ordered in terms of increasing 1-particle energy levels. The maximum 1-particle energy occupied is called

$$\boxed{\epsilon_F = \text{FERMI ENERGY}}$$

The same picture as above can be obtained from the formula for the average number of particles in the 1-particle energy state

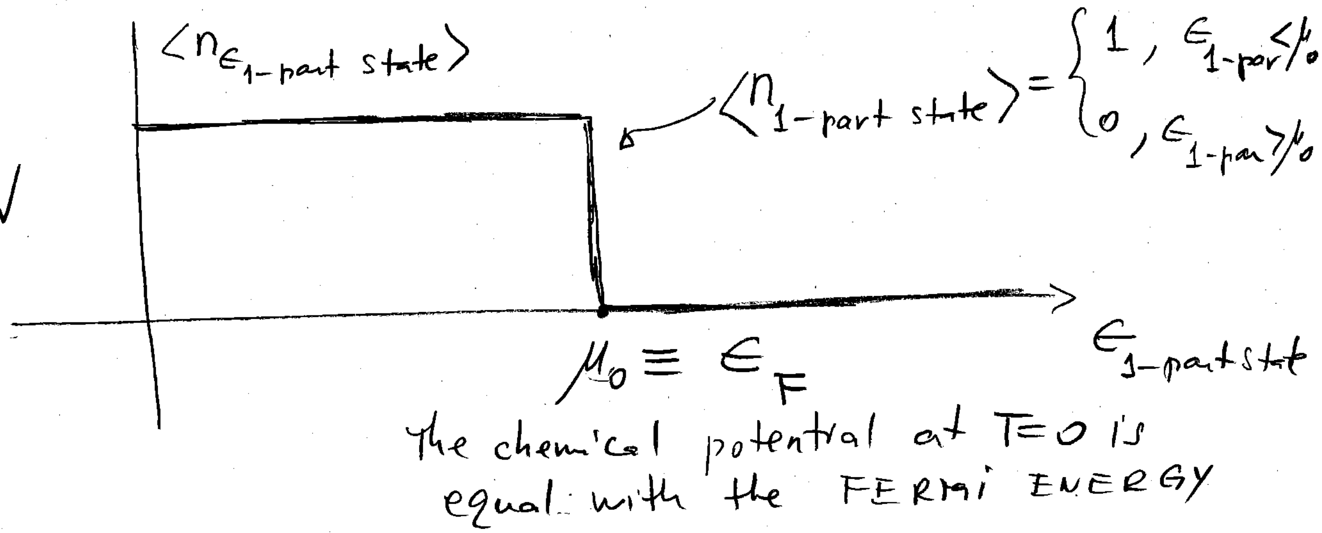
$$\langle n_{\epsilon_{1\text{-part state}}} \rangle = \frac{1}{e^{\frac{\epsilon_{1\text{-part state}} - \mu}{kT}} + 1}$$

When $T \to 0$ the average number of particles in 1-particle energy state becomes a step function

$$\lim_{T \to 0} e^{\frac{\epsilon_{1\text{-part state}} - \mu}{kT}} = \begin{cases} 0 & \text{if } \epsilon_{1\text{-part state}} < \mu_0 \\ \infty & \text{if } \epsilon_{1\text{-part state}} > \mu_0 \end{cases}$$

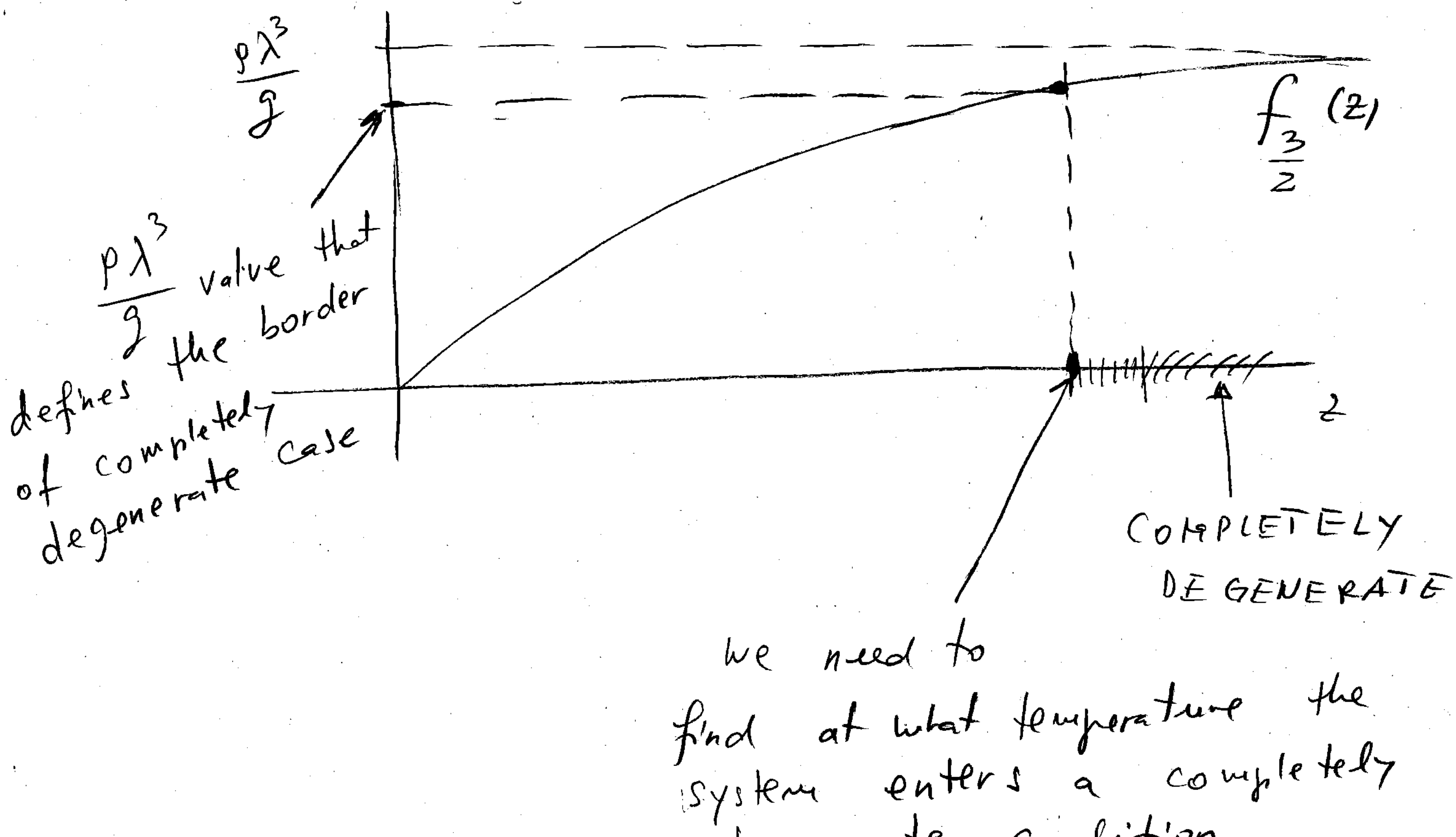
where μ_0 is the chemical potential obtained in formula (5). So for $\langle n_{\epsilon_{1\text{-particle state}}} \rangle$ we have

STEP FUNCTION



The chemical potential at $T=0$ is equal with the FERMI ENERGY

At this point we know what is the behavior of the gas at $T \approx 0$. What we do not know is at what temperature the gas is ENTERING into a completely degenerate situation.



To find the borderline we need to approximate $f_{\frac{3}{2}}(z)$ better than we did in the previous pages.

Sommerfeld showed also that

$$f_{\frac{3}{2}}(z) = \frac{(\ln z)^{\frac{3}{2}}}{\Gamma(\frac{3}{2}+1)}\left[1 + \frac{5\pi^2}{8}(\ln z)^{-2} + \cdots\right] \quad (6)$$

$$f_{\frac{5}{2}}(z) = \frac{(\ln z)^{\frac{5}{2}}}{\Gamma(\frac{5}{2}+1)}\left[1 + \frac{\pi^2}{8}(\ln z)^{-2} + \cdots\right] \quad (7)$$

Now we need to solve for z from

$$\frac{\rho \lambda^3}{g} = f_{\frac{3}{2}}(z)$$

Using the first two terms in (6) we obtain

$$kT \ln z \equiv \mu \simeq \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{\epsilon_F} \right)^2 \right] \qquad (8)$$

For $T=0$ we find $\mu \simeq \epsilon_F$ as it should be; this is given by (5)

$$\epsilon_F = \left(\frac{3N}{4\pi g V} \right)^{\frac{2}{3}} \frac{\hbar^2}{2m}$$

and is independent of temperature. The second term in (8) contains the temperature, and this is what we need to find the borderline into the <u>completely degenerate</u> case. We see from (8) that if

$$\boxed{\frac{kT}{\epsilon_F} \ll 1}$$ Condition for completely degenerate fermion gas

we have $\mu \simeq \epsilon_F$ and we are indeed in a completely degenerate case.

The temperature for which

$$\frac{kT}{\epsilon_F} = 1$$

is called <u>Fermi temperature</u>

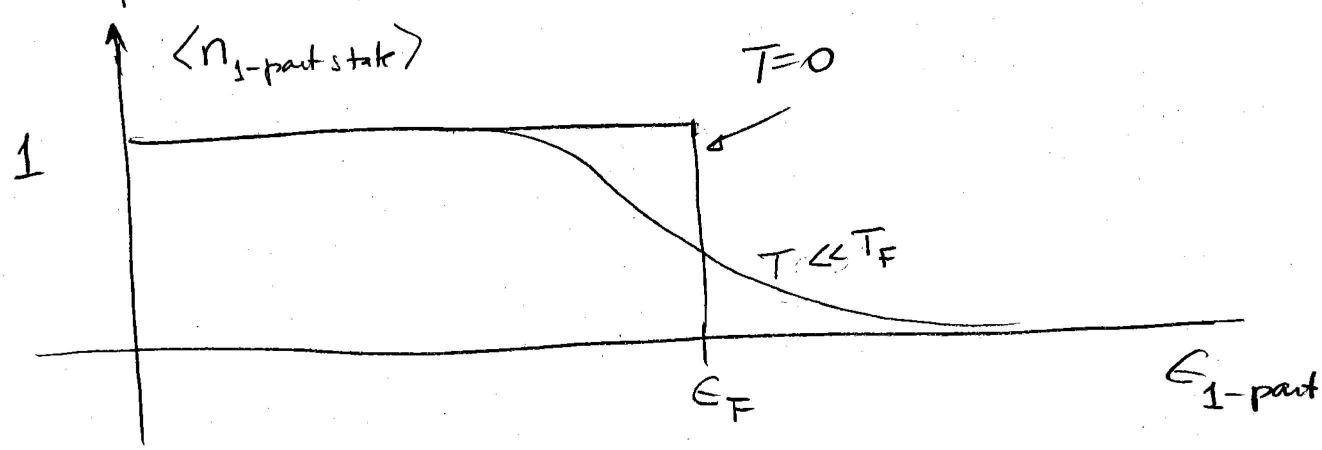
$$\boxed{T_F = \frac{\epsilon_F}{k}}$$

or, inserting the value for ϵ_F

$$\boxed{T_F = \frac{1}{k}\left(\frac{3N}{4\pi g V}\right)^{\frac{2}{3}} \frac{\hbar^2}{2m}}$$

If $\boxed{T \ll T_F}$ COMPLETELY DEGENARTATE FERMI GAS

The average number of particles in the 1-particle state at $T \ll T_F$ is



$$\langle n_{1\text{-part state}} \rangle = \frac{1}{e^{\frac{\epsilon_{1\text{-part state}} - \mu(T)}{kT}} + 1}$$

This $\mu(T)$ depends on temperature and is given by (8)

Now that $T \neq 0$ we will have not only one N-particle state, as it was at $T=0$. However, the N-particle states have a precise structure

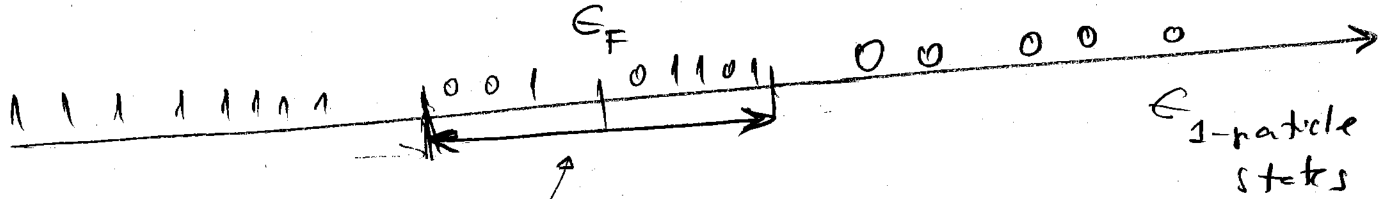
N-particle state at $T \neq 0$ but $T \ll T_F$ is

$$\Big(\underbrace{1,1,1 \cdots 1}, \underbrace{0,0,1,0,1,1,0,1}, \underbrace{0\,0\,0\,0\,0}\Big)$$

many ones up to a 1-particle state with an energy close to ϵ_F

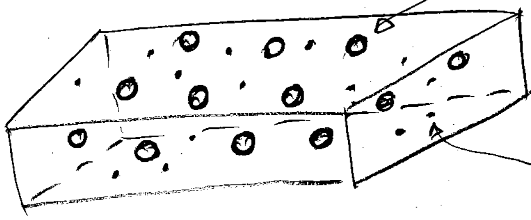
all zeroes for 1-particle states with energy bigger than ϵ_F

a region with mixed zeroes and ones for 1-particle states with energy close to ϵ_F.



this energy interval is approx. kT

Electron gas in metals



To find if the electron gas, which is a nondegenerate or degenerate Fermi gas, we need to estimate the Fermi temperature T_F.

For a metal, like sodium

\# conduction electrons per atom $= 1$

\# atoms per unit lattice cell $= 2$

the lattice cell length $= 4.29\,\mathring{A}$

then

$$\frac{N}{V} = \frac{1 \cdot 2}{(4.29\,\mathring{A})^3}$$

Using

$$\epsilon_F = \left(\frac{3N}{4\pi g V}\right)^{\frac{2}{3}} \frac{\hbar^2}{2m}$$

with $g = 2$ for electrons (electron spin is $\frac{1}{2}$ and $g = 2 \cdot \frac{1}{2} + 1$) and $m =$ electron mass, we get

$$(\epsilon_F)_{\text{Sodium}} = 3.14 \text{ eV}$$

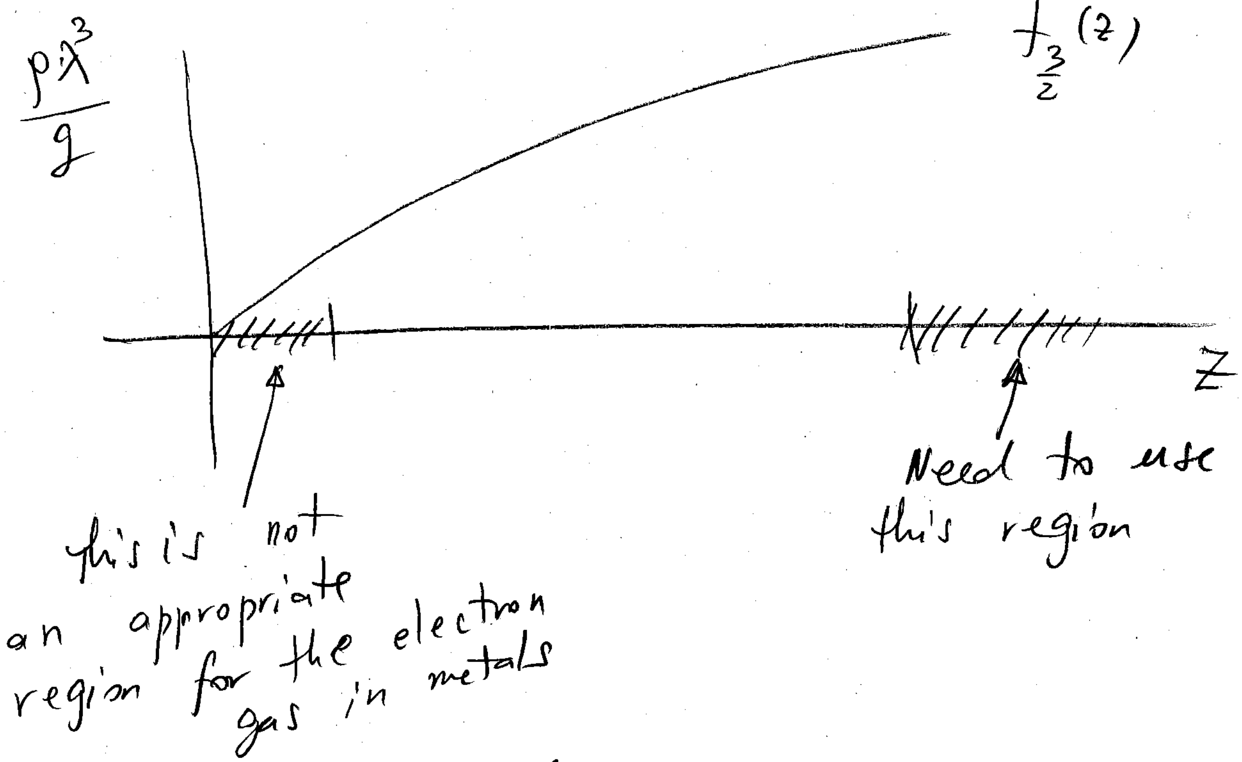
The Fermi temperature of the gas is

$$(T_F)_{\text{Sodium}} = \frac{\epsilon_F}{k} = \underline{\underline{3.64 \cdot 10^4 \text{ K}}}$$

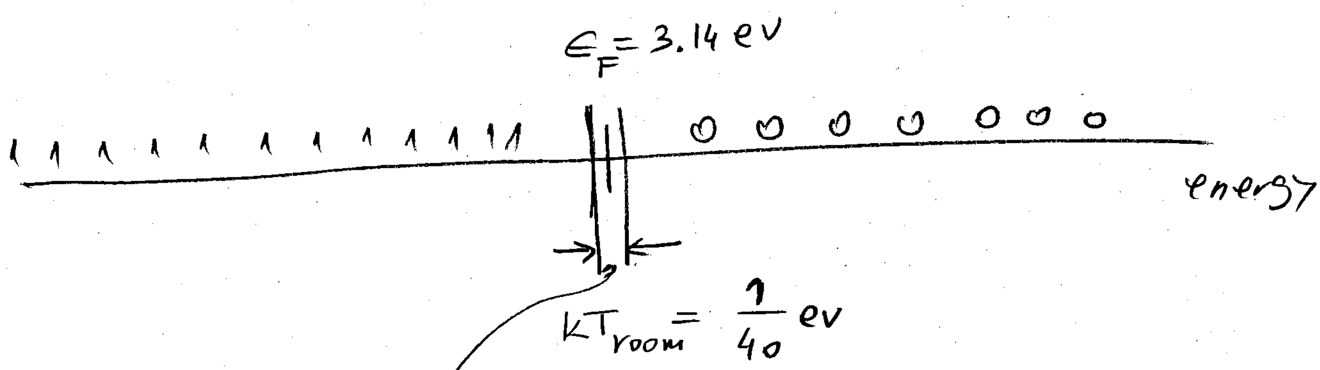
For room temperature $T_{room} = 300$ K we have

$$T_{room} \ll (T_F)_{\text{Sodium}}$$

<u>Conclusion</u>
The electron gas in the sodium metal is completely degenerate



The excited state region around ϵ_F is about kT_{room}, as we pointed before

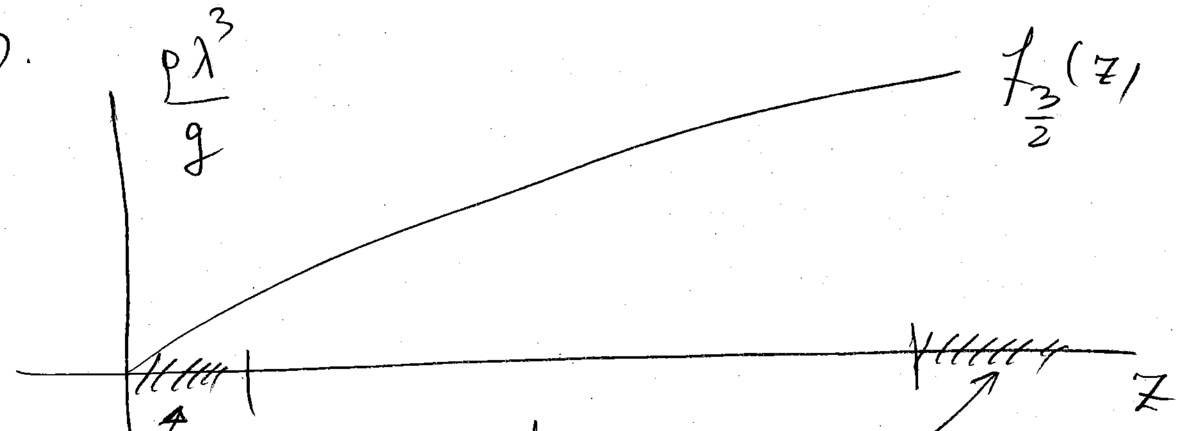


in this narrow region the occupation number for 1-particle states vary, and can take the value 1 or 0.

On the left of the narrow region all the 1-particle states are occupied (only 1's). On the right of the narrow region all the 1-particle states are unoccupied (only 0's).

Sommerfeld Solution to a long standing classical problem

Our conclusion was that the electron gas in the metal is completely degenerate. We will compare now the classical region (normal gas) with the quantum region (completely degenerate case).



For this classical region, the thermodynamics is

$$p = \frac{N}{V} kT$$

$$U = \frac{3}{2} NkT$$

$$C_V = \frac{3}{2} Nk$$

NO TEMPERATURE

For this quantum region of completely degenerate gas, the thermodynamics is

$$p = \frac{2}{5}\frac{N}{V}\epsilon_F\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\epsilon_F}\right)^2+\cdots\right]$$

$$U = \frac{3}{5} N\epsilon_F\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\epsilon_F}\right)^2+\cdots\right]$$

$$C_V = \frac{\pi^2}{2} Nk \frac{kT}{\epsilon_F}$$

TEMPERATURE

Statistical equilibrium of white dwarf stars

The first application of Fermi' statistics appeared in astrophysics - Fowler 1926.

- Hidrogen content is used
  The core is no longer supporeted against gravitational collapse by fusion
- the white dwarf is supported by electron degeneracy pressure
- Model of a white dwarf

mass $M = 10^{33}\, g$ of He

density $\rho = 10^{7}\, \frac{g}{cm^3}$

temperature $T = 10^{7}\, K$

because this temperature is large, the He is ionized. Thus the component of the stars are

N electrons (m_e each)

$\frac{1}{2}N$ He nuclei ($4 m_p$ each)

So $$M = N \cdot m_e + \frac{1}{2} N \cdot 4 m_p = N(m_e + 2m_p) \simeq 2N m_p$$

Electron density

$$n = \frac{N}{V} \simeq \frac{\frac{M}{2m_p}}{\frac{M}{\rho}} = \frac{\rho}{2m_p} \sim 10^{30} \frac{\text{electrons}}{\text{cm}^3}$$

with $g=2$ for electrons, the Fermi energy

is

$$\epsilon_F = \left(\frac{3}{4\pi g}\frac{N}{V}\right)^{\frac{2}{3}} \frac{\hbar^2}{2m_e} \simeq 10^6 \text{ eV}$$

and the Fermi temperature is

$$T_F = 10^{10} \text{ K}$$

Now

$$T = 10^7 \ll 10^{10}$$

So the electron gas in a white dwarf is completely degenerate.

Another observation is that the Fermi energy $\epsilon_F = 10^6$ eV $= 1$ MeV which is comparable with the electron rest mass $mc^2 = 0,511$ MeV.

Conclusion

1) relativistic electrons

2) degenerate electrons

Fowler 1926

Anderson 1929, Stoner 1929-1930, Chandrasekhar 1931-1935