

HH0006 Ideal Gas in Classical Regime

The Fermi and Bose distribution functions are

$$f(\epsilon) = \frac{1}{\lambda e^{\epsilon/\tau} \pm 1} \quad \begin{matrix} +1 \text{ (Fermions)} \\ -1 \text{ (bosons)} \end{matrix}, \quad \lambda = e^{\mu/\tau}$$

If $\lambda^{-1} e^{\epsilon/\tau} \gg 1$, the (± 1) term is not important and can be dropped. In this limit, the distribution fn is

$$f(\epsilon) \approx \lambda^{-1} e^{-\epsilon/\tau}$$

The difference between fermions and bosons disappears \rightarrow classical!

To be concrete, consider the ideal gas in classical regime,

$$\frac{1}{\lambda} e^{\epsilon/\tau} \gg 1 \quad \text{requires} \quad \frac{1}{\lambda} \gg 1 \quad \text{because} \quad \min(\epsilon) = 0.$$

Making use of $\mu = \tau \log(n/n_Q)$ and $\lambda = e^{\mu/\tau}$, the criterion for classical regime becomes rather clear,

$$\frac{1}{\lambda} \gg 1 \quad \rightarrow \quad \frac{n}{n_Q} \ll 1 \quad n_Q = \left(\frac{m\tau}{2\pi\hbar^2} \right)^{\frac{3}{2}}$$



Classical regime: high T, low n

It's important to emphasize that the occupation number for any orbital

$$f(\epsilon) \ll 1$$

quantum stat. is not important.

(I) All about chemical potential.

For system with definite particle number N, the chemical potential can be solved,

$$N = \sum_n \frac{1}{\lambda e^{\epsilon_n/\tau} \pm 1}$$

where $\lambda = e^{\mu/\tau}$ and n stands for orbital index.

It's helpful to convert the sum into integral

$$\sum_n (\dots) = \frac{1}{8} \int_0^\infty 4\pi n^2 dn (\dots) = \frac{\pi}{2} \int_0^\infty dn n^2 (\dots)$$

Since $\varepsilon_n = \frac{\hbar^2 k_n^2}{2m} = \left(\frac{\hbar^2 \pi^2}{2mL^2}\right) n^2$, one changes the variable to energy ε ,

$$\sum_n = \frac{\pi}{4} \left(\frac{\sqrt{2mL}}{\pi\hbar}\right)^3 \int_0^\infty d\varepsilon \sqrt{\varepsilon}$$

Making everything dimensionless $x \equiv \frac{\varepsilon}{\varepsilon_c}$

We come to the useful relation:

$$\sum_n (\dots) = \frac{2}{\sqrt{\pi}} n_Q \cdot V \int_0^\infty dx \sqrt{x} (\dots)$$

very useful expression ☺

Thus, the particle number conservation gives

$$N = \frac{2}{\sqrt{\pi}} n_Q V \int_0^\infty dx \frac{x^{\frac{1}{2}}}{\lambda e^x \pm 1}$$

important relation!

Introduce the polylogarithm function $Li_\nu(z)$.

$$Li_\nu(z) \equiv \sum_{n=1}^{\infty} \frac{z^n}{n^\nu} \rightarrow \int_0^\infty \frac{x^{\nu-1}}{\frac{1}{z} e^x - 1} dx = \Gamma(\nu) Li_\nu(z)$$

For bosons, $\frac{n}{n_Q} = \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}\right) Li_{\frac{3}{2}}(\lambda)$

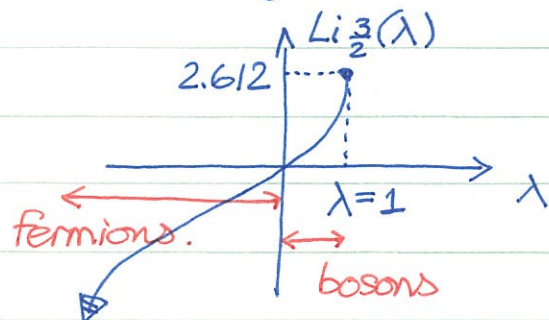
bosons

$$\frac{n}{n_Q} = Li_{\frac{3}{2}}(\lambda)$$

Calculations for fermions are similar, leading to the relation

fermions

$$\frac{n}{n_Q} = -Li_{\frac{3}{2}}(-\lambda)$$



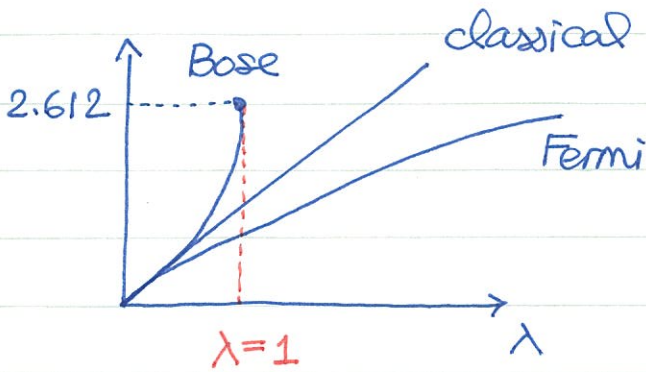
One can also evaluate the integral in classical regime

Classical regime: $N = \frac{2}{\sqrt{\pi}} n_Q V \int_0^\infty dx \lambda x^{\frac{1}{2}} e^{-x}$

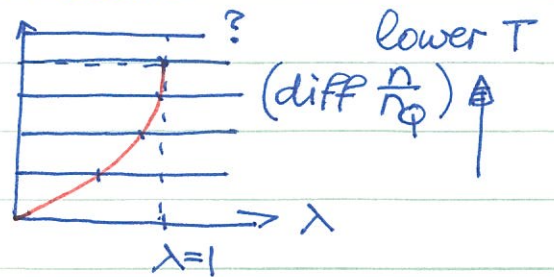
$\frac{N}{n_Q} = \lambda \cdot \frac{2}{\sqrt{\pi}} \int_0^\infty dx x^{\frac{1}{2}} e^{-x} \rightarrow \boxed{\frac{N}{n_Q} = \lambda}$ extremely simple.

$\Gamma(\frac{3}{2}) = \sqrt{\pi}/2$

Now putting all results together for comparison:



There seems to be a problem with bosons



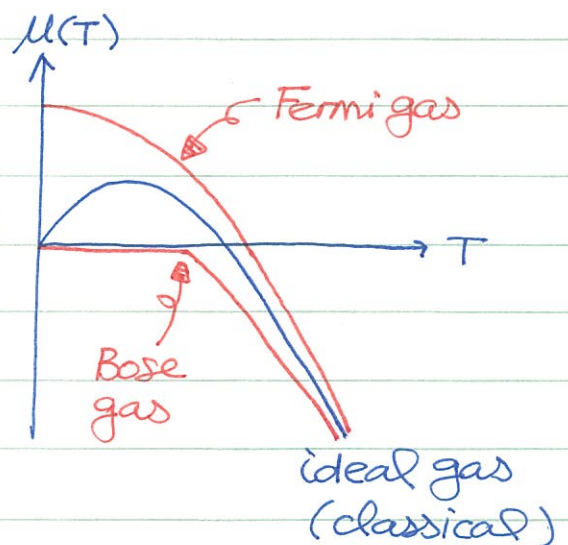
For low enough temperature, $LHS = N/n_Q > 2.612$ and there is no solution for λ (and thus μ)... What does this mean?

$\frac{N}{n_Q} > \int_0^\infty dx \frac{x^{\frac{1}{2}}}{e^x - 1} \cdot \left(\frac{2}{\sqrt{\pi}}\right) = Li_{\frac{3}{2}}(1) \approx 2.612$

The missing particles go to the ground state ϵ_0

$N = N_0 + N_e = N_0 + 2.612 n_Q V$ $[N = N_0 \text{ at } T=0 \text{ because } n_Q=0 \text{ there.}]$

To obtain $\mu = \mu(T)$ needs some work. The logical flows to get the chemical potential are presented in above. The final result can be summarized on the right.

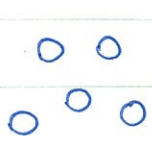


(II) Corrections from internal degrees of freedom.

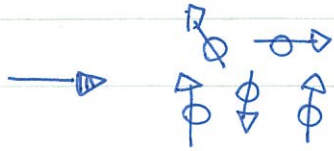
In classical regime, $\frac{n}{n_\phi} = \lambda = e^{\mu/\tau} \rightarrow \mu = \tau \log(n/n_\phi)$

Other quantities can be obtained as described in Kittel's book. (page 162 - page 171).

Let's take an alternative route to understand the internal degrees of freedom.



1 state



$(2S+1)(2S+1) \dots (2S+1)$ states

$(2S+1)^N$

The spin gives rise to $(2S+1)$ configurations.

$g \rightarrow (2S+1)^N g$

Therefore, entropy

$\sigma \rightarrow \sigma + N \log(2S+1)$



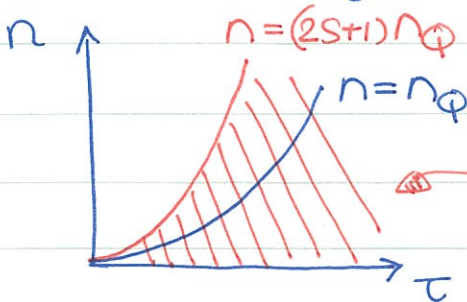
One can obtain the free energy correction

$\frac{\partial F_{int}}{\partial \tau} = -\sigma_{int} \rightarrow F_{int} = -N\tau \log(2S+1)$

and the chemical potential is shifted by $\frac{\partial F_{int}}{\partial N} = -\tau \log(2S+1)$

$\mu = \tau \log\left(\frac{n}{n_\phi}\right) - \tau \log(2S+1)$

It's interesting to see that the activity $\lambda = e^{\mu/\tau} = \frac{n}{(2S+1)n_\phi}$



larger classical regime.

The internal degrees of freedom help the ideal gas more "classical".

But, if the internal degrees of freedom are not equally distributed, one must go back and derive the Gibbs sum first. Starting from $\varepsilon = \varepsilon_n + \varepsilon_{int}$,

$$\mathcal{Z} = 1 + \lambda \sum_{int} e^{-(\varepsilon_n + \varepsilon_{int})/\tau} + (\text{higher orders})$$

In the classical regime, higher-order terms can be ignored,

$$\mathcal{Z} = 1 + \lambda Z_{int} e^{-\varepsilon_n/\tau}$$

$$Z_{int} = \sum_{int} e^{-\varepsilon_{int}/\tau}$$

τ for one particle.

The occupation distribution is

$$f(\varepsilon_n) = \frac{1}{\mathcal{Z}} \lambda Z_{int} e^{-\varepsilon_n/\tau} \approx \lambda Z_{int} e^{-\varepsilon_n/\tau}$$

Sum over all orbitals and the total particle number should add up to N .

$$N = \sum_n f(\varepsilon_n) = \lambda Z_{int} \sum_n e^{-\varepsilon_n/\tau} = Z_1 = n_\phi V.$$

$$\rightarrow \frac{N}{n_\phi} = \lambda Z_{int}$$

$$\lambda = e^{\mu/\tau} \rightarrow \mu = \tau \log \frac{N}{n_\phi} - \tau \log Z_{int}$$

check. For free spin, $Z_{int} = (2S+1)$.

$\mu = \tau \log(\frac{N}{n_\phi}) - \tau \log(2S+1)$ agrees with previous results $\ddot{\smile}$



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