A Schekochihin, Stat Phys Lectures, Oxford HT-2012

§15. Degenerate Fermi Gas.

Recall that our general scheme for dealing with a quantum gas was (see pp 126-127):

1) Calculate μ from

$$N = \sum_i \bar{n}_i = \frac{(2S+1)Vm^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}\int_0^\infty \frac{d\varepsilon\,\sqrt{\varepsilon}}{e^{\beta(\varepsilon-\mu)}+1} \quad (1)$$

keeping just +, for fermions

Using the above,

2) Calculate mean energy:

$$U = \sum_i \varepsilon_i \bar{n}_i = \frac{(2S+1)Vm^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}\int_0^\infty \frac{d\varepsilon\,\varepsilon^{3/2}}{e^{\beta(\varepsilon-\mu)}+1} \quad (2)$$

which is, completely generally, also

$$U = -\frac{3}{2}\Phi = \frac{3}{2}PV$$

so, knowing U, we immediately know the equation of state, $P = \frac{2}{3}\cdot\frac{U}{V}$ (pressure $\leftrightarrow$ energy density)

and can also compute heat capacity:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

Finally, if we want entropy, either for its own sake or, say, to calculate C_P, we have $\Phi = U - TS - \mu\bar{N}$,

so
$$S = \frac{U - \Phi - \mu\bar{N}}{T} = \frac{\frac{5}{3}U - \mu N}{T} \quad \left[\text{or} = -\left(\frac{\partial\Phi}{\partial T}\right)_{V,\mu}\right]$$

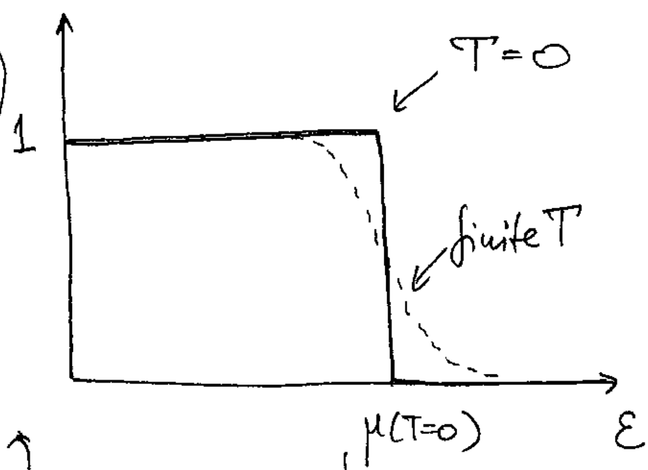
Thus, full construction of thermodynamics hinges on our ability to calculate the integrals in (1) and (2).

So let us now implement this program for a degenerate Fermi gas. We are assuming that $\beta \to \infty$, so

$$\frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

this is just $n_{\vec{k}}$ (occ. # of state with a given momentum and spin)

see p.124



This distribution replaces Maxwell's in the treatment of degenerate gas

So, at T=0, particles just stack up to some fixed energy

this is called Fermi energy:

$$\boxed{\varepsilon_F = \mu(T=0)}$$

At finite T, the step function will be smoothed out, with the width of the smoothing region $\sim k_B T$.

15.1 Energy and Eqn of State

The part of our programme pertaining to the calculation of μ (or ε_F as we now call it at $T=0$), energy and eqn of state is now extremely easy:

1) $$\int_0^\infty \frac{d\varepsilon\sqrt{\varepsilon}}{e^{\beta(\varepsilon-\mu)}+1} \approx \int_0^{\varepsilon_F} d\varepsilon\sqrt{\varepsilon} = \frac{2}{3}\varepsilon_F^{3/2} \overset{\text{from (1)}}{=} \frac{\sqrt{2}\pi^2\hbar^3}{2S+1}\underbrace{\left(\frac{N}{V}\right)}_{=n}\frac{1}{m^{3/2}}$$

$$\boxed{\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{2S+1}\right)^{2/3}} = \frac{\hbar^2 k_F^2}{2m}$$

$$k_F = \left(\frac{6\pi^2 n}{2S+1}\right)^{1/3}$$ — the max wave number up to which the particles stack up.

So this

- tells us what μ is (for use in (2))
- tells us the max energy particles can have (i.e. which levels are occupied)
- tells us how good the $T=0$ approximation is:

indeed, clearly, this picture is fine as long as the smearing of the step function is narrower than the step function itself, i.e.

$$k_B T \ll \varepsilon_F \iff T \ll T_F = \frac{\varepsilon_F}{k_B}$$

this is exactly the same (up to numerical factors) as the degeneration temperature (see p. 133) ~ 10^4 K for electrons in metals.

Note that "low" temperature might not actually be so low if the particle density is high (and mass small)

Eg., for electrons in white dwarves (HW), Fermi energy can be as large as ~ MeV $\iff T_F \sim 10^{10}$ K and we must in fact consider relativistic electron gas (similar calculations as above, but redo everything with the relativistic formula for $\varepsilon(\vec{k})$ – see p. 125 onwards; in fact it is a good exercise to go through the calculations on pp 125 – 135 for $\varepsilon = \hbar k c$)

2) Now calculate energy from (2):

$$U = \underbrace{\frac{(2S+1)Vm^{3/2}}{\sqrt{\pi}\,\pi^2\hbar^3}}_{= N\cdot\frac{1}{\frac{2}{3}\varepsilon_F^{3/2}}} \underbrace{\int_0^{\varepsilon_F} d\varepsilon\, \varepsilon^{3/2}}_{= \frac{2}{5}\varepsilon_F^{5/2}} = \frac{3}{5} N \varepsilon_F ,$$

whence, immediately, the equation of state:

$$p = \frac{2}{3}\frac{U}{V} = \frac{2}{5} n \varepsilon_F = \frac{\hbar^2}{5m}\left(\frac{6\pi^2}{2S+1}\right)^{2/3} n^{5/3}$$

independent of temperature. It can be said that the gas behaves as a "pure mechanism" – i.e. entropy is not involved. Indeed (from p134),

Ex. $TS = \frac{5}{3}U - \mu N = 0$, as it should be at $T=0$.

Note. that the equation of state we have derived is actually just (keep N const)

$$PV^{5/3} = \text{const}$$

the adiabatic law, which, as we know from pp127–129, holds completely generally – but it is only the eqn of state when $T=0$.

From this we can obtain some experimentally verifiable quantities, e.g. "the bulk modulus"

$$B = -V\frac{\partial p}{\partial V} = \frac{2}{3} n \varepsilon_F .$$

for els in metals

15.2 Heat Capacity

We are not done, however, because we can't calculate heat capacity yet. Indeed, ~~we~~ we took $T \to 0$, so everything is independent of temperature, so we know

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = 0 \text{ at } T = 0$$

But this is not really a great surprise.
We'd like to have a formula for $C_V(T)$ – and for that, we need to calculate finite-temperature corrections to our lowest-order ($T=0$) approximation of the integrals in (1) and (2).

This requires a little bit of maths:
We are interested in integrals of the form

$$I = \int_0^\infty \frac{d\varepsilon\, f(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1} \qquad \begin{aligned} f(\varepsilon) &= \sqrt{\varepsilon} \text{ in (1)} \\ &= \varepsilon^{3/2} \text{ in (2)} \end{aligned}$$

Change variables: $\beta(\varepsilon-\mu) = x$, i.e. $\varepsilon = \mu + k_B T x$.
Then

$$I = k_B T \int_{-\mu/k_BT}^{\infty} \frac{dx\, f(\mu + k_B T x)}{e^x+1} =$$

here we have changed $x \to -x$

$$= k_B T \int_0^{\mu/k_BT} \frac{dx\, f(\mu - k_B T x)}{e^{-x}+1} + k_B T \int_0^\infty \frac{dx\, f(\mu + k_B T x)}{e^x+1}$$

but $\dfrac{1}{e^{-x}+1} = 1 - \dfrac{1}{e^x+1}$, so we have

$$I = k_BT\underbrace{\int_0^{\mu/k_BT} dx\, f(\mu - k_BTx)}_{\text{// revert tip to } \varepsilon \quad \int_0^{\mu} d\varepsilon\, f(\varepsilon)} - k_BT\int_0^{\mu/k_BT} \frac{dx\, f(\mu-k_BTx)}{e^x+1} + k_BT\int_0^{\infty}\frac{dx\, f(\mu+k_BTx)}{e^x+1}$$

extend to ∞ at the price of an exponentially small error (because $\mu/k_BT \gg 1$)

$$\approx \int_0^{\mu} d\varepsilon\, f(\varepsilon) + k_BT\int_0^{\infty}\frac{dx}{e^x+1}\Big[\underbrace{f(\mu+k_BTx) - f(\mu-k_BTx)}_{\simeq\ 2k_BTx\, f'(\mu)}\Big]$$

(if necessary, can keep higher-order terms)

$$= \int_0^{\mu} d\varepsilon\, f(\varepsilon) + 2(k_BT)^2 f'(\mu)\underbrace{\int_0^{\infty}\frac{dx\, x}{e^x+1}}_{\text{pure number} = \frac{\pi^2}{12}} + \ldots$$

[redacted] (see, e.g. LL §58 on how to compute this)

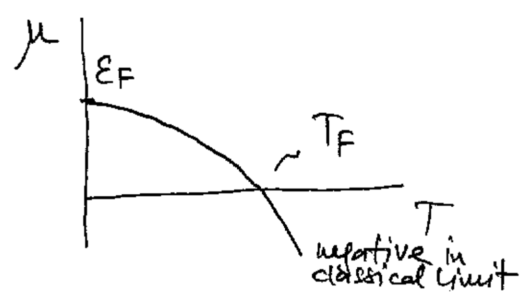
So, for $f(\varepsilon) = \sqrt{\varepsilon}$, we have, from (1),

$$N = \underbrace{\frac{(2S+1)Vm^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}}_{= \frac{N}{\frac{2}{3}\varepsilon_F^{3/2}}}\left[\frac{2}{3}\mu^{3/2} + 2(k_BT)^2\cdot\frac{\pi^2}{12}\cdot\frac{1}{2\sqrt{\mu}} + \ldots\right]$$

$$\mu^{3/2} = \varepsilon_F^{3/2} - \frac{\pi^2}{8}\frac{1}{\sqrt{\mu}}(k_BT)^2 + \ldots$$

$$\boxed{\mu \approx \varepsilon_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \ldots\right]}$$

So this is the corrected expression for $\mu(T)$



Now set $f(\varepsilon) = \varepsilon^{3/2}$ and calculate energy from (2):

$$U = \frac{N}{\frac{2}{3}\varepsilon_F^{3/2}}\left[\frac{2}{5}\mu^{5/2} + 2(k_BT)^2\frac{\pi^2}{12}\frac{3}{2}\sqrt{\mu} + \dots\right]$$

sub. our expression for μ

$$\approx \frac{N}{\frac{2}{3}\varepsilon_F^{3/2}}\left[\frac{2}{5}\varepsilon_F^{5/2} - \frac{\cancel{2}}{\cancel{5}}\varepsilon_F^{5/2}\cdot\frac{\cancel{5}}{\cancel{2}}\frac{\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \right.$$

$$\left. + 2\cdot\frac{\pi^2}{12}\cdot\frac{3}{2}(k_BT)^2\varepsilon_F^{1/2} + \dots\right]$$

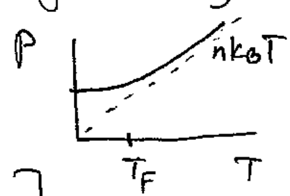
$$= N\left[\frac{3}{5}\varepsilon_F - \varepsilon_F\frac{\pi^2}{8}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \varepsilon_F\frac{3\pi^2}{8}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right]$$

$$= N\varepsilon_F\left[\frac{3}{5} + \frac{\pi^2}{4}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right]$$

Thus,

$$\boxed{U = \frac{3}{5}N\varepsilon_F\left[1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right]}$$

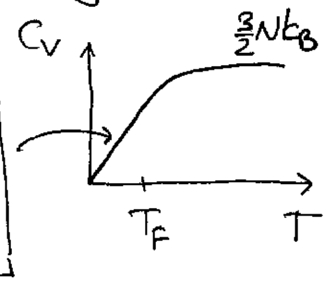
corrected expression for $U(T)$



Equation of state:

$$P = \frac{2}{3}\frac{U}{V} = \frac{2}{5}n\varepsilon_F\left[1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right]$$

Heat capacity:



$$\boxed{C_V = \left(\frac{\partial U}{\partial T}\right)_V = Nk_B\frac{\pi^2}{2}\frac{k_BT}{\varepsilon_F} + \dots}$$

Thus, the heat capacity $C_V \propto T$ at low T — this is the dominant part of the heat capacity of a metal at low T because the heat capacity due to lattice vibrations is $\propto T^3$ at low T.