D. "Low temperature" physics of a Fermi Gas

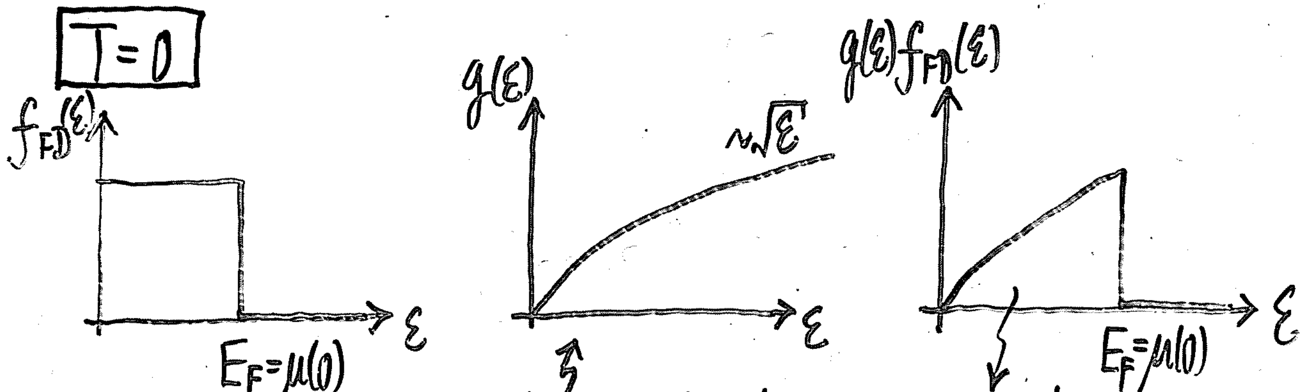
$$\underbrace{0 < kT \ll E_F}\,(= kT_F)$$

In this case, the Fermi gas is said to be degenerate.

(a) Key physics idea

$kT \ll E_F \Rightarrow$ the physics is given by the small change in $f_{FD}(\varepsilon)$, when compared with $T=0$ case.

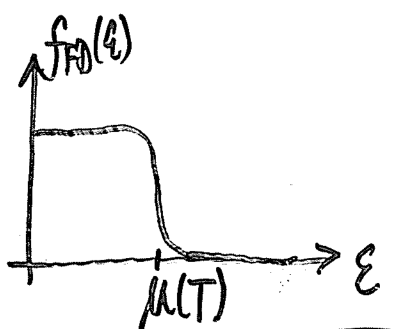
$\boxed{T=0}$

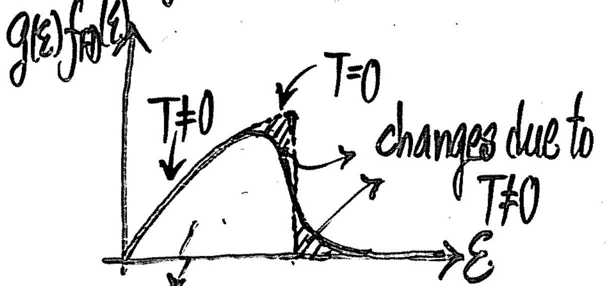


does NOT depend on temperature

Area under curve $= \int_0^{E_F} g(\varepsilon) f_{FD}(\varepsilon) = N$

$\boxed{T\neq 0 \ (T \ll T_F)}$



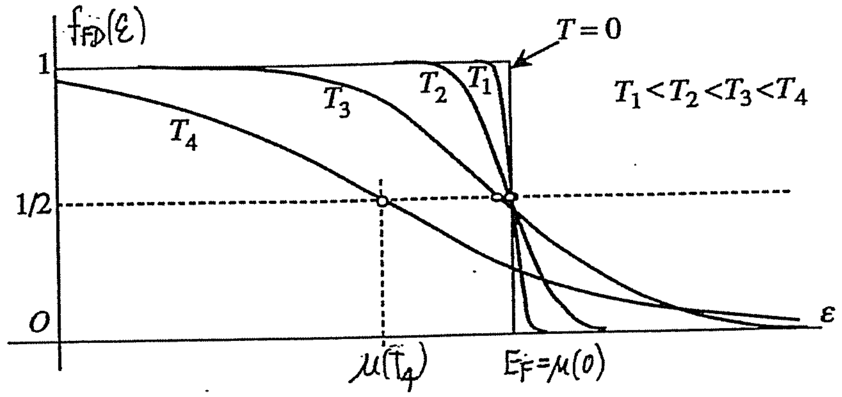


Area under ε
$= \int_0^{\infty} g(\varepsilon) f_{FD}(\varepsilon) = N$

(the same N)

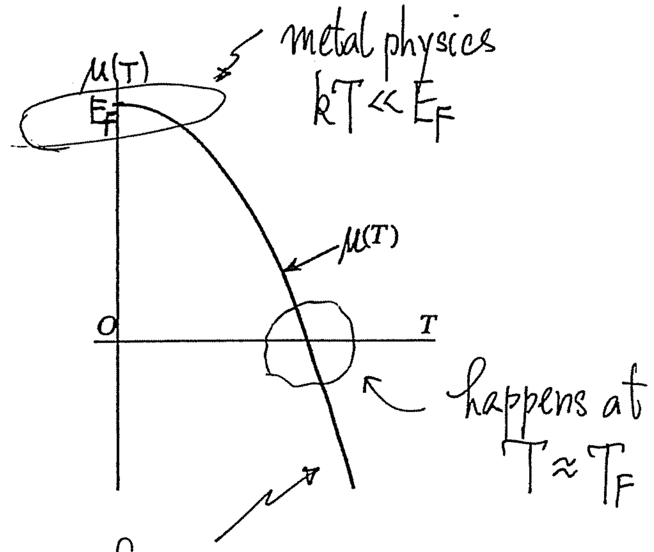
$\therefore$ changes in physics at $T\neq 0$ are due to small changes in the electron occupations near E_F!

3D Ideal Fermi Gas

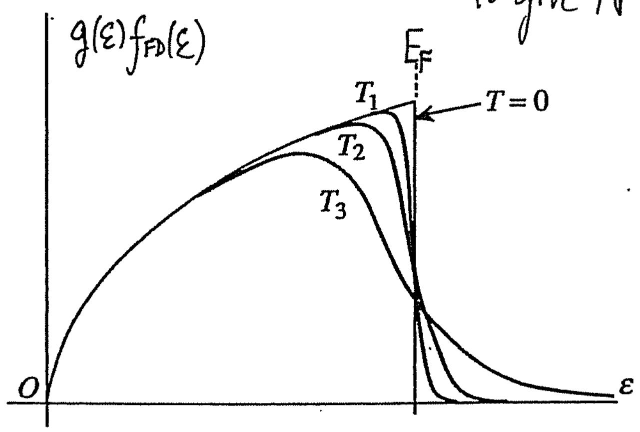


μ shifts

μ shifts so as to keep $\int_0^\infty g(\varepsilon) f(\varepsilon)$ fixed to give N



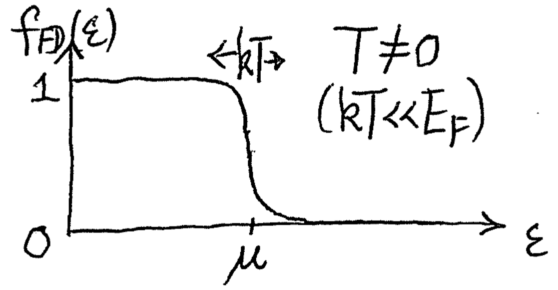
for $T > T_F$ (or $T \gg T_F$)
$f_{FD}(\varepsilon)$ has a tail for $\varepsilon > 0$ that behaves like the Maxwell-Boltzmann distribution. Thus, μ is negative as in a classical ideal gas.



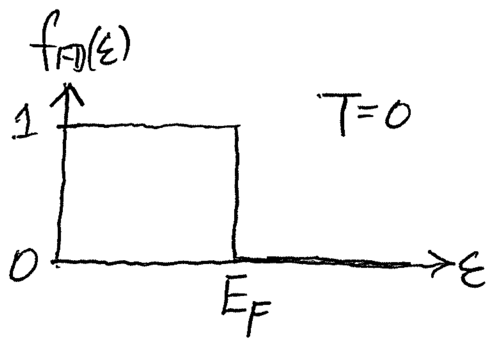
Areas under curves give N

Criterion of $\mu(T)$

- We expect the changes in μ and in E are small and $\sim \left(\frac{kT}{E_F}\right)^{\alpha}$ (α is some power) because



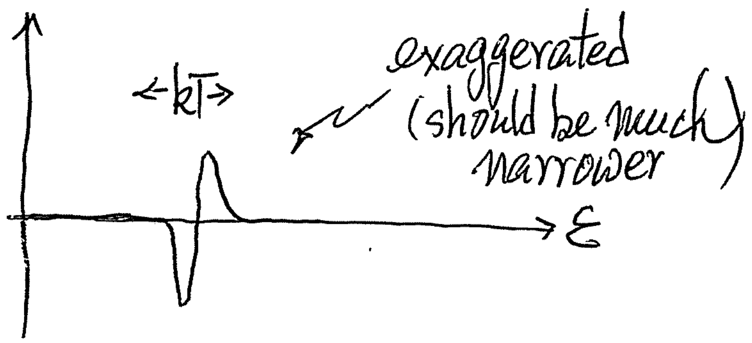
and



differ <u>only slightly</u> <u>AND</u> differ only in a range of $\sim kT$ near E_F

- States deep below E_F : $T=0$ occupied, $T>0$ occupied } no change
- States way above E_F : $T=0$ empty, $T>0$ empty } no change
- Occupation changes only for states near E_F

$f_{FD}^{T\neq0}(\varepsilon) - f_{FD}^{T=0}(\varepsilon)$



$\therefore$ $\underbrace{\left.\begin{array}{l}\mu(T) - E_F \\ E(T) - E(0)\end{array}\right\}}_{\text{changes}}$ determine by states very close to E_F "Fermi Surface effect"

- With this in mind and for $T \ll T_F$ ($kT \ll E_F$), we recognize $\frac{kT}{E_F} \ll 1$ as the <u>small parameter</u> in the low-temperature regime
- Thus, we expect

$$\mu(T) = \underset{\mu(T=0)}{E_F}\left[1 + \underbrace{(\overset{\text{small correction}}{\text{something}})}_{\text{goes like } a\left(\frac{kT}{E_F}\right) + b\left(\frac{kT}{E_F}\right)^2 + \cdots \text{ (tiny)}}\right] \quad \text{(C9)}$$

$$E(T) = E(0)\left[1 + (\text{something})\right] \quad \text{(C10)}$$

<u>Recall</u>: metals at room temperature

$$\frac{kT}{E_F} \sim 0.01 \quad , \quad \left(\frac{kT}{E_F}\right)^2 \sim 10^{-4}$$

- This picture (task) helps us get through the messy mathematics. Keep in mind: We want to find the <u>lowest order correction</u>, i.e., the first term in "something".
- From Eq. (C9), we expect $\mu(T) \approx E_F$ (shift is tiny). The following results are good when $0 < kT \ll \mu$.

(b) A useful formula : "Sommerfeld Expansion"

We need to evaluate $\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}$ and $\int_0^\infty \frac{\varepsilon^{3/2}\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}$

for $\beta\mu \gg 1$ or $kT \ll \mu$.

$$\boxed{I = \int_0^\infty \frac{f(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon \approx \int_0^\mu f(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(kT)^2 f'(\mu) + \cdots} \quad (C11)$$

$f(\varepsilon)$ is some function of ε

note upper limit is μ

$f'(\mu) \equiv \left.\frac{df(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=\mu}$

- Eq. (9) is valid for $kT \ll \mu$ (good for low-temperatures)
- Eq. (9) is called the Sommerfeld Expansion

(c) The shift of μ with temperature : $\mu(T)$

$\mu(T=0) = E_F$

For a 3D Fermi gas : $\mu(T)$

$$N = \int_0^\infty \underbrace{g(\varepsilon)}\, \frac{1}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon \qquad (\text{determines } \mu)$$

DOS plays the role of $f(\varepsilon)$ in Eq. (C11)

- But for a system, N or N/V (e.g. electron density in a metal) is the same for different T.

LHS = N = Same number "N" at $T=0$

$$= \frac{2}{3}\underbrace{\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}}_{} E_F^{3/2} \qquad (\text{see p. FG-13})$$

$$= \frac{2}{3} A\, E_F^{3/2}$$

$$\therefore N \overset{T=0 \text{ result}}{=} \frac{2}{3} A E_F^{3/2} \underset{(\text{any } T)}{=} \int_0^\infty A \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}+1}\,d\varepsilon$$

$$\underset{(kT \ll E_F)}{\approx} \int_0^\mu A\,\varepsilon^{1/2}\,d\varepsilon + \frac{\pi^2}{6}(kT)^2 A\left(\frac{d}{d\varepsilon}\varepsilon^{1/2}\right)_{\varepsilon=\mu} + \underbrace{\cdots}_{\text{ignore}}$$

(Sommerfeld Expansion)

[μ is the unknown]

$$= A\,\frac{2}{3}\mu^{3/2} + A\,\frac{\pi^2}{12}\frac{(kT)^2}{\mu^{1/2}}$$

$$= \frac{2}{3} A \mu^{3/2}\left[1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right]$$

$$\Rightarrow E_F^{3/2} = \mu^{3/2}\left[1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right]$$

Start to see the small parameter!

$$\therefore \mu(T) = E_F\left[1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right]^{-2/3}$$

$$\approx E_F\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{\mu}\right)^2 + \underbrace{\cdots}_{\text{ignore}}\right]$$

$$\approx E_F\left[1 - \underbrace{\frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2}_{\text{leading correction}}\right]$$

shifts downward

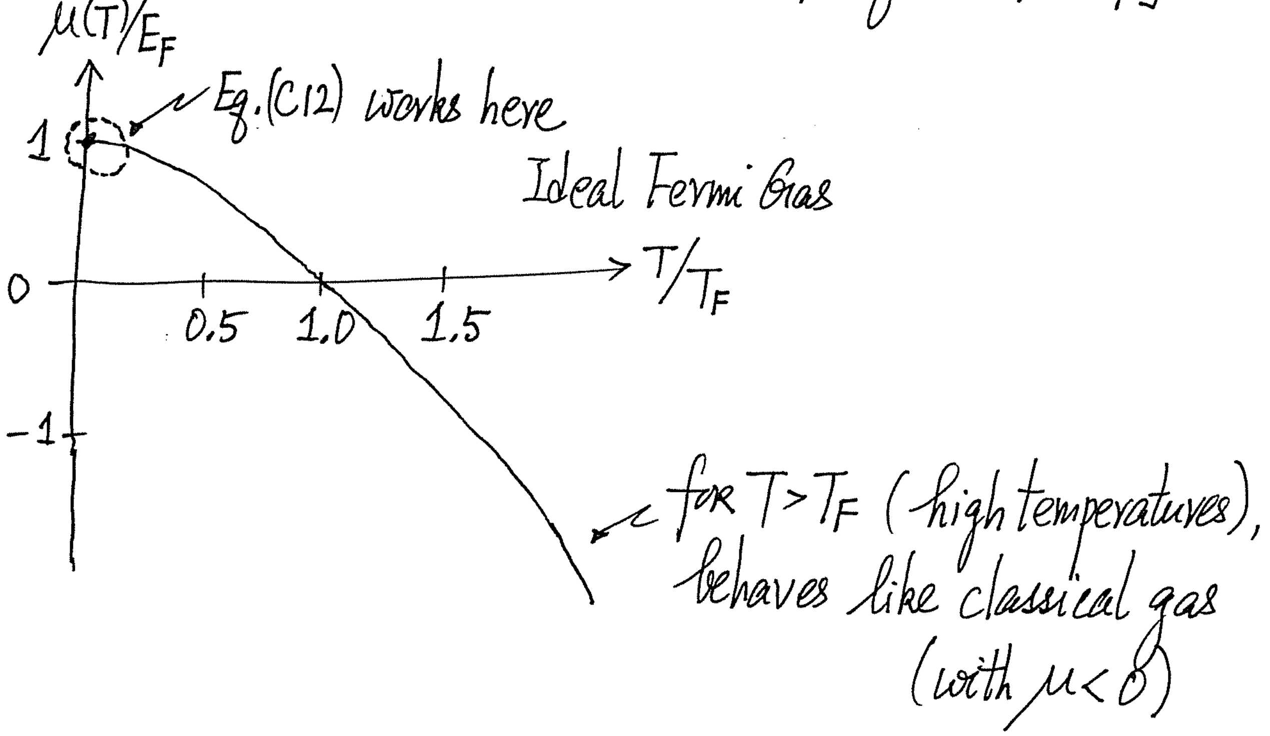
- Key result: The lowest order correction is

$$\boxed{\mu(T) = E_F\left(1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right)} \qquad (C12)$$

  - $\mu(T)$ does shift with T
  - Shifts downward (3D, non-relativistic)
  - first order is already of order $\left(\frac{kT}{E_F}\right)^2$

    [e.g. 10^{-4} for metals at room temperature]
  - Next correction term $\sim \left(\frac{kT}{E_F}\right)^4$ [tiny! Can be ignored!]
  - So, $\mu(T)$ shifts but the shift is small

    [$\mu(T)$ is still close to E_F for $kT \ll E_F$]

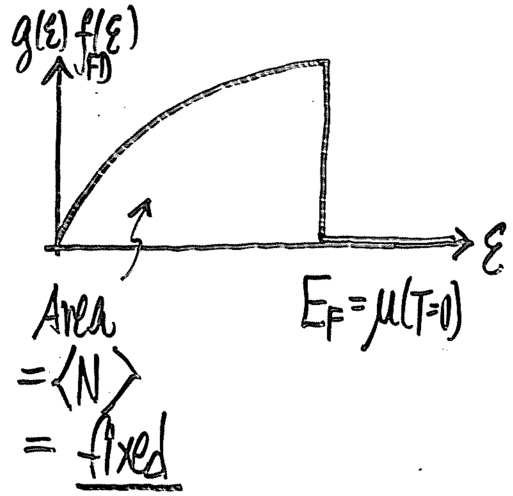


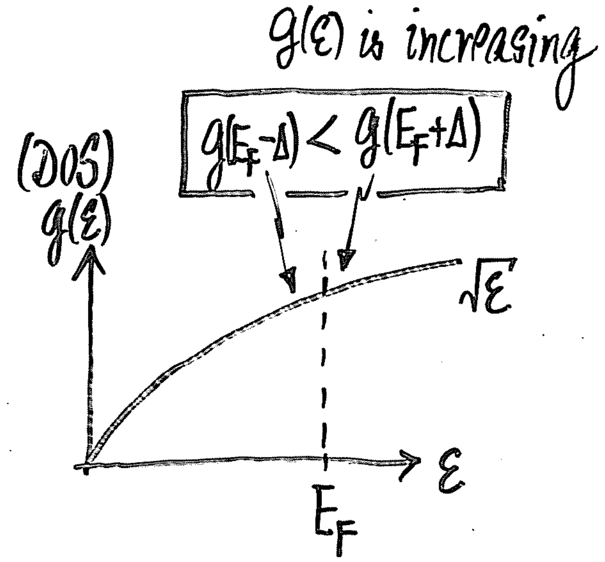
Why does $\mu(T)$ shift downwards: the physics?

[3D box, non-relativistic]

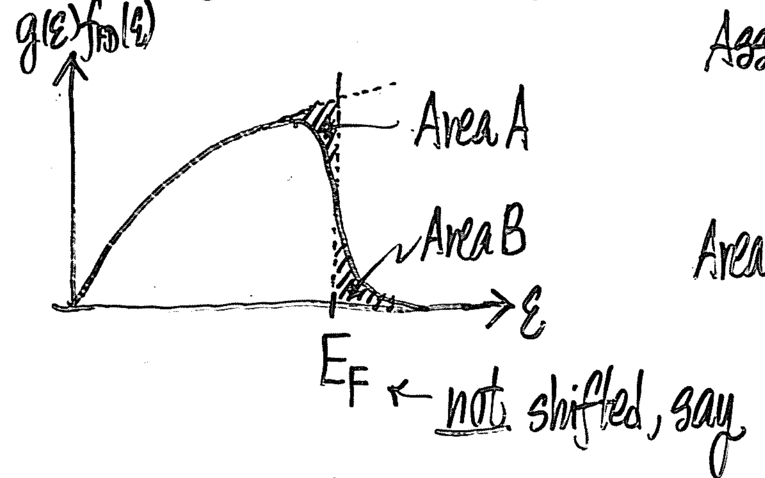
$$N = \int_0^\infty g(\varepsilon) f_{FD}(\varepsilon)\, d\varepsilon$$

$\boxed{T=0}$





$\boxed{T \neq 0}$ What if (which is wrong) μ does not change?



Assume $\mu(T) = E_F$ ← wrong!

Area under curve $\neq N$!

- Area A < Area B because $g(\varepsilon \gtrsim E_F) > g(\varepsilon \lesssim E_F)$ and $f_{FD}(\varepsilon)$ is "symmetrical" about μ

\# missing particles with energy $< E_F$ due to thermal excitations $<$ $\neq$ \# particles with energy $> E_F$ due to thermal excitations

trouble! [not right!]

$\therefore$ μ must shift so as to give N

- Shifting up or down?
  - $g(\varepsilon) \sim \sqrt{\varepsilon}$ (increases with ε)
  - $\mu(T)$ shifts toward the side of smaller density of states (smaller $g(\varepsilon)$) so as to keep area equal to N

(d) Total Energy $E(T)$

$$E(T) = \int_0^\infty g(\varepsilon)\cdot\varepsilon\cdot\frac{1}{e^{\frac{\varepsilon-\mu}{kT}}+1}\,d\varepsilon$$

$$= \int_0^\infty A\,\frac{\varepsilon^{3/2}}{e^{\frac{\varepsilon-\mu}{kT}}+1}\,d\varepsilon$$

$kT \ll E_F$

$$\approx A\left[\int_0^\mu \varepsilon^{3/2}d\varepsilon + \frac{\pi^2}{6}(kT)^2\left(\frac{d}{d\varepsilon}\varepsilon^{3/2}\right)_{\varepsilon=\mu} + \cdots\right]$$ Sommerfeld expansion

$$= A\left[\frac{2}{5}\mu^{5/2} + \frac{\pi^2}{4}(kT)^2\mu^{1/2}\right]$$

$$= A\frac{2}{5}\mu^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right]$$

$\boxed{\text{Note: } \mu(T) \text{ is known}}$

$$= \underbrace{A\frac{2}{5}E_F^{5/2}}\left(\frac{\mu}{E_F}\right)^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right]$$

Note Manipulation Technique

$$= E(T=0)\left(\frac{\mu}{E_F}\right)^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right]$$

(Total energy at T=0, known)

$$E(T) \cong E(0)\left[1-\frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right]^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{E_F}\right)^2\right]$$

$$\approx E(0)\left[1-\frac{5\pi^2}{24}\left(\frac{kT}{E_F}\right)^2\right]\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{E_F}\right)^2\right]$$

$$\approx E(0)\left[1+\left(\frac{5}{8}-\frac{5}{24}\right)\pi^2\left(\frac{kT}{E_F}\right)^2\right] \quad \text{(ignored } \left(\frac{kT}{E_F}\right)^4\text{)}$$

$$= E(0)\left[1+\underbrace{\frac{5\pi^2}{12}\left(\frac{kT}{E_F}\right)^2}\right] \quad (C13)$$

leading term in "something", order $\left(\frac{kT}{E_F}\right)^2$
[total energy increases, but not by much]

Rewrite result of $E(T)$:

$$E(T) = E(0) + \frac{5\pi^2}{12}\cdot\underbrace{E(0)}\cdot\left(\frac{kT}{E_F}\right)^2$$

$$= E(0) + \frac{5\pi^2}{12}\cdot\left(\frac{3}{5}NE_F\right)\cdot\left(\frac{kT}{E_F}\right)^2$$

$$= E(0) + \frac{5\pi^2}{12}\cdot\frac{3}{5}\cdot\overbrace{\frac{2}{3}g(E_F)E_F}\cdot E_F\cdot\left(\frac{kT}{E_F}\right)^2$$

$$\Rightarrow \boxed{E(T) = E(0) + \underbrace{\frac{\pi^2}{6}g(E_F)(kT)^2} \quad (C14)}$$

increase in energy at finite T ($T < T_F$)

Heat Capacity

$$\boxed{C = \frac{\partial E}{\partial T} = \underbrace{\frac{\pi^2}{3}g(E_F)\cdot k^2}T = \gamma T} \quad (C15)$$

linear in T

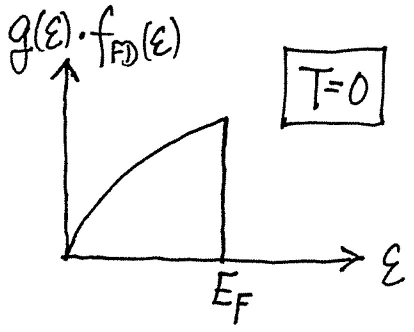
pre-factor $\sim g(E_F)$

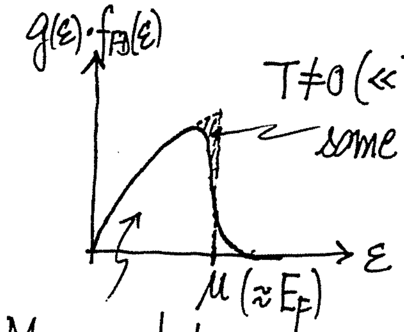
A Hand-Waving Argument

$$E(T) = E_0 + (\text{pre-factor})\, g(E_F)(kT)^2 \qquad (C14)$$

and hence $C \sim T$ (C15)

for ideal Fermi Gas

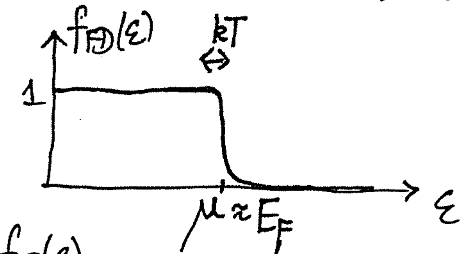




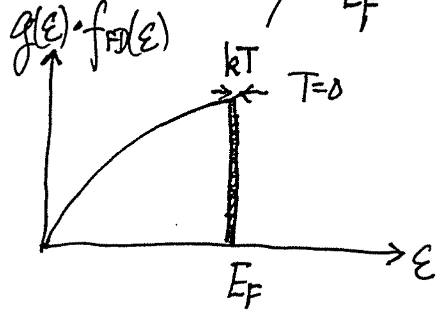
some particles are thermally excited (energy increases)

Many particles are not affected (∵ Pauli Exclusion principle)

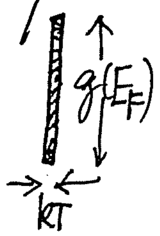
- Compared with T=0 situation, only occupancy of s.p. states in an interval $\sim kT$ near E_F are affected



recall: $\dfrac{kT}{E_F} \sim 0.01$ for metals

- 

Number of particles that can be thermally excited

$\approx$ 

$\approx \underbrace{g(E_F)\cdot kT}_{\text{this is a number}}$

- Each excited particle gains $\sim kT$ in energy

$$\therefore\ E(T) \approx E(T=0) + g(E_F)\cdot kT\cdot kT$$

$$= E(0) + g(E_F)(kT)^2 \qquad \text{[almost correct!]}$$

[c.f. Eq.(C14), just a pre-factor $\frac{\pi^2}{6}$ (order "1") is missing]

Thus, $C = \underbrace{2}_{\frac{\pi^2}{3}}\, g(E_F)\, k^2 T \propto T$

[comparing with Eq.(C15), "2" should be $\frac{\pi^2}{3}$. Not bad!]

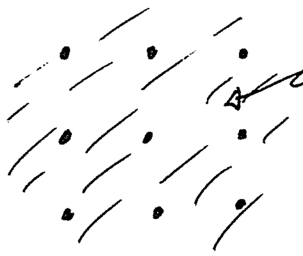
∴ Simple argument gives the correct temperature dependence of $E(T)$ and $C(T)$ at low temperature. It captures the key point that only a small portion of particles near the Fermi energy can be affected. "Fermi Surface Effect"

Heat Capacity of Metals

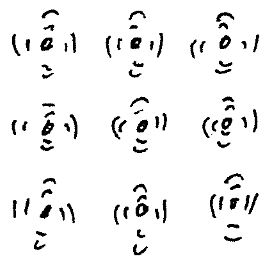
$C_V \sim T$ (due to conduction electrons) $(T \ll T_F)$

$C_V \sim T^3$ (due to lattice vibrations or "phonons") $(T \ll \Theta_D)$

Θ_D: Debye temperature



Sea of electrons (Fermi Gas) $C_V \sim T$



ions vibrate "phonons" [oscillators] (Debye Model) $C_V \sim T^3$

Expect to see in metals

$$\boxed{C_V = \underbrace{\gamma T}_{\text{Statistical Physics of Fermi Gas}} + \underbrace{b T^3}_{\text{Statistical Physics of quantum oscillators}}} \qquad \text{(C16)}$$

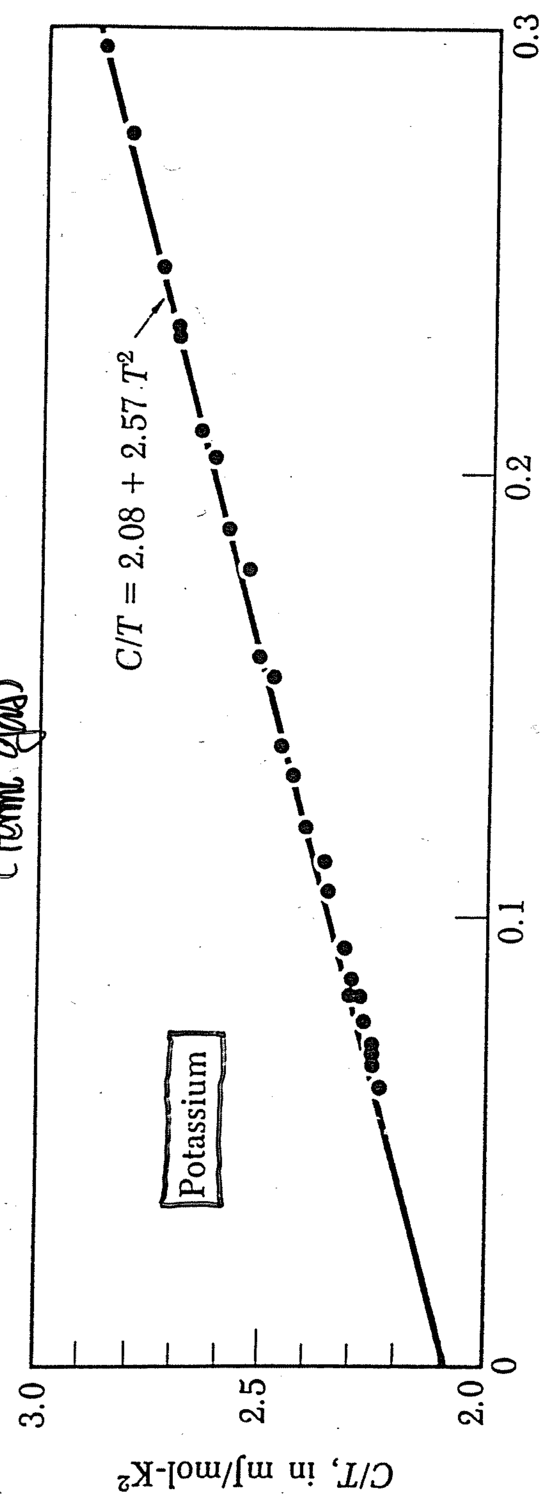
[see this term only at very low temperature when $\sim T^3$ term becomes tiny]

$\therefore$ Plot $\frac{C_V}{T}$ vs T^2 should give a straight line

Low-temp. data

$$C = \underbrace{\gamma T}_{\substack{\text{electrons contribution} \\ \text{(Fermi Gas)}}} + \underbrace{bT^3}_{\substack{\text{from lattice vibration ("phonons")} \\ \text{(Bosons)}}} \Rightarrow \frac{C}{T} = \gamma + bT^2$$

$\Downarrow$ Plot $\frac{C}{T}$ vs T^2



Experimental heat capacity values for potassium, plotted as C/T versus T^2.

In Potassium, the "$4s^1$" electrons contribute to conduction and form a sea of electrons.

note: at very low temperature

- Both electronic and lattice vibrational contributions are observed.
- Can extract γ experimentally
- Theoretically, $\gamma = \frac{\pi^2}{3} k^2 g(E_F)$. $\therefore$ Measure $\gamma \Rightarrow$ information on $g(E_F)$

$g(E_F) = G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E_F}$

Remarks

- Some numbers: Cu $\begin{cases} n = 8.5\times10^{22}/cm^3 \\ E_F \sim 7eV \;;\; T_F \sim 8.2\times10^4 K \\ \gamma(\text{free electron}) \sim 0.5\, mJ\cdot mol^{-1}\cdot K^{-2} \\ \gamma(\text{exp't}) \sim 0.7\, mJ\cdot mol^{-1}\cdot K^{-2} \end{cases}$

  [not bad for simply treating the sea of conduction electrons as an ideal Fermi gas]

- We will be very wrong to treat the Fermi Gas as a classical gas.
  - Classical Gas: $E = N\cdot 3\cdot(\frac{1}{2}kT)$ Equipartition "theorem"

    $\Rightarrow C_V^{classical} = \frac{3}{2}Nk$ (independent of T)
  - Fermi Gas: $C_V^{Fermi} = \frac{\pi^2}{3} g(E_F)\, kT$ (But $N = \frac{2}{3}g(E_F)\cdot E_F$)

    $$= \underbrace{\frac{\pi^2}{2}Nk}_{\approx C_V^{classical}} \underbrace{\left(\frac{kT}{E_F}\right)}_{(10^{-2})\text{ factor for electrons in metal}}$$

$\therefore C_V^{classical} \gg C_V^{Fermi\,Gas}$

$C_V^{classical}$ has no T-dependence

Behavior of $C_V^{classical}$ is inconsistent with exp'tal data.

[This is, again, an effect due to Pauli Exclusion Principle]

Summary

(a) $T=0$ [Completely degenerate Fermi Gas] (spin-half)

$$N = \frac{2}{3}g(E_F)E_F \;;\; E_F \equiv \mu(T=0) = \frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3} \propto n^{2/3}$$

$$= \frac{\hbar^2}{2m}k_F^2 \text{ with } k_F = (3\pi^2 n)^{1/3}$$

$$\underbrace{E}_{T=0\text{ total energy}} = \frac{3}{5}NE_F \;;\; pV = \frac{2}{3}E \;;\; \underbrace{p}_{T=0\text{ pressure}} = \frac{2}{5}\frac{N}{V}E_F \sim \left(\frac{N}{V}\right)^{5/3}$$

[Key physics: Pauli Exclusion Principle piles fermions up in s.p. states]

(b) $T\neq0$ and $kT\ll\mu$ [Degenerate Fermi Gas]

$$\mu(T) = E_F\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right]$$

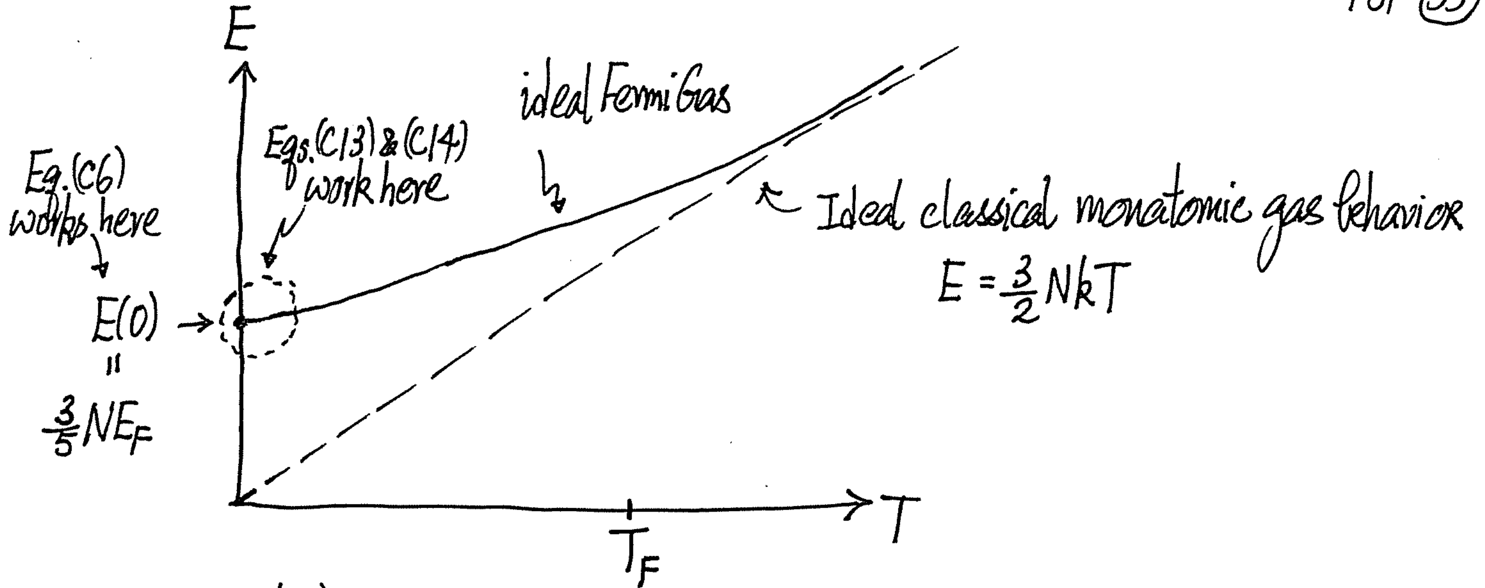
$$E(T) = E(0)\left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_F}\right)^2\right]$$

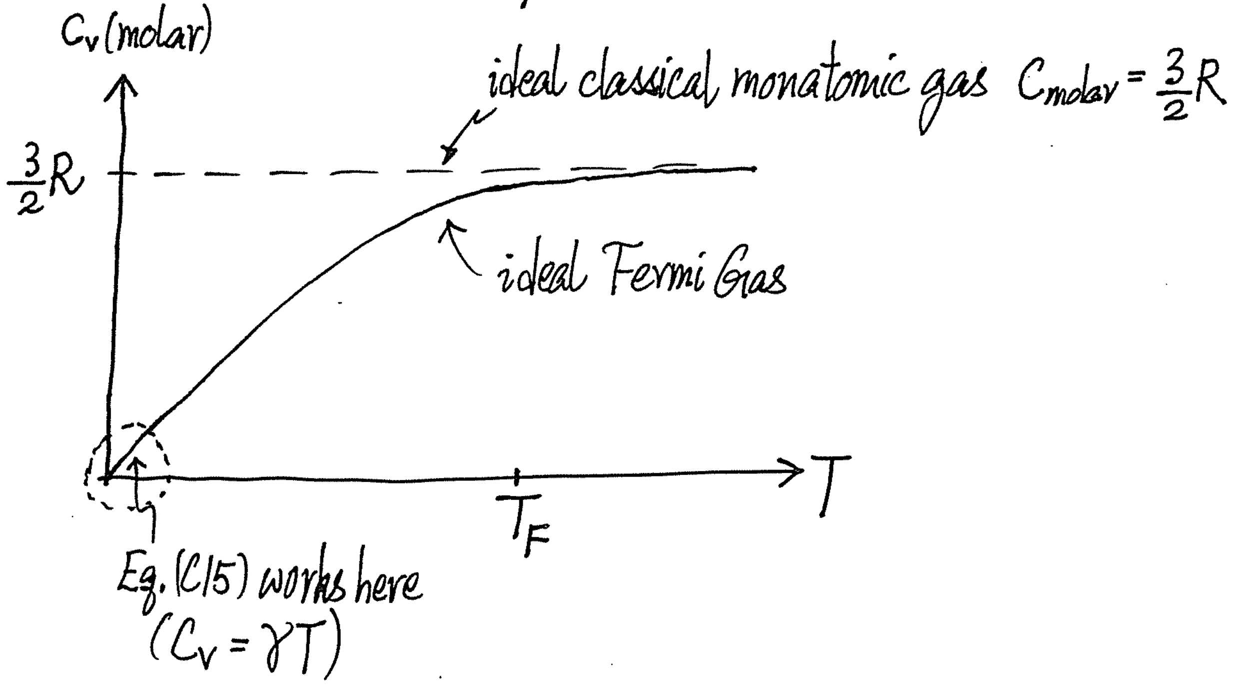
$$= E(0) + \frac{\pi^2}{6}g(E_F)(kT)^2$$

$$C_V(T) = \frac{\pi^2}{3}g(E_F)k^2T = \frac{\pi^2}{2}Nk\left(\frac{kT}{E_F}\right) = \gamma T$$

$$p = \frac{2}{3}\frac{E}{V}$$

[Key physics: Only changes near E_F matter]





- Analytic Results can be obtained at $T=0$ and $T \ll T_F$.
- For general temperatures, $\mu(T)$ and $E(T)$ can be obtained by the general equations Eqs.(3) and (5) in Sec. A, using numerical methods.