Ideal Fermi gas

General properties:

$$\boxed{\begin{aligned} -pV = \Omega &= -k_BT \sum_\alpha \ln\left(1+e^{-\beta(\varepsilon_\alpha-\mu)}\right) \\ N &= \sum_\alpha \langle n_\alpha \rangle = \sum_\alpha \frac{1}{e^{\beta(\varepsilon_\alpha-\mu)}+1} \\ U &= \sum_\alpha \frac{\varepsilon_\alpha}{e^{\beta(\varepsilon_\alpha-\mu)}+1} \end{aligned}}$$

μ is determined from $\rightarrow$ (the equation for N) and can range $-\infty<\mu<\infty$

Non-relativistic gas in 3d: $\alpha = \{\vec{k}, \sigma\}$

$$\varepsilon_\alpha = \frac{\hbar^2\vec{k}^2}{2m}$$

$$\boxed{\begin{aligned} N &= \frac{V(2s+1)}{\lambda^3} f^-_{3/2}(z) \\ U &= \frac{3}{2}pV \\ \frac{p}{k_BT} &= \frac{(2s+1)}{\lambda^3} f^-_{5/2}(z) \end{aligned}}$$

$$f^-_\nu(z) = \frac{1}{(\nu-1)!}\int_0^\infty dy \, \frac{y^{\nu-1}}{z^{-1}e^{y}+1}$$

$$\left.\rho(\varepsilon) = (2s+1)\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon^{1/2}\right\}$$ – density of states in 3d.

High-temperature behaviour – considered generally earlier

Low-temperature behaviour: $z = e^{\beta\mu}$ ($\mu \approx \varepsilon_F$) is large. can proceed by studying asymptotic behaviour of $f^-_\nu(z)$ at large z. However, it is much more informative – and physical – to proceed more directly. "Solid state physics" approach where the degenerate Fermi gas of electrons is the most important system.

$T = 0$ behaviour $\rightarrow$ ground state of the electron gas

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \quad , \quad \vec{k} = \left(\frac{2\pi}{L_x} n_x \, , \frac{2\pi}{L_y} n_y \, , \frac{2\pi}{L_z} n_z \right)$$

d^3k contains
$$\frac{d^3k}{\left(\frac{2\pi}{L_x}\right)\cdot\left(\frac{2\pi}{L_y}\right)\left(\frac{2\pi}{L_z}\right)} = L_x L_y L_z \frac{d^3k}{(2\pi)^3} =$$

$$= \text{Vol} \cdot \frac{d^3k}{(2\pi)^3} \text{ states.}$$

(without including spin degeneracy).

Fill states up from $k=0$ up to some k_F

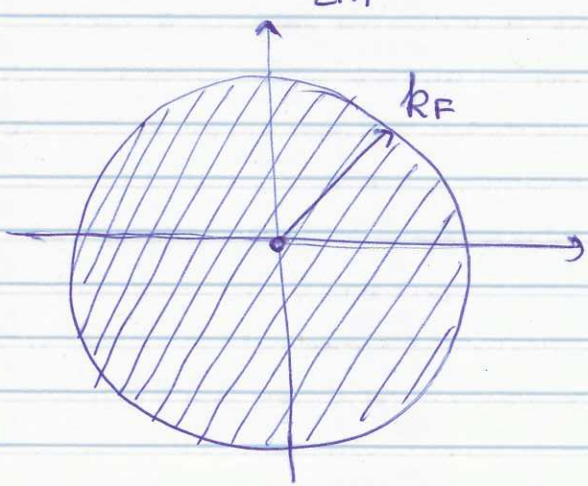
$$N = \underset{\substack{\| \\ 2S+1 = 2 \text{ for electrons}}}{g} \cdot V \cdot \frac{\frac{4}{3}\pi k_F^3}{(2\pi)^3} = V \frac{g k_F^3}{6\pi^2}$$

$$\boxed{k_F = \left(\frac{6\pi^2 n}{g} \right)^{1/3}} \qquad \mu(T=0) = \frac{\hbar^2 k_F^2}{2m} \equiv \varepsilon_F$$

Example: In metals, $O(1)$ electron per atom
$\rightarrow$ spacings between electrons $\sim$ Å , $n^{1/3} \sim$ Å^{-1} $\sim k_F$

$$\Rightarrow v_F = \frac{\hbar k_F}{m_e} \sim 10^8 \frac{cm}{sec} \sim 0.01 \text{ speed of light!}$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} \sim k_B \cdot 10^5 \, K \, !$$



Even at absolute zero temperature, electrons are actually moving around with huge velocities $\sim 1\%$ of c.

T=0 fermions cont'd

Ground state energy

$$E = gV \int^{k_F} \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m}$$

$$N = gV \int^{k_F} \frac{d^3k}{(2\pi)^3} \cdot 1$$

$$\Rightarrow \boxed{\frac{E}{N} = \frac{\hbar^2}{2m} \frac{\int_0^{k_F} k^2 dk \cdot k^2}{\int_0^{k_F} k^2 dk} = \frac{\hbar^2}{2m} \frac{k_F^5/5}{k_F^3/3} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}\varepsilon_F} \sim \left(\frac{N}{V}\right)^{2/3}$$

$$E(N,V) = \frac{c N^{5/3}}{V^{2/3}}$$

"Thermo-dynamics": $dU = \overset{0}{TdS} - pdV + \mu dN$

$$\boxed{\mu = \left(\frac{\partial U}{\partial N}\right) = \frac{5}{3}\frac{cN^{5/3-1}}{V^{2/3}} = \frac{5}{3}\frac{U}{N} = \varepsilon_F} \checkmark$$

$$\boxed{p = -\frac{\partial U}{\partial V} = \frac{2}{3}\frac{U}{V}} \checkmark$$ (general result holding for any T)

$$p = \frac{2}{3} \cdot \frac{\frac{3}{5} N\varepsilon_F}{V} = \frac{2}{5}\frac{N}{V}\varepsilon_F \sim \left(\frac{N}{V}\right)^{5/3}$$

– "fermion degeneracy pressure" due to Pauli exclusion

Example: * Bulk modulus $B = -V\frac{\partial P}{\partial V} = \frac{5}{3}P$.

compressibility $\varkappa = -\frac{1}{V}\frac{\partial V}{\partial p} = \frac{1}{B}$ – is measurable mechanical response property of materials.

Electron contribution constitutes significant fraction (~50%) of the bulk modulus of metals.

(of electrons (relativistic)

* Fermion degeneracy pressure is the main balancing source in white dwarf stars (← why those interested in astrophysics need to know statmech!)

Pauli spin susceptibility of electrons

$\alpha = \{\vec{k}, \sigma\}$ $\qquad\qquad$ $\varepsilon_{\vec{k},\sigma} = \dfrac{\hbar^2 k^2}{2m} \mp \mu_B B$

$$N_\uparrow = \sum_k \frac{1}{e^{\beta(\varepsilon_k^0 - \mu_B B - \mu)} + 1} = N_0(T, \mu + \mu_B B)$$

$$N_\downarrow = \sum_k \frac{1}{e^{\beta(\varepsilon_k^0 + \mu_B B - \mu)} + 1} = N_0(T, \mu - \mu_B B)$$

$$N_0(T,\mu) = \sum_k \frac{1}{e^{\beta(\varepsilon_k^{(0)} - \mu)} + 1} \; ; \quad N(T,\mu) = 2N_0(T,\mu)$$

$$M = \mu_B (N_\uparrow - N_\downarrow) = \mu_B \big(N_0(T, \mu + \mu_B B) - N_0(T, \mu - \mu_B B) \big)$$

$$\approx 2\mu_B^2 B \frac{\partial N_0}{\partial \mu} = \mu_B^2 B \frac{\partial N}{\partial \mu}$$

$$\boxed{\chi_{tot} = \lim_{B \to 0} \frac{M(B)}{B} = \mu_B^2 \frac{\partial N}{\partial \mu}}$$ – general result

Per volume $\qquad \chi = \dfrac{\mu_B^2}{V} \dfrac{\partial N}{\partial \mu}$

At $T = 0$ $\qquad N \sim k_F^3 \sim \varepsilon_F^{3/2}$, $\mu = \varepsilon_F$

$$\frac{\partial N}{\partial \mu} = \frac{3}{2} \frac{N}{\varepsilon_F}$$

$$\boxed{\chi = \frac{N}{V} \frac{3\mu_B^2}{2\varepsilon_F}}$$ = finite # at $T=0$

more general result valid for arbitrary dispersion (e.g., electrons in Bloch bands)

$\underline{T=0}$

$$\chi = n\,\frac{3}{2}\frac{\mu_B^2}{\varepsilon_F} = \underbrace{\rho(\varepsilon_F)}_{\text{(including spin)}}\cdot \mu_B^2$$

$$\left(n = \int^{\varepsilon_F} \rho(\varepsilon)\,d\varepsilon = \int_0^{\varepsilon_F} c\,\varepsilon^{1/2}\,d\varepsilon = c\,\frac{\varepsilon_F^{3/2}}{3/2} = \rho(\varepsilon_F)\,\frac{2}{3}\varepsilon_F \right).$$

At high temperature $\approx$ classical gas,

$$\mu = k_B T \ln\left(\frac{N}{V}\left(\frac{h^2}{2\pi m k_B T}\right)^{3/2}\right)$$

$$N = \frac{V}{\lambda^3} e^{\mu/k_B T}$$

$$\frac{\partial N}{\partial \mu} = \frac{N}{k_B T}$$

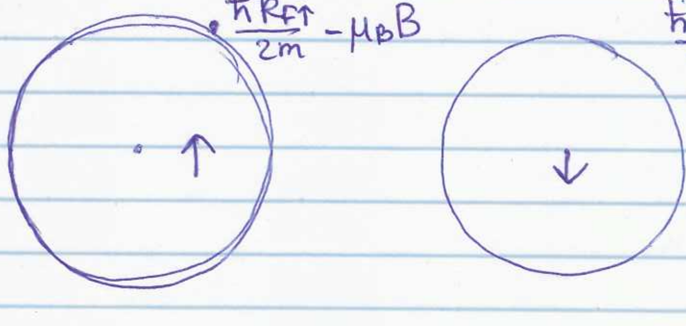
$$\chi = n\,\frac{\mu_B^2}{k_B T} \quad \text{— Curie susceptibility}$$

At high temperature = classical gas = spin part is indep. of the kinetic energy part (was in one HW) and spins behave as free $\to$ Curie susceptibility

However, at low temperatures — quantum degenerate regime — there is no such factorization!

$k_B T$ is replaced by the degeneracy scale $\sim \varepsilon_F$

$$\frac{\hbar^2 k_{F\uparrow}^2}{2m} - \mu_B B \qquad\qquad \frac{\hbar^2 k_{F\downarrow}^2}{2m} + \mu_B B$$



$$\frac{\hbar^2 k_{F\uparrow}^2}{2m} - \mu_B B = \frac{\hbar^2 k_{F\downarrow}^2}{2m} + \mu_B B$$

$$k_{F\uparrow}^3 + k_{F\downarrow}^3 = k_{F0}^3 \cdot 2$$

Sommerfeld theory for electrons in metals

Low-temperature properties of the Fermi gas

(Degenerate Fermi gas ; $k_B T \ll E_F$)

e.g. electrons in metals $E_F \sim 10^5\,K$

Various properties → need integrals like

$$I = \int_0^\infty d\varepsilon\, \phi(\varepsilon)\, n_F(\varepsilon) \quad , \quad n_F(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

e.g.

- $N = \int_0^\infty d\varepsilon\, \rho(\varepsilon)\, n_F(\varepsilon) \quad , \quad \phi(\varepsilon) = \rho(\varepsilon)$
- $E = \int_0^\infty d\varepsilon\, \rho(\varepsilon)\, \varepsilon\, n_F(\varepsilon) \quad , \quad \phi(\varepsilon) = \varepsilon\rho(\varepsilon)$

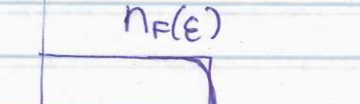
At low temperature, all action is near $\varepsilon \approx \mu \approx \varepsilon_F$.

~~For example,~~ To see this, write $\phi(\varepsilon) = \frac{d}{d\varepsilon}\Psi \; ; \quad \Psi(\varepsilon) = \int_0^\varepsilon \phi(\varepsilon')d\varepsilon'$

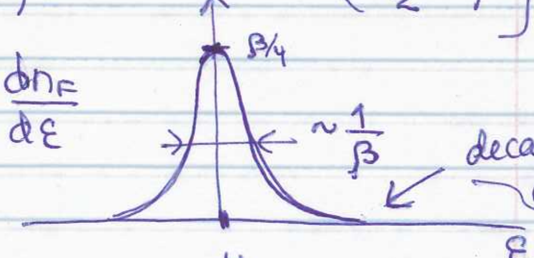
$$I = \int_0^\infty d\varepsilon \frac{d\Psi}{d\varepsilon} n_F(\varepsilon) = \Psi(\varepsilon) n_F(\varepsilon)\Big|_0^\infty - \int_0^\infty \Psi(\varepsilon)\frac{dn_F}{d\varepsilon}d\varepsilon$$

$$-\frac{dn_F}{d\varepsilon} = \frac{\beta\, e^{\beta(\varepsilon-\mu)}}{\left(e^{\beta(\varepsilon-\mu)}+1\right)^2} = \frac{\beta}{4\cosh^2\left(\frac{\beta(\varepsilon-\mu)}{2}\right)}$$

$\int_{-\infty}^{+\infty}\left(-\frac{dn_F}{d\varepsilon}\right) = 1$



$-\frac{dn_F}{d\varepsilon}$



decays as $e^{-\beta|\varepsilon-\mu|}$

For $T \to 0$, $\underbrace{-\frac{dn_F}{d\varepsilon}}_{} = \delta(\varepsilon-\mu)$

↑ derivative of a step function

$\frac{d}{dx}\theta(x) = \delta(x)$

$$\boxed{I = \Psi(\infty)\overset{0}{\cancel{n_F(\infty)}} - \overset{0}{\cancel{\Psi(0)}}n_F(0) + \int_0^\infty \Psi(\varepsilon)\cdot\left(-\frac{dn_F}{d\varepsilon}\right)d\varepsilon}$$ — can replace the lower limit by $-\infty$

Write $\Psi(\varepsilon) = \Psi(\mu) + \Psi'(\mu)(\varepsilon-\mu) + \Psi''(\mu)\frac{(\varepsilon-\mu)^2}{2} + \ldots$

$$I = \cancel{\Psi(\infty) n_F(\infty)}^{\,0} - \underbrace{\Psi(0)}_{=\phi} n_F(0) + \Psi(\mu)\int_0^\infty \frac{\beta}{4\cosh^2\frac{\beta(\varepsilon-\mu)}{2}}\,d\varepsilon$$

$$+ \Psi'(\mu)\int_0^\infty \frac{\beta}{4\cosh^2\frac{\beta(\varepsilon-\mu)}{2}}\cdot(\varepsilon-\mu)\,d\varepsilon + \frac{1}{2}\Psi''(\mu)\int_0^\infty \frac{\beta}{4\cosh^2\frac{\beta(\varepsilon-\mu)}{2}} \times (\varepsilon-\mu)^2\,d\varepsilon$$

~~next order~~ is $(k_B T)^4$!

With accuracy $\sim e^{-\beta\varepsilon_F}$, we can replace $\int_0^\infty \to \int_{-\infty}^{+\infty}$

$$\boxed{I \approx \Psi(\mu)\int_{-\infty}^{+\infty}\frac{dx}{4\cosh^2\frac{x}{2}} + \phi + \frac{1}{2}\Psi''(\mu)(k_BT)^2\int_{-\infty}^{+\infty}\frac{x^2}{4\cosh^2\frac{x}{2}}\,dx + O\left((k_BT)^4\right) + O\left(e^{-\varepsilon_F/k_BT}\right)}$$

Table integrals

$$\int_{-\infty}^{+\infty}\frac{dx}{4\cosh^2\frac{x}{2}} = 1$$

– OK since $-\frac{dn_F}{d\varepsilon} = \delta(\varepsilon-\mu)$

$$\int_{-\infty}^{+\infty}\frac{x^2}{4\cosh^2\frac{x}{2}}\,dx = \frac{\pi^2}{3}$$

$$\boxed{\begin{aligned} I &= \Psi(\mu) + \frac{\pi^2}{6}(k_BT)^2\Psi''(\mu) + O\left((k_BT)^4\right) \\ &= \int_0^\mu \phi(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_BT)^2\phi'(\mu) + O\left((k_BT)^4\right) \\ &= \int_0^{\varepsilon_F}\phi(\varepsilon)\,d\varepsilon + \int_{\varepsilon_F}^{\mu}\phi(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_BT)^2\phi'(\mu) + O\left((k_BT)^4\right) \end{aligned}}$$

We will see that $\mu \approx \varepsilon_F + O\left((k_BT)^2\right)$, so

$$\phi'(\mu) \approx \phi'(\varepsilon_F) + \phi''(\varepsilon_F)\cdot \underbrace{(\mu-\varepsilon_F)}_{\sim (k_BT)^2}$$

$$\int_{\varepsilon_F}^{\mu} \phi(\varepsilon)\,d\varepsilon \approx \int_{\varepsilon_F}^{\mu} \Big(\phi(\varepsilon_F) + \phi'(\varepsilon)(\varepsilon-\varepsilon_F)\Big)\,d\varepsilon =$$

$$= \phi(\varepsilon_F)\underbrace{(\mu-\varepsilon_F)}_{(k_BT)^2} + \phi'(\varepsilon_F)\underbrace{\frac{(\mu-\varepsilon_F)^2}{2}}_{(k_BT)^4} + \ldots$$

$$\boxed{I \approx \int_0^{\varepsilon_F} \phi(\varepsilon)\,d\varepsilon + \phi(\varepsilon_F)\left(\mu(T)-\varepsilon_F\right) + \frac{\pi^2}{6}(k_BT)^2\phi'(\varepsilon_F) + O\left((k_BT)^4\right)}$$

* Number of particles N: $\quad \phi(\varepsilon) = \rho(\varepsilon)$

$$N = \underbrace{\int_0^{\varepsilon_F} \rho(\varepsilon)\,d\varepsilon}_{N\,@\,T=0} + \rho(\varepsilon_F)(\mu-\varepsilon_F) + \frac{\pi^2}{6}(k_BT)^2\rho'(\varepsilon_F) + O\left((k_BT)^4\right)$$

$$\Rightarrow \boxed{\mu-\varepsilon_F \approx -\frac{\pi^2}{6}(k_BT)^2\frac{\rho'(\varepsilon_F)}{\rho(\varepsilon_F)} + O\left((k_BT)^4\right)}$$

* Internal energy U: convenient to consider

$$\phi(\varepsilon) = \rho(\varepsilon)\cdot(\varepsilon-\varepsilon_F)$$

$$\int_0^\infty \phi(\varepsilon)n_F(\varepsilon)\,d\varepsilon = \int_0^\infty \rho(\varepsilon)\,\varepsilon\, n_F(\varepsilon)\,d\varepsilon - \varepsilon_F\underbrace{\int_0^\infty \rho(\varepsilon)n_F(\varepsilon)\,d\varepsilon}_{N}$$

$$\boxed{U(T) = \int_0^\infty \rho(\varepsilon)\,\varepsilon\, n_F(\varepsilon)\, d\varepsilon} = N\cdot\varepsilon_F + \int_0^\infty \underbrace{\rho(\varepsilon)(\varepsilon-\varepsilon_F)}_{=\phi(\varepsilon)} n_F(\varepsilon)\, d\varepsilon$$

$\phi(\varepsilon_F)=0$

$\phi'(\varepsilon_F)=\rho(\varepsilon_F)$

$$\approx N\cdot\varepsilon_F + \int_0^{\varepsilon_F} \rho(\varepsilon)(\varepsilon-\varepsilon_F)\,d\varepsilon + \frac{\pi^2}{6}\rho(\varepsilon_F)(k_BT)^2$$

$$= \boxed{U(T=0) + \frac{\pi^2}{6}\rho(\varepsilon_F)(k_BT)^2} + O\left((k_BT)^4\right)$$

* Specific heat

$$\boxed{C(T) = \frac{\pi^2}{3}\rho(\varepsilon_F)(k_BT)\cdot k_B}$$

Remarks ⊛ The results are for general system of noninteracting Fermions — can be any dimension ($d=1,2,3,\ldots$) and any external potential (particles in a box; particles in a crystal - periodic potential).

The only input information is density of states at the Fermi energy $\rho(\varepsilon_F)$ — as long as it is non-vanishing. (If $\rho(\varepsilon_F)=0$ — e.g. for "Dirac Fermions" - graphene in 2d — would need to do calculation more carefully)

⊛ Specific heat per particle

$$\frac{C(T)}{N} = k_B \frac{\frac{\pi^2}{3}\rho(\varepsilon_F)(k_BT)}{\int_0^{\varepsilon_F}\rho(\varepsilon)\,d\varepsilon}$$

e.g. in 3d $\quad \rho(\varepsilon) = \alpha\, \varepsilon^{1/2}$

generally

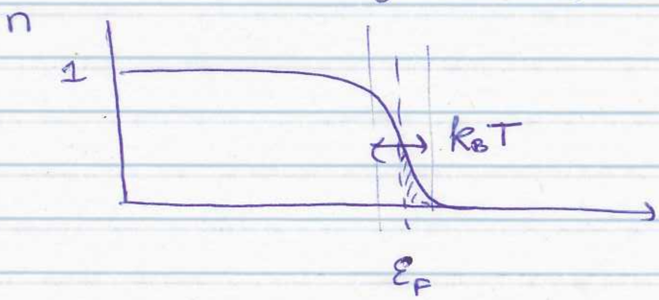
$$\frac{\rho(\varepsilon_F)}{\int_0^{\varepsilon_F} \rho(\varepsilon)\,d\varepsilon} = \frac{\alpha\, \varepsilon_F^{1/2}}{\alpha \frac{\varepsilon_F^{3/2}}{3/2}} = \frac{3}{2\varepsilon_F} \sim \frac{1}{\varepsilon_F}$$

$$\frac{C(T)}{N} = k_B \frac{\pi^2}{2} \frac{k_B T}{\varepsilon_F} \sim k_B \frac{k_B T}{\varepsilon_F}$$

~ classical C per particle

suppression due to quantum degeneracy

⊛ Qualitative argument for $U \sim \rho(\varepsilon_F)(k_B T)^2$:



$$U(T) - U(T=0) \sim$$

$$\sim \underbrace{\rho(\varepsilon_F)\cdot k_B T}_{\text{number of populated states above } \varepsilon_F} \; \underbrace{k_B T}_{\text{typical excitation energy.}}$$

⊛ For typical metals, $\varepsilon_F \sim 10^5 K$, so at room T

$\frac{k_B T}{\varepsilon_F} \sim 10^{-2}$, $\frac{C}{N} \sim 10^{-2} k_B$ – much smaller than the classical value and negligible compared to contribution from lattice vibrations

⊛ Specific heat of solids:

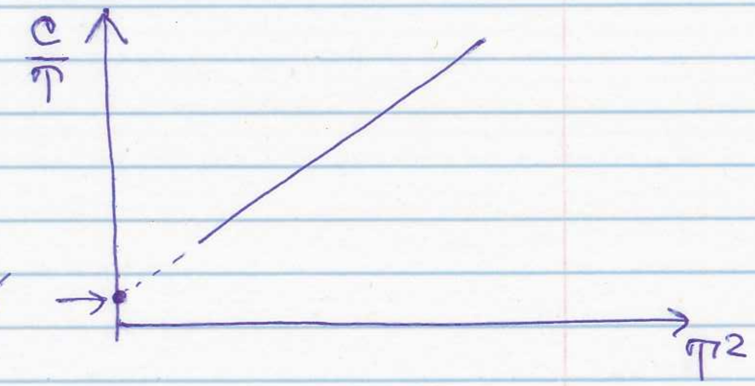
$$C = C_{vib.} + C_{el.}$$

- At room T, C is dominated by lattice vibrations (~$3k_B$ per ion)
- At low T

$$C_{vib} = AT^3$$

$$C_{el} = \gamma T$$

$$C = \gamma T + AT^3$$



Holds very generally for metals — success of Somerfeld theory!

Band structure $\to \rho(\varepsilon_F)$; Interactions $\to$ quasiparticles

From γ, we can extract density of states at the Fermi level:

$$\gamma = \frac{\pi^2}{3}\rho(\varepsilon_F)k_B.$$

<u>Other results for free electron gas in 3d:</u>

- $$U^{(T)} = \underbrace{U(T=0)}_{\frac{3}{5}N\varepsilon_F} + \frac{\pi^2}{6}\underbrace{\rho(\varepsilon_F)}_{\propto \varepsilon_F^{1/2} = \frac{N}{\varepsilon_F}\cdot\frac{3}{2}}(k_B T)^2 = \frac{3}{5}N\varepsilon_F\left(1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right)$$

- $$pV = \frac{2}{3}U = \frac{2}{5}N\varepsilon_F\left(1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right) = -\Omega$$

$$\Omega = U - TS - \mu N$$

- Helmholtz free energy

$$F = \Omega + \mu N = \mu N - pV = \left(\varepsilon_F \;\; \frac{\pi^2}{6}(k_BT)^2\frac{1}{2}\frac{1}{\varepsilon_F}\right)N -$$

$$- \frac{2}{5} N \varepsilon_F \left(1 + \frac{5\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right) =$$

$$= \frac{3}{5} N \varepsilon_F - \frac{3\pi^2}{12} N \varepsilon_F \left(\frac{k_B T}{\varepsilon_F}\right)^2 ;$$

- Entropy $$\boxed{S = -\left(\frac{\partial F}{\partial T}\right)_{N,V} = \frac{\pi^2}{2} N k_B \frac{k_B T}{\varepsilon_F}}$$

Alternative calculation of the entropy:

$$S(T) - \underbrace{S(0)}_{=0} = \int_0^T \frac{C_V}{T} dT = \gamma T = C_V =$$

$$= N k_B \frac{\pi^2}{2} \frac{k_B T}{\varepsilon_F}$$