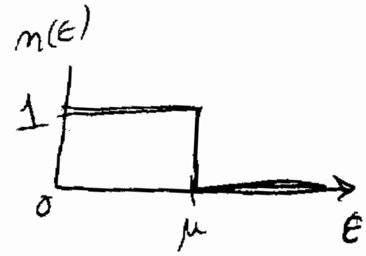
Sommerfeld model of electrons in a conductor

Fermi gas – high density / low temperature limit
"degenerate" fermi gas

Consider first $T \to 0$

$$\langle n(\epsilon)\rangle = \frac{1}{e^{\beta(\epsilon-\mu)}+1}$$



as $T \to 0$ $\quad e^{\beta(\epsilon-\mu)} \to \begin{cases} \infty & \epsilon > \mu \\ 0 & \epsilon < \mu \end{cases}$

$$\Rightarrow \langle n(\epsilon)\rangle \to \begin{cases} 0 & \epsilon > \mu \\ 1 & \epsilon < \mu \end{cases}$$

$\Rightarrow$ all states with $\epsilon < \mu$ are filled, all states with $\epsilon > \mu$ are empty. This is the $T=0$ ground state of the Fermi gas. We therefore see that $\mu(T=0)$ is the energy of the highest energy single particle state that is occupied in the ground state. One calls this energy the <u>Fermi-energy</u>

$$\epsilon_F \equiv \mu(T=0)$$

at $T=0$

$$N = g_s \sum_{\vec{k} \text{ s.t. } \frac{\hbar^2 k^2}{2m} \le \epsilon_F} 1 \qquad \text{count occupied states}$$

$$= g_s \frac{V}{(2\pi)^3} 4\pi \int_0^{k_F} dk\, k^2 = \frac{g_s V}{6\pi^2} k_F^3 \qquad \text{where } \frac{\hbar^2 k_F^2}{2m} = \epsilon_F$$

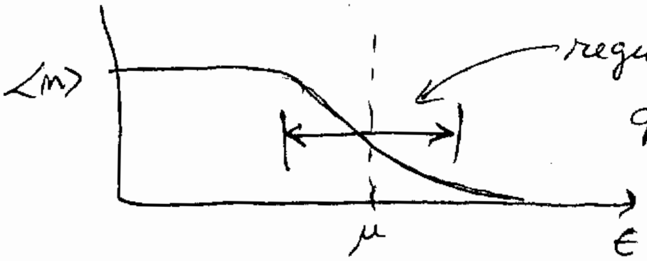
$$n \equiv \frac{N}{V} = \frac{g_s}{6\pi^2} k_F^3 = \frac{g_s}{6\pi^2}\left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2}$$

or

$$\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{g_s}\right)^{2/3}, \quad k_F = \left(\frac{6\pi^2 n}{g_s}\right)^{1/3}$$

relation between $\mu(T=0)$ and density $n = N/V$

Now at finite T



region of energy where $\langle n \rangle$ differs from ground state ($T=0$) is a region of order $k_B T$ about μ.

So the $T \simeq 0$ approx is good when $k_B T \ll \mu$

~~Since $\mu(T) \approx \mu(0) = \epsilon_F$ we have~~

Using $\mu \approx \mu(0) = \epsilon_F$ we have

$$k_B T \ll \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{g_s}\right)^{2/3} \Rightarrow \frac{2\pi m k_B T}{h^2} \ll \frac{1}{4\pi}\left(\frac{6\pi^2 n}{g_s}\right)^{2/3}$$

$$\Rightarrow \lambda^2 \gg 4\pi\left(\frac{g_s}{6\pi^2 n}\right)^{2/3}$$

$$\Rightarrow n\lambda^3 \gg \frac{(4\pi)^{3/2}}{6\pi^2} g_s = \frac{4}{3\sqrt{\pi}} g_s$$

so this is equivalent to a low T or a high density limit $n\lambda^3 \gg 1$ – called the "degenerate" limit.

(just as the classical limit $z \simeq n\lambda^3 \ll 1$ was a high T low density limit)

Fermi temperature $T_F = \epsilon_F / k_B$. Degenerate limit is $T \ll T_F$

For electrons in a metal, $T_F \simeq 10000\,K$.
So electrons in a metal are always in the degenerate limit.

Energy in the degenerate limit $T=0$

$$\frac{E}{V} = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\, \epsilon \qquad g(\epsilon) = C\sqrt{\epsilon}$$

with $C = \left(\frac{2\pi m}{h^2}\right)^{3/2} \frac{2g_s}{\sqrt{\pi}}$.

density of states

$$n = \frac{N}{V} = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)$$

$$\Rightarrow \frac{E}{V} = C\int_0^{\epsilon_F} d\epsilon\, \epsilon^{3/2} = \frac{2}{5} C \epsilon_F^{5/2}$$

$$n = \frac{N}{V} = C\int_0^{\epsilon_F} d\epsilon\, \epsilon^{1/2} = \frac{2}{3} C \epsilon_F^{3/2}$$

$$\Rightarrow \frac{E}{V} = \frac{3}{5}\frac{N}{V}\epsilon_F$$

$$\frac{E}{V} = \frac{3}{5} n \epsilon_F \quad \text{or} \quad \boxed{\frac{E}{N} = \frac{3}{5}\epsilon_F}$$

energy per volume   energy per particle

Above gives $T=0$ results. To get behavior at low $T>0$, or to get quantities such as $C_V = \left(\frac{\partial E}{\partial T}\right)_V$, we need to get the next order terms in a low temperature expansion.

In general we need to do integrals of the form

$$\int d\epsilon \frac{\tilde{\phi}(\epsilon)}{z^{-1}e^{\beta\epsilon}+1} = \int d\epsilon\, \tilde{\phi}(\epsilon)\, n(\epsilon) \quad , \quad \tilde{\phi}(\epsilon) \text{ some function}$$

ex: to compute n, $\tilde{\phi}(\epsilon) = g(\epsilon)$; to compute $\frac{E}{V}$, $\tilde{\phi}(\epsilon) = g(\epsilon)\epsilon$

transform variables to $x = \beta\epsilon$.

Then we want to do integrals of the form

$$\Phi \equiv \int_0^\infty dx \, \frac{\phi(x)}{z^{-1}e^x+1}$$

$\phi(x)$ is any function of x.

For example, to get the "standard" function $f_n(z)$, we use $\phi(x) = \frac{1}{\Gamma(n)} x^{n-1}$

Define $\xi = \beta\mu = \ln z$

$$\Phi = \int_0^\infty dx \, \frac{\phi(x)}{e^{x-\xi}+1}$$

Define $\psi(x) \equiv \int_0^x \phi(x')dx'$, $f(x) \equiv \frac{1}{\left[e^{x-\xi}+1\right]}$ fermi function

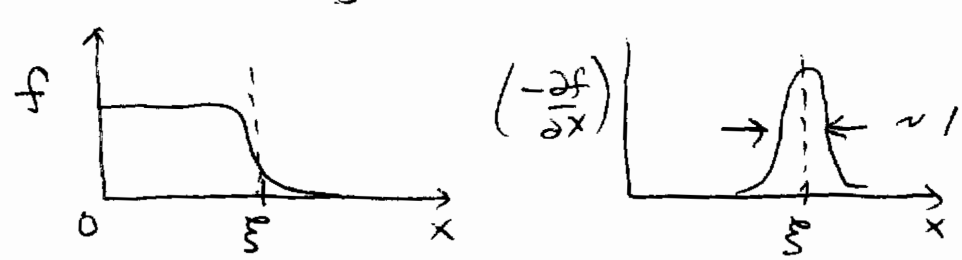
$$\Phi = \int_0^\infty dx \left(\frac{\partial\psi}{\partial x}\right) f(x) \quad \text{integrate by parts}$$

$$= \psi(x) f(x)\Big|_0^\infty + \int_0^\infty dx \, \psi(x)\left(-\frac{\partial f}{\partial x}\right)$$

$$= \int_0^\infty dx \, \psi(x)\left(-\frac{\partial f}{\partial x}\right)$$

since $\psi(0) = 0$ and $f(\infty) = 0$, 1st term vanishes

Now we use the fact that at low T, $\left(-\frac{\partial f}{\partial x}\right)$ is strongly peaked about $x = \xi$



$\xi \gg 1$

$\xi \sim \frac{\epsilon_F}{k_B T}$ large expand $\psi(x)$ about $x=\xi$

$$\psi(x) = \sum_{n=0}^{\infty} \frac{d^n\psi}{dx^n}\Big|_{x=\xi} \frac{(x-\xi)^n}{n!}$$

$$\Rightarrow \quad \Phi = \sum_{n=0}^{\infty} \frac{d^n\psi}{dx^n}\Big|_{x=\xi} \int_0^{\infty} dx \, \frac{(x-\xi)^n}{n!}\left(-\frac{\partial f}{\partial x}\right)$$

since $\left(-\frac{\partial f}{\partial x}\right)$ is zero except for a region of order 1 about $x=\xi \gg 1$, we can replace the lower limit of the integral by $-\infty$ without any noticeable change

Then we can make a change of variables $y = x-\xi$ and the integrals become

$$\int_{-\infty}^{\infty} dy \, \frac{y^n}{n!}\left(-\frac{\partial f}{\partial y}\right) \qquad \text{where } f(y) = \frac{1}{e^y+1}$$

Now $$-\frac{\partial f}{\partial y} = \frac{e^y}{(e^y+1)^2} = \frac{e^y}{e^{2y}+2e^y+1} = \frac{1}{e^y+2+e^{-y}}$$

is <u>symmetric</u> about $y=0$.

$\Rightarrow$ all the integrals for n odd vanish!

To sum over only n even terms, let $n \to 2n$

$$\Phi = \sum_{n=0}^{\infty} \frac{d^{2n}\psi}{dx^{2n}}\bigg|_{x=\xi} \int_{-\infty}^{\infty} dy \, \frac{y^{2n}}{(2n)!} \left(-\frac{\partial f}{\partial y}\right)$$

let $a_n \equiv \int_{-\infty}^{\infty} dy \, \frac{y^{2n}}{(2n)!} \left(-\frac{\partial f}{\partial y}\right)$, $a_0 = \int_{-\infty}^{\infty} dy \left(-\frac{\partial f}{\partial y}\right) = 1$

The a_n are <u>just numbers</u> that be computed.
They contain <u>no system parameters</u> whatsoever

For $n \geq 1$ one can show

$$a_n = 2\left(1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \frac{1}{5^{2n}} - \cdots\right)$$

$$= \left(2 - \frac{1}{2^{2(n-1)}}\right) \zeta(2n)$$

where $\zeta(n) = 1 + \frac{1}{2^n} + \frac{1}{3^n} + \frac{1}{4^n} + \cdots$ is the Riemann zeta function

In particular $a_1 = \frac{\pi^2}{6}$, $a_2 = \frac{7\pi^4}{360}$

$$\Phi = \sum_{n=0}^{\infty} a_n \frac{d^{2n}\psi}{dx^{2n}}\bigg|_{x=\xi} = \psi(\xi) + \sum_{n=1}^{\infty} a_n \frac{d^{2n}\psi}{dx^{2n}}\bigg|_{x=\xi}$$

use $\frac{d\psi}{dx} = \phi$ to finally get $\qquad \psi(x) = \int_0^x dx' \phi(x')$

$$\Phi = \int_0^{\xi} dx \, \phi(x) + \sum_{n=1}^{\infty} a_n \frac{d^{2n-1}\phi}{dx^{2n-1}}\bigg|_{x=\xi}$$

$$= \int_0^{\xi} dx \, \phi(x) + \frac{\pi^2}{6}\frac{d\phi}{dx}\bigg|_{x=\xi} + \frac{7\pi^4}{360}\frac{d^3\phi}{dx^3}\bigg|_{x=\xi} + \cdots$$

This gives a power series in temperature.

To see this, transform back to the energy variable
$x = \beta\epsilon \;, \quad \epsilon = k_B T x$

$$\Phi \equiv \int_0^\infty d\epsilon \, \frac{\phi(\epsilon)}{z^{-1} e^{\beta\epsilon}+1} = k_B T \left\{ \int_0^\infty dx \, \frac{\phi(k_B T x)}{z^{-1} e^{x}+1} \right\}$$

using $$k_B T \int_0^{\xi = \mu/k_B T} dx \, \phi(k_B T x) = \int_0^\mu d\epsilon \, \phi(\epsilon)$$

and $$\frac{d\phi}{dx} = \frac{d\phi}{d\epsilon}\frac{d\epsilon}{dx} = \frac{d\phi}{d\epsilon} k_B T$$

we get

$$\Phi = \int_0^\infty d\epsilon \, \phi(\epsilon) n(\epsilon)$$

$$\boxed{\Phi = \int_0^\mu d\epsilon \, \phi(\epsilon) + \frac{\pi^2}{6}(k_B T)^2 \left.\frac{d\phi}{d\epsilon}\right|_{\epsilon=\mu} + \frac{7\pi^4}{360}(k_B T)^4 \left.\frac{d^3\phi}{d\epsilon^3}\right|_{\epsilon=\mu} + \cdots}$$

Example

① density $$n = \frac{N}{V} = \int_0^\infty d\epsilon \, g(\epsilon) n(\epsilon) \quad \Rightarrow \phi(\epsilon) \equiv g(\epsilon)$$

$$n = \int_0^\mu d\epsilon \, g(\epsilon) + \frac{\pi^2}{6}(k_B T)^2 \left.\frac{dg}{d\epsilon}\right|_{\epsilon=\mu} + \cdots$$

Now as $T \to 0$, $\mu \to \epsilon_F$ the fermi energy

$$n = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon) + \int_{\epsilon_F}^{\mu} d\epsilon\, g(\epsilon) + \frac{\pi^2}{6}(k_B T)^2 \left.\frac{dg}{d\epsilon}\right|_{\epsilon=\mu}$$

But ϵ_F was determined by $n = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon)$

$$\Rightarrow \int_{\epsilon_F}^{\mu} d\epsilon\, g(\epsilon) = -\frac{\pi^2}{6}(k_B T)^2 \left.\frac{dg}{d\epsilon}\right|_{\epsilon=\mu}$$

since left hand side is $O(kT)^2$ is small, we can approx ~~the right hand side as~~ it as

$$\int_{\epsilon_F}^{\mu} d\epsilon\, g(\epsilon) \approx (\mu - \epsilon_F)\, g(\epsilon_F)$$

$$\Rightarrow (\mu - \epsilon_F) \simeq -\frac{\pi^2}{6} \frac{(k_B T)^2}{g(\epsilon_F)} \left.\frac{dg}{d\epsilon}\right|_{\epsilon=\mu}$$

so $\mu - \epsilon_F \sim O(k_B T)^2$ is small, so to lowest order can evaluate $\frac{dg}{d\epsilon}$ on right hand side at $\epsilon = \epsilon_F$ instead of $\epsilon = \mu$

$$\boxed{\mu(T) \simeq \epsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{g'(\epsilon_F)}{g(\epsilon_F)}} \qquad g' = \frac{dg}{d\epsilon}$$

Shows that chemical potential μ decreases from ϵ_F by $O(kT)^2$ at low T

For free electrons where $g(\epsilon) = C\sqrt{\epsilon}$

$$g'(\epsilon) = \tfrac{1}{2}C\frac{1}{\sqrt{\epsilon}}$$

$$\mu(T) \simeq \epsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{1}{2\epsilon_F} = \epsilon_F - \frac{\pi^2}{12}\frac{(k_B T)^2}{\epsilon_F}$$

$$\boxed{\mu(T) \simeq \epsilon_F\left(1 - \frac{1}{3}\left(\frac{\pi k_B T}{2\epsilon_F}\right)^2\right) = \epsilon_F\left(1 - \frac{1}{3}\left(\frac{\pi}{2}\frac{T}{T_F}\right)^2\right)}$$

correction is small for metals at room temp as $T_F \sim 10{,}000\,^\circ K$

② energy $\frac{E}{V} = \int_0^\infty d\epsilon\, g(\epsilon)\,\epsilon\, n(\epsilon) \Rightarrow \phi(\epsilon) = g(\epsilon)\,\epsilon$

$$u = \frac{E}{V} = \int_0^\mu d\epsilon\, g(\epsilon)\,\epsilon + \frac{\pi^2}{6}(k_B T)^2\left[g(\mu) + \mu g'(\mu)\right]$$

$$= \underbrace{\int_0^{\epsilon_F} d\epsilon\, g(\epsilon)\,\epsilon}_{\substack{= u(0) \\ \text{ground state} \\ \text{energy density}}} + \underbrace{\int_{\epsilon_F}^{\mu} d\epsilon\, g(\epsilon)\,\epsilon}_{\substack{\simeq (\mu - \epsilon_F) g(\epsilon_F)\epsilon_F \\ \text{as before}}} + \frac{\pi^2 (k_B T)^2}{6}\left[g(\mu) + \mu g'(\mu)\right]$$

replace $\mu \approx \epsilon_F$ as before

$$u(T) = u(0) + (\mu - \epsilon_F)\, g(\epsilon_F)\,\epsilon_F + \frac{\pi^2 (k_B T)^2}{6}\left[g(\epsilon_F) + \epsilon_F g'(\epsilon_F)\right]$$

$$= u(0) + \left[-\frac{\pi^2}{6}(k_B T)^2 \frac{g'(\epsilon_F)}{g(\epsilon_F)}\right] g(\epsilon_F)\,\epsilon_F + \frac{\pi^2 (k_B T)^2}{6}\left[g(\epsilon_F) + \epsilon_F g'(\epsilon_F)\right]$$

$$\boxed{u(T) = u(0) + \frac{\pi^2 (k_B T)^2}{6} g(\epsilon_F)}$$

Specific heat per volume

$$c_V \equiv \frac{C_V}{V} = \frac{1}{V}\left(\frac{dE}{dT}\right)_V = \left(\frac{du}{dT}\right)_V$$

$$\boxed{c_V = \frac{\pi^2}{3} k_B^2 T\, g(\epsilon_F)}$$

for free electrons we can write $g(\epsilon) = C\sqrt{\epsilon}$

$$n = \int_0^{\epsilon_F} d\epsilon\, g(\epsilon) = \frac{2}{3} C \epsilon^{3/2} \Rightarrow C = \frac{3}{2}\frac{n}{\epsilon^{3/2}}$$

$$\Rightarrow g(\epsilon_F) = \frac{3}{2}\frac{n}{\epsilon_F^{3/2}} \cdot \epsilon_F^{1/2} = \frac{3}{2}\frac{n}{\epsilon_F}$$ density of states at fermi energy

$$\boxed{c_V = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right) n k_B}$$

or total specific heat $C_V = V c_V$ $\qquad nV = N$

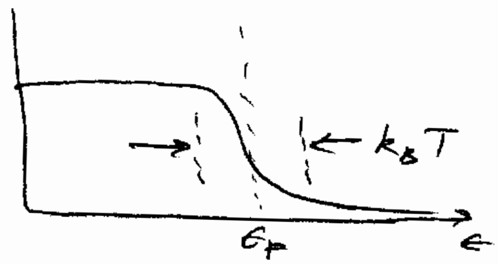
$$C_V = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right) N k_B$$

⇒ specific heat due to fermi gas of electrons in a conductor is $C_V \sim T$ at low temperatures

We already saw that specific heat due to ionic vibrations (phonons) in a solid went like $C_V \sim T^3$ at low temperatures (Debye model)

⇒ electronic contribution to C_V dominates at sufficiently low T.

Simple estimate of C_V



when increase temperature to $k_B T$, the electrons near the fermi energy ϵ_F will increase their energy by an amount $\sim k_B T$. The number of such electrons ~~is roughly~~ per unit volume is roughly

$$\underbrace{g(\epsilon_F)}_{\text{density of states at } \epsilon_F}\underbrace{(k_B T)}_{\text{energy interval about } \epsilon_F \text{ of states which get excited}}$$

$\Rightarrow$ increase in energy per unit volume is

$$\Delta u \sim \underbrace{(g(\epsilon_F) k_B T)}_{\#\text{ electrons excited}}\underbrace{(k_B T)}_{\text{excitation energy per excited electron}} \sim g(\epsilon_F)(k_B T)^2$$

for free electrons

$$\Rightarrow C_v = \frac{d\Delta u}{dT} \sim g(\epsilon_F) k_B^2 T = \frac{3}{2}\frac{n}{\epsilon_F} k_B^2 T = \frac{3}{2} n k_B \left(\frac{T}{T_F}\right)$$

The previous calculation gives the precise numerical coefficient electronic specific heat per volume

$$C_V^{elec} = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right)\frac{N}{V}k_B \left(1 + o\left(\frac{k_B T}{\epsilon_F}\right)^2\right)$$

compare to classical result $C_V^{classical} = \frac{N}{V}k_B$

The correct result for degenerate fermi gas is a factor $\frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right) = \frac{\pi^2}{2}\left(\frac{T}{T_F}\right)$ smaller than classical result by factor $\sim \frac{10^2}{10^4} = 10^{-2}$ at room temperature

also, classical C_V is indep of T, whereas fermi gas result is $\propto T$.

At low T, the ionic contribution to C_V is

$$C_V^{ion} = \frac{12\pi^4}{5}\left(\frac{T}{\Theta_D}\right)^3\frac{N}{V}k_B$$

$$\frac{C^{elec}}{C^{ion}} = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right)\frac{5}{12\pi^4}\left(\frac{\Theta_D}{T}\right)^3 \simeq \frac{5}{24\pi^2}\left(\frac{\Theta_D}{T_F}\right)\left(\frac{\Theta_D}{T}\right)^2$$

$$\simeq 1 \quad \text{when} \quad T^* = \sqrt{\frac{5}{24\pi^2}\left(\frac{\Theta_D}{T_F}\right)}\,\Theta_D \approx 0.15\left(\frac{\Theta_D}{T_F}\right)^{1/2}\Theta_D$$

for metals, $T_F \sim 10^4\,{}^\circ K$, $\Theta_D \sim 10^2\,{}^\circ K$

$$T^* = 0.15\sqrt{10^{-2}}\,\Theta_D \simeq 0.015\,\Theta_D$$

So ionic contrib to C_V dominates over electronic contrib until $T \lesssim 0.01\,\Theta_D$ ie at $O(1)\,{}^\circ K$. The electronic contrib dominates at lower temperatures.

Pauli paramagnetism of electron gas

electron has intrinsic spin $\underbrace{\vec{\sigma}}_{\vec{S}=\frac{1}{2}\hbar\vec{\sigma}}$ with intrinsic magnetic moment $\vec{\mu} = -\mu_B\vec{\sigma}$ $\quad \mu_B = \dfrac{|e|\hbar}{2mc}$ is Bohr magneton

In an external magnetic field $\vec{B}$, there is an interaction energy $-\vec{\mu}\cdot\vec{B} = \mu_B\sigma B$ where $\sigma = \pm 1$ for spins parallel and antiparallel to $\vec{B}$. The energy spectra for up and down electron spins becomes

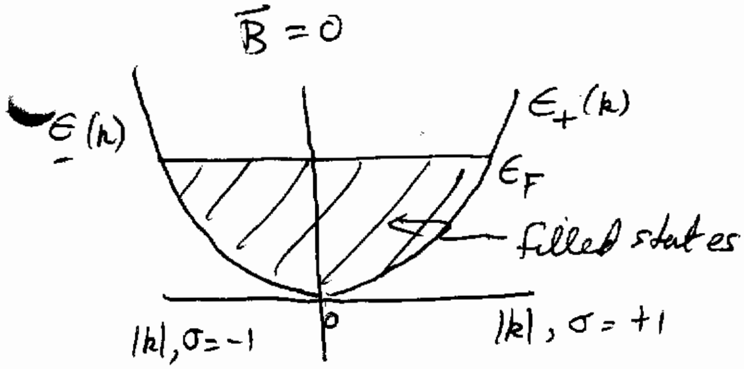
$$\epsilon_\pm(\vec{k}) = \epsilon(\vec{k}) \pm \mu_B B$$

where $\epsilon(\vec{k})$ is spectrum at $\vec{B}=0$

Since $\uparrow$ and $\downarrow$ electrons now have different energy spectra, we should treat them as two different populations of particles $\Rightarrow$ ~~they~~ they will be in equilibrium when their chemical potentials are equal, ie $\mu_+ = \mu_-$

this will induce a net magnetization in the system.

To see this, consider free electrons at $T=0$

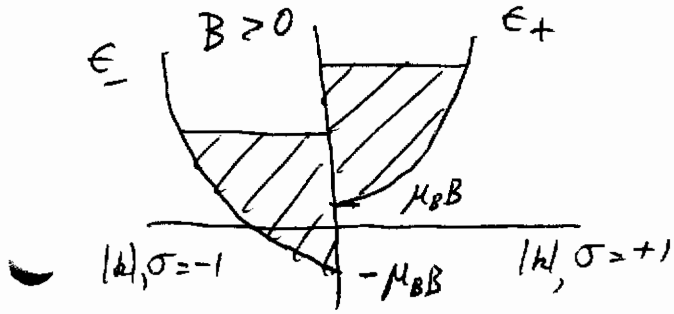


when $\vec{B} = 0$, $\epsilon_+(\vec{k}) = \epsilon_-(\vec{k})$

ground state occupations look as shown on the left. Equal numbers of ↑ and ↓ electrons

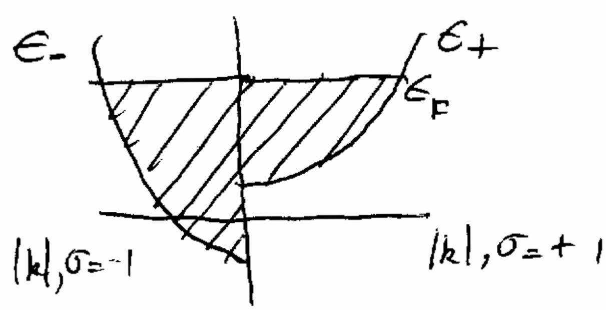
$n_+ = n_-$

when $\vec{B}$ is turned on, if there were no redistribution of electron spins, the situation would look like



Clearly the system can lower its energy by transferring ↑ electrons to ↓ electrons.

At equilibrium the system will look like



again the two populations have the same max energy ϵ_F. But there are now more ↓ electrons than ↑ electrons

magnetization $\frac{M}{V} = -\mu_B (n_+ - n_-) > 0$

$\frac{\vec{M}}{V}$ is parallel to $\vec{B}$ $\Rightarrow$ <u>paramagnetic effect</u>