contribution to B.

T > 0: The Fermi-Dirac Distribution

A Fermionic state $\vec{k}\sigma$ with energy $\varepsilon_{\vec{k}}$ may be empty, or filled with one fermion. The grand partition function of the state is

$$\mathcal{Z} = 1 + e^{-\beta(\varepsilon_{\vec{k}} - \mu)}.$$

The probability that the state is empty is

$$p = \frac{1}{\mathcal{Z}}.$$

The probability that it is occupied is

$$P = \frac{e^{-\beta(\varepsilon_{\vec{k}} - \mu)}}{Z}.$$

The average # of Fermions in this state is thus

$$\langle n_{\vec{k}\sigma} \rangle = \frac{e^{-\beta(\varepsilon_{\vec{k}} - \mu)}}{1 + e^{-\beta(\varepsilon_{\vec{k}} - \mu)}}$$

$$= \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} + 1}$$

$$\boxed{f(E) = \frac{1}{e^{\beta(E-\mu)} + 1}}$$

Fermi-Dirac distribution

Phys. 528 Lecture 15

The Fermi gas

Consider N noninteracting spin-1/2 fermions in a cubic box of volume $V = L^3$ subject to periodic boundary conditions (for simplicity; bcs don't matter for bulk behavior).

Energy eigenstates

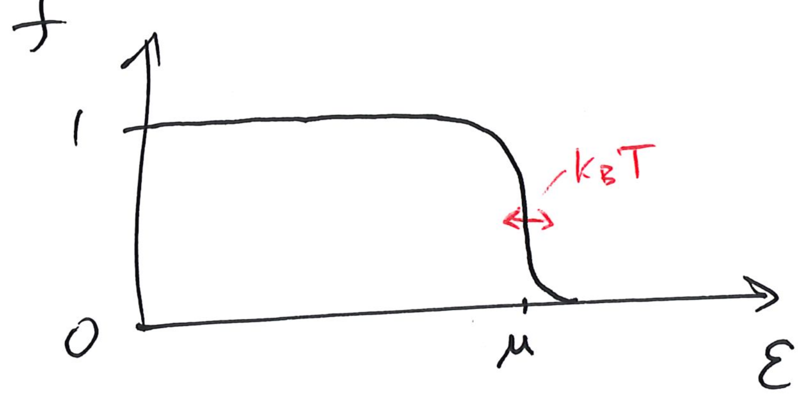
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

$$\text{BCs} \Rightarrow \quad \vec{k} = \frac{2\pi\vec{n}}{L}, \quad n_i \in \mathbb{Z}$$

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

states occupied according to Fermi-Dirac distribution

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



1) Ground state

$$\lim_{T\to 0} f(\varepsilon) = \theta(\varepsilon_F - \varepsilon),$$

where $\varepsilon_F \equiv \lim_{T\to 0} \mu(T)$.

Total # of particles

$$N = \sum_{\sigma=\uparrow}^{\downarrow} \sum_{\vec{k}} \theta(\varepsilon_F - \varepsilon_{\vec{k}}) = 2\sum_{\vec{k}} \theta(k_F - |\vec{k}|)$$

$$\simeq 2\int d^3n \, \theta(k_F - |\vec{k}|)$$

$$= \frac{2V}{(2\pi)^3} \int d^3k \, \theta(k_F - |\vec{k}|)$$

$$N = 2\int \frac{d^3x\, d^3p}{h^3}$$

$$= \frac{2V}{h^3}\frac{4\pi}{3}p_F^3$$

$$\frac{N}{V} = \frac{8\pi}{3}\left(\frac{p_F}{h}\right)^3 = \frac{k_F^{\,3}}{3\pi^2}$$

$$E_0 = 2\int \frac{d^3x\, d^3p}{h^3}\frac{p^2}{2m}$$

$$= \frac{V}{mh^3}\int d^3p\, p^2$$

$$= \frac{4\pi V}{mh^3}\int_0^{p_F} p^4\, dp = \frac{4\pi V}{mh^3}\frac{p_F^5}{5}$$

$$= \frac{8\pi V}{5}\left(\frac{p_F}{h}\right)^3\frac{p_F^2}{2m} = \frac{3}{5}N\varepsilon_F$$

$$N = \frac{V}{4\pi^3} \frac{4\pi}{3} k_F^3 = \frac{k_F^3 V}{3\pi^2}$$

$$\boxed{k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = \text{Fermi wavevector}}$$

Fermi energy

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$$

Fermi velocity

$$v_F = \frac{\hbar k_F}{m} = \frac{\hbar}{m}\left(\frac{3\pi^2 N}{V}\right)^{1/3}$$

Total energy

$$E_0 = 2 \sum_{\vec{k}} \varepsilon_{\vec{k}}\, \theta(k_F - |\vec{k}|)$$

$$= \frac{2V}{(2\pi)^3} \int d^3k \, \frac{\hbar^2 \vec{k}^2}{2m}\, \theta(k_F - |\vec{k}|)$$

$$= \frac{V}{\pi^2} \frac{\hbar^2}{2m} \int_0^{k_F} k^4 \, dk = \frac{V k_F^3}{5\pi^2} \frac{\hbar^2 k_F^2}{2m}$$

$$\boxed{E_0 = \frac{3}{5} N \varepsilon_F}$$

The average energy per particle in the ground state is $\frac{3}{5}$ of the Fermi energy!

Typical Fermi gas parameters are exhibited by the conduction electrons in copper:

V_F	ε_F	$T_F \equiv \varepsilon_F / k_B$
1.56×10^3 km/s	7.0 eV	8.2×10^4 K
$\sim \frac{c}{200}$		

Fermi pressure

$$P = - \left. \frac{\partial E_0}{\partial V} \right|_{N,S} \qquad (S = 0 \text{ @ } T = 0)$$

$$E_0 = \frac{3}{5} N \varepsilon_F = \frac{3\hbar^2}{10m} N \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

$$P = - \left. \frac{\partial E_0}{\partial V} \right|_N = \frac{\hbar^2}{5m} \frac{N}{V} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

$$\boxed{P = \frac{2}{5}\frac{N}{V}\varepsilon_F}$$

In copper, one has

$$P_{Cu} = \frac{2}{5} n \varepsilon_F = 0.4\,(8.5\times10^{22}\,cm^{-3})\,7.0\,eV$$

$$= 1.1\times10^{11}\,N/m^2 \approx 10^6\,Atm\ !$$

The Fermi pressure exherts a repulsive force equivalent to one million atmospheres of pressure?

Q: Why doesn't a penny explode under this tremendous pressure?

A: The repulsive force of the Fermi pressure is balanced by an equally strong attractive force between the negatively charged electrons and the positive ions.

Bulk modulus

Although the Fermi pressure is not directly measurable since it is in balance with the Coulomb forces, the Bulk modulus, which characterizes the compressibility of a solid, is measurable:

$$B \equiv -V \frac{\partial P}{\partial V}\bigg|_{N,T} = \frac{\hbar^2}{3m}\frac{N}{V}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$$

$$B = \frac{5}{3} P$$

The bulk moduli of many simple metals are fairly close to the values predicted by the Fermi gas model.

2) <u>Thermal effects</u> At 300K, $T \ll T_F$, so one can treat

Bulk moduli (10^{10} Dynes/cm^2)

metal	Free electron B	measured B
Li	23.9	11.5
Na	9.23	6.42
K	3.19	2.81
Rb	2.28	1.92
Cs	1.54	1.43
Cu	63.8	134.3
Ag	34.5	99.9

The bulk moduli of the heavier alkali metals are rather well described by the free electron model. The discrepancy can be explained to some extent by the fact that the interaction of an electron with the lattice tends to increase its <u>effective mass</u>, decreasing the bulk modulus.

However, in the noble metals, the bulk modulus significantly <u>exceeds</u> the free electron value. This is a sign that the ionic core electrons play an important role in the noble metals. They give an additional repulsive thermal excitations as a small perturbation. The chemical potential $\mu = \mu(T)$ is determined by

$$N = \int_0^\infty d\varepsilon \, g(\varepsilon) f(\varepsilon) ,$$

where $g(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \varepsilon^{1/2}$ is the density of states. Once μ is known, we can calculate the total energy

$$E(T) = \int_0^\infty d\varepsilon \; \varepsilon \, g(\varepsilon) f(\varepsilon) .$$

Sommerfeld expansion

For fermionic systems, we often need to compute averages over $f(\varepsilon)$:

$$\langle A \rangle = \int_{-\infty}^{\infty} d\varepsilon \; A(\varepsilon) f(\varepsilon) ,$$

where $f(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}+1}$.

Assuming $A(-\infty) = 0$, we can integrate by parts:

$$\langle A \rangle = \int_{-\infty}^{\infty} d\varepsilon \left[\int_{-\infty}^{\varepsilon} d\varepsilon' A(\varepsilon') \right] \left(-\frac{\partial f}{\partial \varepsilon} \right)$$

$-\dfrac{\partial f}{\partial \varepsilon} > 0$ is sharply peaked about $\varepsilon = \mu$, and has unit integral.

$$\lim_{T \to 0} \left(-\frac{\partial f}{\partial \varepsilon} \right) = \delta(\varepsilon - \varepsilon_F).$$

Thus we can expand

$$\int_{-\infty}^{\varepsilon} d\varepsilon' A(\varepsilon') = \int_{-\infty}^{\mu} d\varepsilon' A(\varepsilon') + \int_{\mu}^{\varepsilon} d\varepsilon' A(\varepsilon')$$

using

$$A(\varepsilon') = A(\mu) + A'(\mu)(\varepsilon' - \mu) + \cdots$$
$$= \sum_{n=0}^{\infty} \left. \frac{d^n A}{d\varepsilon^n} \right|_{\varepsilon=\mu} \frac{(\varepsilon' - \mu)^n}{n!}$$

$$\int_{\mu}^{\varepsilon} d\varepsilon' A(\varepsilon') = A(\mu)(\varepsilon-\mu) + A'(\mu)\frac{(\varepsilon-\mu)^2}{2} + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{d^n A(\mu)}{d\mu^n} \frac{(\varepsilon-\mu)^{n+1}}{(n+1)!}.$$

$-\frac{\partial f}{\partial \varepsilon}$ is an even function of $\varepsilon-\mu$, so only the even terms in the series contribute to $\langle A \rangle$.

$$\langle A \rangle = \int_{-\infty}^{\mu} d\varepsilon\, A(\varepsilon) + \sum_{n=1}^{\infty} \frac{d^{2n-1} A(\mu)}{d\mu^{2n-1}} \frac{1}{(2n)!}$$

$$\times \int_{-\infty}^{\infty} d\varepsilon\, (\varepsilon-\mu)^{2n} \left(-\frac{\partial f}{\partial \varepsilon}\right)$$

Let $x = \beta(\varepsilon-\mu)$.

$$\langle A \rangle = \int_{-\infty}^{\mu} d\varepsilon\, A(\varepsilon) + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \frac{d^{2n-1} A(\mu)}{d\mu^{2n-1}},$$

where $a_n = \frac{1}{(2n)!} \int_{-\infty}^{\infty} dx \frac{x^{2n}}{(e^{\frac{x}{2}} + e^{-\frac{x}{2}})^2}.$

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

So

$$\langle A \rangle = \int_{-\infty}^{\mu} d\varepsilon\, A(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 A'(\mu) + \frac{7\pi^4}{360}(k_B T)^4 A'''(\mu) + \cdots$$

Chemical potential

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

$$\simeq \int_{-\infty}^{\mu} d\varepsilon\, g(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 g'(\mu)$$

$$= \underbrace{\int_{-\infty}^{\varepsilon_F} d\varepsilon\, g(\varepsilon)}_{N} + \int_{\varepsilon_F}^{\mu} d\varepsilon\, g(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 g'(\mu)$$

$$0 \cong (\mu - \varepsilon_F)\, g(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2 g'(\varepsilon_F)$$

$$\mu \simeq \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)}$$

$$\boxed{\mu \simeq \varepsilon_F - \frac{\pi^2}{12} \frac{(k_B T)^2}{\varepsilon_F}}$$

$$g(\varepsilon_F) = \frac{3N}{2\varepsilon_F}$$

$$\mu \simeq \varepsilon_F \left(1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F} \right)^2 \right).$$

Note that the correction term is $\mathcal{O}(T/T_F)^2 \ll 1$ @ 300K for typical Fermi systems such as conduction electrons in metals.

Energy

$$E(T) = \int_0^\infty d\varepsilon\, \varepsilon g(\varepsilon) f(\varepsilon)$$

$$\simeq \int_0^\mu d\varepsilon\, \varepsilon g(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 \frac{d}{d\mu}\left(\mu g(\mu)\right)$$

$$= \underbrace{\int_0^{\varepsilon_F} d\varepsilon\, \varepsilon g(\varepsilon)}_{\frac{3}{5} N \varepsilon_F} + \int_{\varepsilon_F}^{\mu} d\varepsilon\, \varepsilon g(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 \overbrace{\left(g(\mu) + \mu g'(\mu)\right)}^{\frac{3}{2} g(\mu)}$$

$$E(T) \simeq E_0 + (\mu - \varepsilon_F)\varepsilon_F g(\varepsilon_F) + \frac{\pi^2}{4}(k_B T)^2 g(\varepsilon_F)$$

$$E(T) \simeq E_0 + \frac{\pi^2}{6}(k_B T)^2 g(\varepsilon_F)$$

$$E(T) \simeq E_0 + \frac{\pi^2}{4}(k_B T)^2 \frac{N}{\varepsilon_F}$$

$$\boxed{C_V = \left.\frac{\partial E}{\partial T}\right|_V \simeq \frac{\pi^2}{2} N k_B \frac{k_B T}{\varepsilon_F}}$$

Compare to the specific heat in the classical theory:

$$C_V\Big|_{class.} = \frac{3}{2} N k_B$$

$$\frac{C_V}{C_V\big|_{class.}} = \frac{\pi^2}{3} \frac{k_B T}{\varepsilon_F} \ll 1 \quad \text{typically}$$

The large suppression is due to the fact that only electrons within $\sim k_B T$ of the Fermi surface are available for thermal excitation.