Free Fermi Gas $(T=0)$

- Simple, solvable model. Turns out to capture many features of real metals, despite drastic oversimplification.

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m}$$

- N = # electrons ($N \sim 10^{22}-10^{23}$ electrons per cm^3 of typical metals)
- m need not be electron mass in free space: $m \to m^*$ "effective mass"
- We'll consider $d=3$, can do for any d.

- First: 1-electron problem:

$$H^{(1)} = \frac{\vec{p}^{\,2}}{2m} \; ; \quad [r_\mu, p_\nu] = i\hbar \delta_{\mu\nu} \quad (\mu, \nu = x, y, z)$$

- Put system in periodic box, volume $V = L^3$, periodic boundary conditions on wavefunction:

$$\psi(x,y,z) = \psi(x+L, y, z) = \psi(x, y+L, z) = \cdots$$

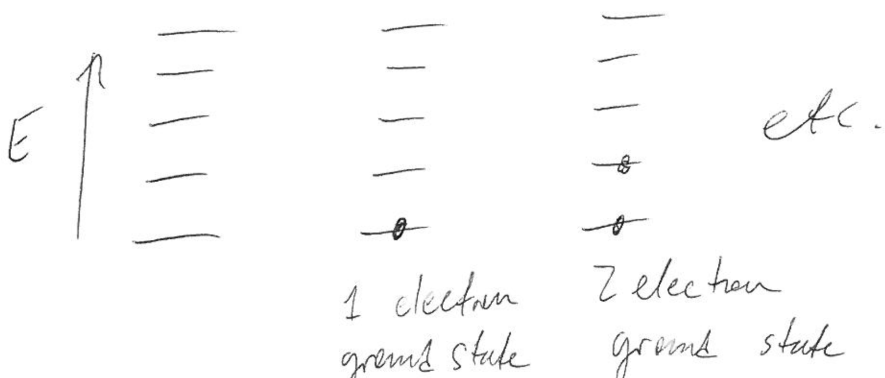
- Energy eigenstates: $|\vec{p}\rangle$; $\vec{k} = \frac{\vec{p}}{\hbar} = \frac{2\pi n_x}{L}\hat{x} + \frac{2\pi n_y}{L}\hat{y} + \frac{2\pi n_z}{L}\hat{z}$

$$(1)\quad H^{(1)}|\vec{p}\rangle = E_{\vec{p}}|\vec{p}\rangle = \frac{\vec{p}^{\,2}}{2m}|\vec{p}\rangle$$

$$(2)\quad \langle\vec{r}|\vec{p}\rangle = \frac{1}{\sqrt{V}}e^{i\vec{p}\cdot\vec{r}/\hbar} = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}$$

- Back to N-electron problem:

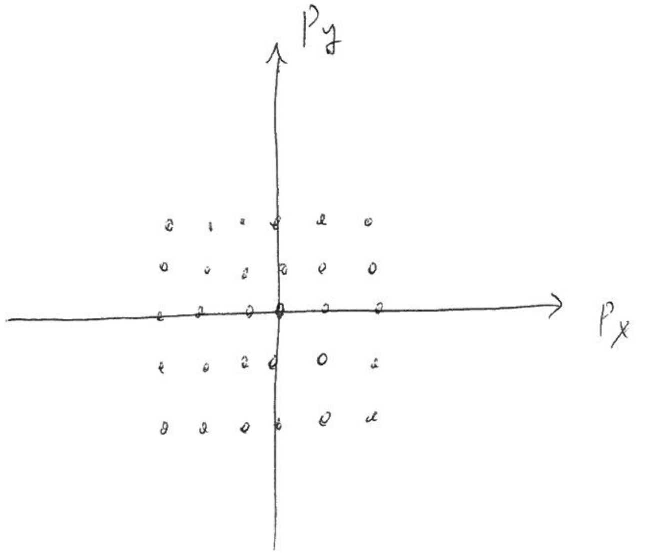
- Many-electron ground state is obtained by filling energy levels from the bottom (Pauli principle)



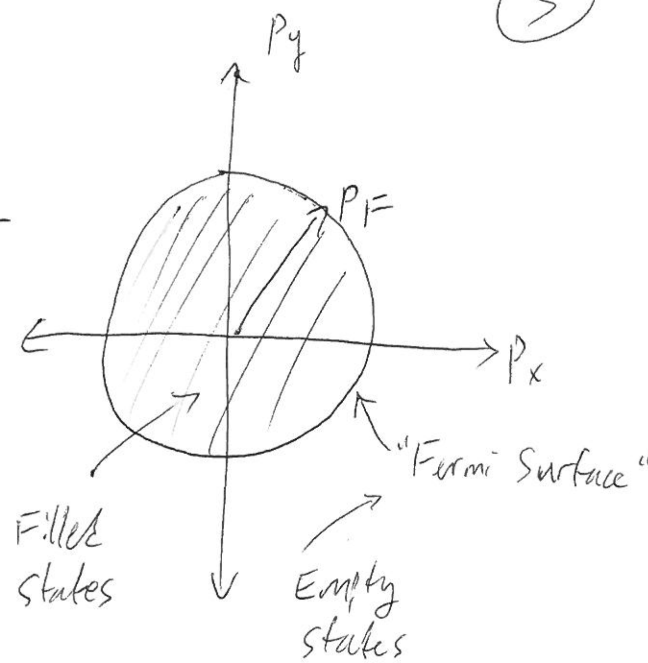
- Electrons have spin-$1/2$ $\Rightarrow$ Fill each discrete $\vec{p}$ with 2 electrons (States $|\vec{p}\uparrow\rangle$ & $|\vec{p}\downarrow\rangle$)

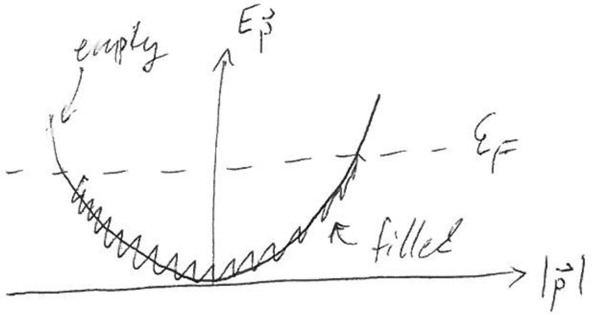
- We will be interested in "thermodynamic" limit":

$$L\to\infty,\quad N\to\infty,\quad n=\frac{N}{V}\to \text{const.}$$



Large-L $\longrightarrow$





- Fill to maximum energy

$$\varepsilon_F = \frac{p_F^2}{2m}$$

$\varepsilon_F \rightarrow$ Fermi energy

$p_F \rightarrow$ " momentum

$k_F = \frac{p_F}{\hbar} \rightarrow$ " wave vector

$T_F = \frac{\varepsilon_F}{k_B} \rightarrow$ " temperature

☆ Fermi surface is the crucial feature of the metallic state. It is manifest in many physical properties.

Number of electrons

$$\Theta(x) = \begin{cases} 1 & ; \ x \geq 0 \\ 0 & ; \ x < 0 \end{cases}$$

$$N = 2 \sum_{\vec{k}} \Theta(k_F - |\vec{k}|)$$

- Limit $V \to \infty$, k-points become close together $\quad \Big\} \frac{2\pi}{L}$

k-space volume per k-point $= \left(\frac{2\pi}{L}\right)^3 = \frac{(2\pi)^3}{V}$

$$\Rightarrow N \to 2 \sum_{\vec{k}} \frac{d^3k}{\left((2\pi)^3/V\right)} \Theta(k_F - |\vec{k}|)$$

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

$$= \frac{2V}{8\pi^3} \frac{4\pi}{3} k_F^3$$

$\Rightarrow$ density $\boxed{n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}}$

We obtained a
Useful result for k-space sums :

$$\boxed{\sum_{\vec{k}} \longleftrightarrow V \int \frac{d^3k}{(2\pi)^3}}$$

Density of states

- Do this another way, using "density of states,"

defined by: $$D(\varepsilon) = \frac{2}{V}\sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}}) \rightarrow 2\int \frac{d^3k}{(2\pi)^3}\, \delta(\varepsilon - \varepsilon_{\vec{k}})$$

(NB: ~~does not~~ includes spin)

- Physical meaning: ~~#~~ $D(\varepsilon)\,d\varepsilon$ is the # of states per unit volume in the interval ~~d~~ $[\varepsilon, \varepsilon + d\varepsilon]$

- Useful since many physical quantities depend on ~~the value~~ $\vec{k}$ only through $\varepsilon_{\vec{k}}$. Also, can define $D(\varepsilon)$ for electrons moving in a crystal lattice. (later)

- Express n in terms of $D(\varepsilon)$:

$$n = \frac{2}{V}\sum_{\vec{k}} \Theta(k_F - |\vec{k}|) = \frac{2}{V}\int_{-\infty}^{\infty} d\varepsilon \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})\,\Theta(k_F - |\vec{k}|)$$

$$= \frac{2}{V}\int_{-\infty}^{\infty} d\varepsilon \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})\,\Theta(\varepsilon_F - \varepsilon_{\vec{k}})$$

$$= \int_{-\infty}^{\infty} d\varepsilon\, D(\varepsilon)\,\Theta(\varepsilon_F - \varepsilon) = \int_{0}^{\varepsilon_F} D(\varepsilon)\, d\varepsilon$$

no states with $\varepsilon < 0$.

- Calculation of $D(\varepsilon)$:

$$D(\varepsilon) = 2\int \frac{d^3k}{(2\pi)^3}\,\delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right)$$

$$= 2\cdot\frac{4\pi}{(2\pi)^3}\int_0^\infty dk\,k^2\,\delta\left(\varepsilon - \frac{\hbar^2k^2}{2m}\right)$$

$u = \frac{\hbar^2 k^2}{2m}$ change of variables

$$\Rightarrow \boxed{D(\varepsilon) = \frac{m}{\pi^2\hbar^3}\sqrt{2m\varepsilon}}$$

Application: ground state energy:

$$\frac{E_0}{V} = \frac{2}{V}\sum_{\vec{k}} \varepsilon_{\vec{k}}\,\Theta(\varepsilon_F - \varepsilon_{\vec{k}}) = \int_0^{\varepsilon_F} d\varepsilon\,\varepsilon\,D(\varepsilon) = \frac{2}{5}\frac{m\sqrt{2m}}{\pi^2\hbar^3}\varepsilon_F^{5/2}$$

g.s. energy per electron:

$$\frac{E_0}{N} = \left(\frac{E_0}{V}\right)\left(\frac{V}{N}\right) = \frac{3}{5}\varepsilon_F \quad \text{(after some algebra)}$$

(compare to classical gas, $\frac{E}{N} = \frac{3}{2}k_BT \to 0$ at $T \to 0$)

[G.S. energy not so interesting in its own right, but can use to calculate thermodynamic quantities — see A&M Ch. 2]

<u>Another application</u>: "Electronic compressibility"

(NB: Not same as "real" compressibility, which is discussed in A&M.)

$$K_e \equiv \frac{\partial n}{\partial \varepsilon_F}$$; change in density for small change in ε_F

Recall $n = \int_{-\infty}^{\infty} d\varepsilon\, D(\varepsilon)\, \Theta(\varepsilon_F - \varepsilon)$

$$\Rightarrow K_e = \int_{-\infty}^{\infty} d\varepsilon\, D(\varepsilon)\, \delta(\varepsilon_F - \varepsilon) = D(\varepsilon_F)$$

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

• Only depends on $D(\varepsilon)$ at $\varepsilon = \varepsilon_F$; only electrons near (in this case, ~~exactly~~ on) the Fermi surface contribute. This is true for many (most?) physical properties at low temperature. To understand why this is so, we need to start thinking about excitations and finite-T properties, where excited states contribute.