

§2. Electron gas

* Free electron gas (Sommerfeld theory)

$$H = -\frac{\hbar^2}{2m} \sum_{j=1}^{N_e} \vec{\nabla}_j^2 = \sum_{j=1}^{N_e} H_j \quad N_e: \# \text{ of electrons}$$

Single electron case:

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

$$H_j \phi_{\vec{k}}(\vec{r}_j) = \varepsilon_{\vec{k}} \phi_{\vec{k}}(\vec{r}_j) \quad \rightarrow \varepsilon_{\vec{k}} = \frac{\hbar^2 |\vec{k}|^2}{2m}$$

Total energy: $E = \sum_{j=1}^{N_e} \varepsilon_{\vec{k}_j}$

Pauli's exclusion principle: Electrons must occupy different single-particle states!

One single-particle state can accommodate two electrons.

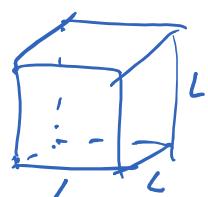
spin: \uparrow, \downarrow

Periodic boundary ("box quantization"):

$$\phi_{\vec{k}}(\vec{r}_j + L\hat{x}) = \phi_{\vec{k}}(\vec{r}_j + L\hat{y}) = \phi_{\vec{k}}(\vec{r}_j + L\hat{z})$$

$$\Rightarrow e^{i\vec{k} \cdot L\hat{x}} = e^{i\vec{k} \cdot L\hat{y}} = e^{i\vec{k} \cdot L\hat{z}} = 1$$

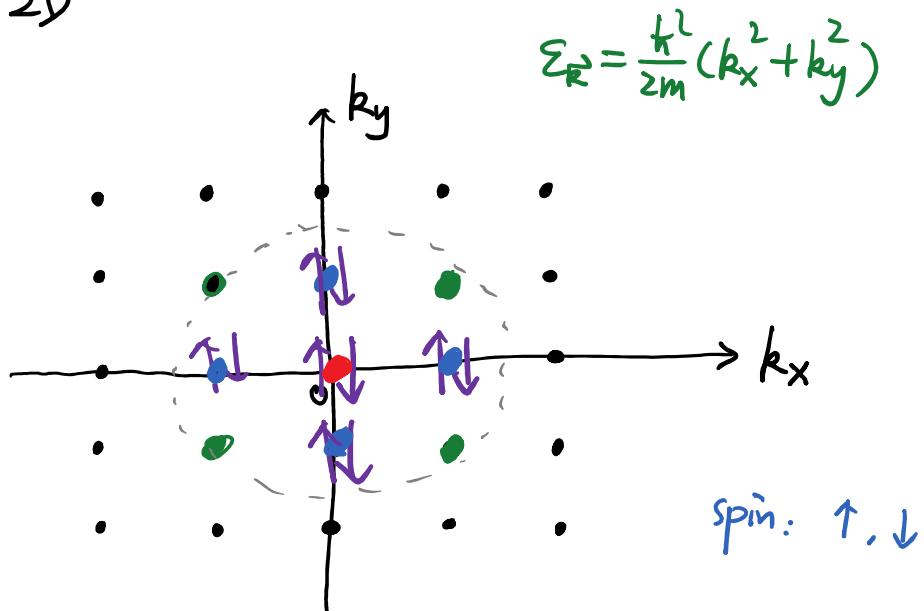
$$k_x, k_y, k_z = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots$$



discrete, makes the states countable!

- Ground state: Fermi sphere

Example: 2D



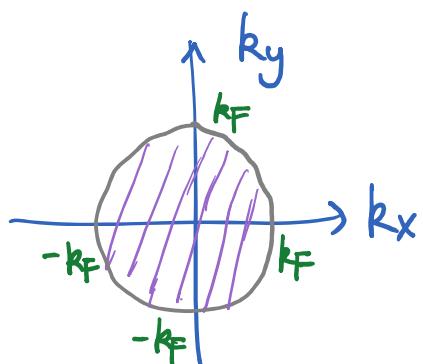
≥ electrons: $(k_x, k_y) = (0, 0)$ occupied

10 electrons: $(k_x, k_y) = (0, 0), (0, \pm \frac{2\pi}{L}),$

\vdots $(\pm \frac{2\pi}{L}, 0)$ occupied

L large \rightarrow \vec{k} points dense

Many electrons form Fermi sphere.

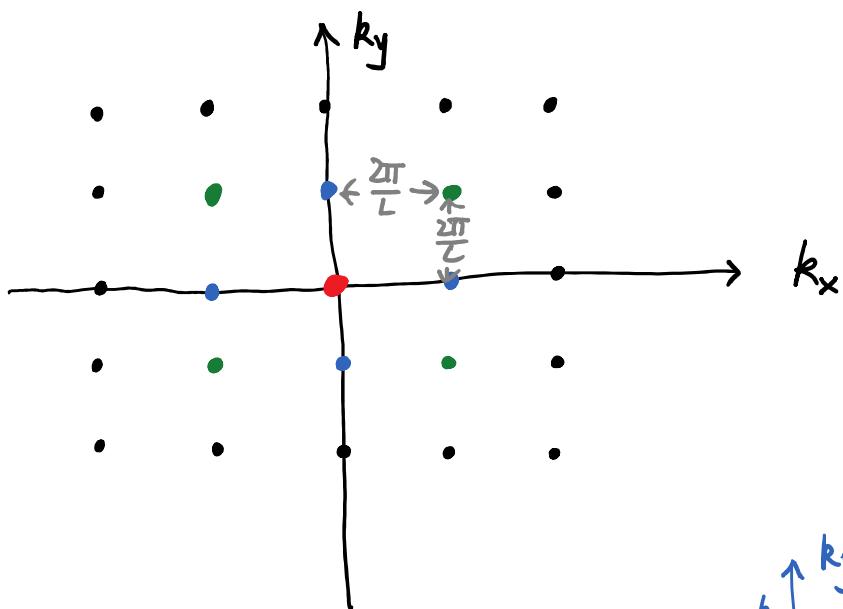


$\hbar k_F$: Fermi momentum

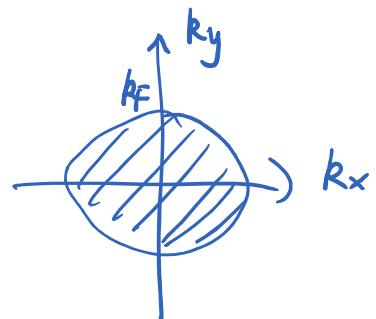
k_F : Fermi wave vector

$\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$: Fermi energy

$T_F = \frac{\epsilon_F}{k_B}$: Fermi temperature
(metal: $\sim 10^4$ K)



: Q How many \vec{k} -points are there
in the Fermi sphere?



(How many electrons are there in the Fermi sphere?)

3D: volume of the Fermi sphere $\frac{4\pi}{3}k_F^3\Omega =$

Each \vec{k} point has volume $(\frac{2\pi}{L})^3$

\Rightarrow # of \vec{k} points within Fermi sphere

$$= \frac{\Omega}{(\frac{2\pi}{L})^3} = \frac{\Omega V}{(2\pi)^3} \quad (\text{"real-space" volume } V=L^3)$$

$$\Rightarrow \# \text{ of electrons : } \frac{\Omega}{(\frac{2\pi}{L})^3} \cdot 2 = N_e$$

$\frac{4}{3}\pi k_F^3$ spin

$$\frac{4}{3}\pi k_F^3 \cdot \frac{V}{(2\pi)^3} \cdot 2 = N_e$$

\Rightarrow Density of electrons:

$$n = \frac{N_e}{V} = \frac{4\pi}{3} k_F^3 \cdot \frac{1}{(2\pi)^3} \cdot 2 = \frac{1}{3\pi^2} k_F^3$$

$$k_F = (3\pi^2 n)^{1/3}$$

k_F is determined by electron density!

Exercise: Generalize this to 1D and 2D.

We still need to work out the explicit form of the many-electron wave function for the Fermi sphere:

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_e}) = ?$$

Product of single-particle wave function does NOT work!

$$\phi_{\vec{k}_1}^{\uparrow}(\vec{r}_1) \phi_{\vec{k}_2}^{\uparrow}(\vec{r}_2) \cdots \phi_{\vec{k}_{N_e/2}}^{\uparrow}(\vec{r}_{N_e/2}) \cdot (\text{spin-}\downarrow \text{ part})$$

$\vec{r}_i \leftrightarrow \vec{r}_j$ should only give a minus sign!

Electrons are fermions \Rightarrow Many-electron wave functions must be totally antisymmetric!

Solution : slater determinant

$$\Psi(\vec{r}_1, \dots, \vec{r}_{N_e}) = \det \begin{pmatrix} \phi_{\vec{R}_1}^{\uparrow}(\vec{r}_1) & \phi_{\vec{R}_1}^{\uparrow}(\vec{r}_2) & \dots & \phi_{\vec{R}_1}^{\uparrow}(\vec{r}_{N_e/2}) \\ \phi_{\vec{R}_2}^{\uparrow}(\vec{r}_1) & \phi_{\vec{R}_2}^{\uparrow}(\vec{r}_2) & \dots & \phi_{\vec{R}_2}^{\uparrow}(\vec{r}_{N_e/2}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\vec{R}_{N_e/2}}^{\uparrow}(\vec{r}_1) & \phi_{\vec{R}_{N_e/2}}^{\uparrow}(\vec{r}_2) & \dots & \phi_{\vec{R}_{N_e/2}}^{\uparrow}(\vec{r}_{N_e/2}) \end{pmatrix}$$

$\times (\text{spin-}\downarrow \text{ part})$

$\frac{N_e}{2} \times \frac{N_e}{2}$ matrix

$\vec{r}_i \leftrightarrow \vec{r}_j$: minus sign due to interchange of rows
in the Slater determinant.

$\frac{N_e}{2} \times \frac{N_e}{2}$ matrix : very large when $N_e \sim 10^{23}$!

More convenient approach : second quantization

electron / fermion creation & annihilation operators

$$C_{\vec{R}, \sigma}^+ \quad C_{\vec{R}, \sigma}$$

↑ ↘
 spin

wave vector

Anticommutation relations: $\{A, B\} \equiv AB + BA$

$$\{C_{\vec{k},\sigma}, C_{\vec{k}',\sigma'}\} = \{C_{\vec{k},\sigma}^+, C_{\vec{k}',\sigma'}^+\} = 0$$

$$\{C_{\vec{k},\sigma}, C_{\vec{k}',\sigma'}^+\} = \delta_{\vec{k},\vec{k}'} \delta_{\sigma\sigma'}$$

Hilbert space:

"vacuum": $|0\rangle$ (no electrons)

single-electron state: $C_{\vec{k},\sigma}^+ |0\rangle$

two-electron state:

$$C_{\vec{k}_1,\sigma_1}^+ C_{\vec{k}_2,\sigma_2}^+ |0\rangle = - C_{\vec{k}_2,\sigma_2}^+ C_{\vec{k}_1,\sigma_1}^+ |0\rangle$$

↑
use anticommutation relations!

$$C_{\vec{k}_1,\sigma_1}^+ C_{\vec{k}_1,\sigma_1}^+ |0\rangle = (C_{\vec{k}_1,\sigma_1}^+)^2 |0\rangle = 0$$

Pauli's exclusion principle is encoded automatically!

Within the second quantization framework,
the wave function for the Fermi sphere is simple:

$$|FS\rangle = \prod_{|\vec{k}| < k_F} \prod_{\sigma=\uparrow,\downarrow} C_{\vec{k},\sigma}^+ |0\rangle$$

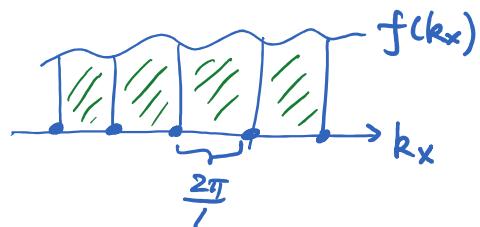
- Ground-state energy

$$E = 2 \sum_{|\vec{k}| < k_F} \frac{\hbar^2 |\vec{k}|^2}{2m}$$

V large: sum over \vec{k} becomes an integral.

1D:

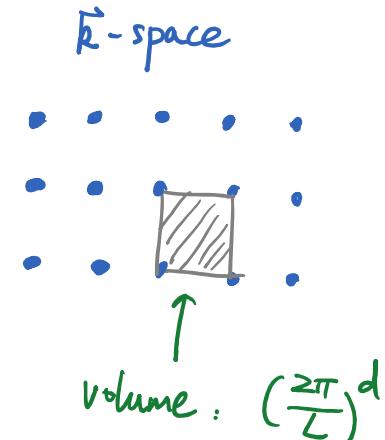
$$\frac{2\pi}{L} \sum_{k_x} f(k_x) \xrightarrow{L \rightarrow \infty} \int dk_x f(k_x)$$



3D:

$$\left(\frac{2\pi}{L}\right)^3 \sum_{\vec{k}} f(\vec{k}) \xrightarrow{L \rightarrow \infty} \int d\vec{k} f(\vec{k})$$

$$\Rightarrow \sum_{\vec{k}} f(\vec{k}) \simeq \frac{V}{(2\pi)^3} \int d\vec{k} f(\vec{k})$$



d: dimension

Ground-state energy:

$$\begin{aligned}
 E &= 2 \frac{V}{(2\pi)^3} \int_{|\vec{k}| < k_F} d\vec{k} \frac{\hbar^2}{2m} |\vec{k}|^2 \\
 &= \frac{V}{4\pi^3} \int_0^{k_F} dk \cdot 4\pi k^2 \cdot \frac{\hbar^2}{2m} k^2 \\
 &\quad \text{with } \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \\
 &= \frac{\hbar^2 k_F^5}{10\pi^2 m} V
 \end{aligned}$$

$$\text{Energy density : } \frac{E}{V} = \frac{\frac{4}{3} \pi^2 k_F^3 n}{10 m}$$

$$\text{Density of electrons : } n = \frac{N_e}{V} = \frac{1}{3\pi^2} k_F^3$$

Energy per electron :

$$\frac{E}{N_e} = \frac{\frac{E}{V}}{\frac{N_e}{V}} = \frac{\frac{3}{10} \pi^2 k_F^2 n}{m} = \frac{3}{5} \underline{\varepsilon_F}$$

Fermi energy

— Density-of-states (DOS)

It is often convenient to think/calculate by using DOS.

$$\begin{aligned} D(\varepsilon) &= 2 \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}}) \\ &= 2 \frac{V}{(2\pi)^3} \int d\vec{k} \delta(\varepsilon - \varepsilon_{\vec{k}}) \end{aligned}$$

$D(\varepsilon)$ counts the "# of states" within a small energy window $\varepsilon \rightarrow \varepsilon + d\varepsilon$.

Example :

$$\sum_{\vec{k}} f(\vec{k}) = \sum_{\vec{k}} \underbrace{\int d\varepsilon \delta(\varepsilon - \varepsilon_{\vec{k}}) f(\vec{k})}_{\stackrel{=}{{}^{\textcolor{red}{\sum}}} \frac{1}{\varepsilon} D(\varepsilon)} \\ = \frac{1}{\varepsilon} \int d\varepsilon D(\varepsilon) f(\varepsilon)$$

of electrons : $N_e = 2 \sum_{|\vec{k}| < k_F} = \int_0^{E_F} d\varepsilon D(\varepsilon)$

Ground-state energy : $E = 2 \sum_{|\vec{k}| < k_F} \varepsilon_{\vec{k}} = \int_0^{E_F} d\varepsilon D(\varepsilon) \varepsilon$

Explicit calculation of $D(\varepsilon)$ for 3D electron gas :

$$D(\varepsilon) \xrightarrow{L \rightarrow \infty} 2 \frac{1}{(2\pi)^3} \int d\vec{k} \delta(\varepsilon - \frac{\hbar^2}{2m} |\vec{k}|^2) \\ = \frac{1}{4\pi^3} \int_0^\infty dk \cdot 4\pi k^2 \underbrace{\delta(\varepsilon - \frac{\hbar^2}{2m} k^2)}$$

use $\delta[f(x)] = \sum_n \frac{\delta(x - x_n)}{|f'(x_n)|}$

x_n : zeros of $f(x)$

$$= \frac{1}{\pi^2} \int_0^\infty dk \cdot k^2 \cdot \frac{m}{\hbar^2 k} \delta(k - \frac{1}{\hbar} \sqrt{2m\varepsilon})$$

$$= \frac{\sqrt{2} V}{\pi^2 \hbar^3} m^{3/2} \sqrt{\varepsilon} \propto \sqrt{\varepsilon}$$

use $\frac{N_e}{V} = \frac{1}{3\pi^2} k_F^3$ and $\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$:

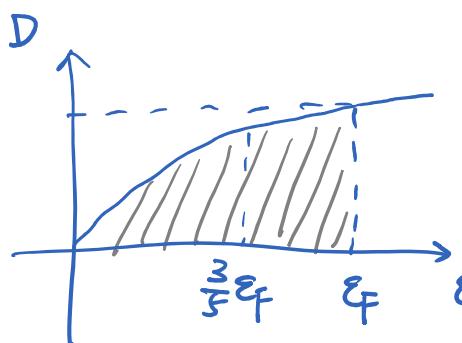
$$D(\epsilon) = \frac{\sqrt{2} V}{\pi^2 \hbar^3} m^{3/2} \sqrt{\epsilon}$$

$$= \frac{\sqrt{2}}{\pi^2 \hbar^3} \frac{3\pi^2 N_e}{k_F^3} m^{3/2} \sqrt{\epsilon}$$

$$= 3\sqrt{2} N_e \underbrace{\left(\frac{m}{\hbar^2 k_F^2} \right)^{3/2}}_{\propto \left(\frac{1}{2\epsilon_F} \right)^{3/2}} \sqrt{\epsilon}$$

$$= \frac{3}{2} \frac{N_e}{\epsilon_F} \underbrace{\left(\frac{\epsilon}{\epsilon_F} \right)^{1/2}}_{\text{red}} \Rightarrow \int_0^{\epsilon_F} d\epsilon D(\epsilon) = N_e \quad \checkmark$$

"sum rule"



$$3D: D(\epsilon) \propto \sqrt{\epsilon}$$

Exercise: $D(\epsilon)$ for electron gas in 1D & 2D

$$1D: D(\epsilon) \propto \frac{1}{\sqrt{\epsilon}}$$

$$2D: D(\epsilon) \propto \text{const.}$$