SFB 1143

Solid State Theory (SS2020)

Lecture 5: Electron gas

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§ 2.1 Free electron gas

- Non-interacting electrons (Sommerfeld theory):

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N_e}\vec{\nabla}_j^2 = \sum_{j=1}^{N_e} H_j$$

Single electron case:

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

$$H_j\,\phi_{\vec{k}}(\vec{r}_j) = \varepsilon_{\vec{k}}\,\phi_{\vec{k}}(\vec{r}_j)$$

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

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

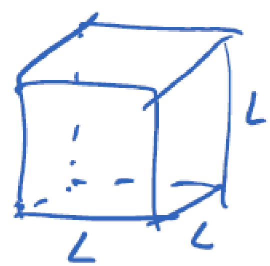
Pauli's exclusion principle!

§ 2.1 Free electron gas

- Box quantization:

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

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



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

discrete, makes the states countable!

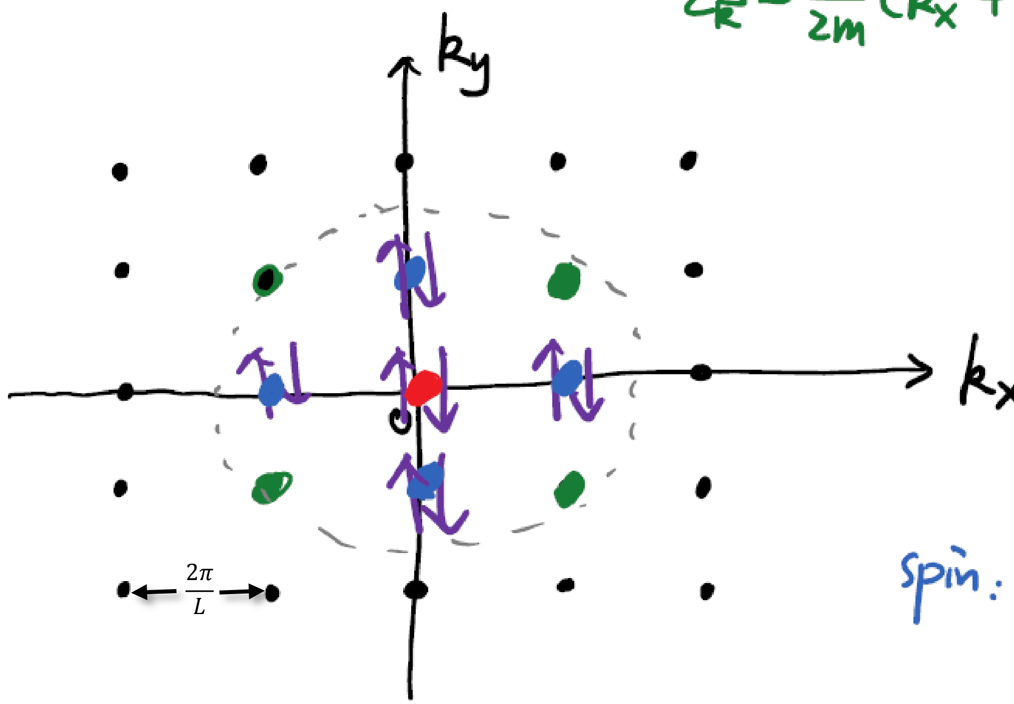
➢ Each $\mathbf{k} = (k_x, k_y, k_z)$ can accommodate two electrons (spin: ↑ and ↓).

§ 2.1 Free electron gas

- Ground state: Fermi sphere

Example : 2D

$$\varepsilon_{\vec{k}} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$$



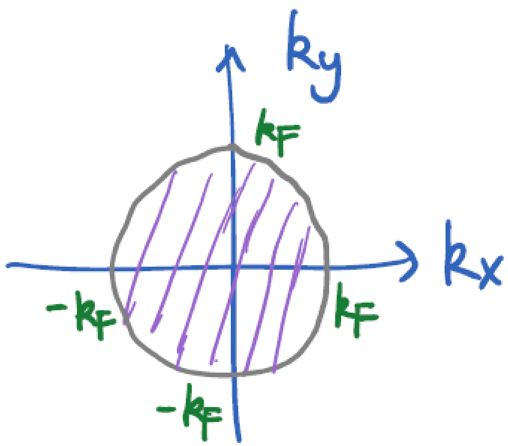
spin: ↑, ↓

§ 2.1 Free electron gas

- Ground state: Fermi sphere

L large → $\vec{k}$ points dense

Many electrons form Fermi sphere.



$\hbar k_F$: Fermi momentum

k_F : Fermi wave vector

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

$T_F = \frac{\varepsilon_F}{k_B}$: Fermi temperature

(metal : $\sim 10^4$ K)

§ 2.1 Free electron gas

Q: How many electrons are there in the Fermi sphere?

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

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

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

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

$\Rightarrow$ # of electrons: $\underbrace{\Omega}_{\frac{4}{3}\pi k_F^3} \frac{V}{(2\pi)^3} \cdot \underbrace{2}_{\text{spin}} = N_e$

§ 2.1 Free electron gas

Q: How many electrons are there in the Fermi sphere?

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

$\Rightarrow$ Density of electrons :

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

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

k_F is determined by electron density !

- Generalize this to 1D and 2D!

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- Many-electron wave function:

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

Product of single-particle wave function does NOT work!

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

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

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

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- Many-electron wave function: Slater determinant

$$\psi(\vec{r}_1, \dots \vec{r}_{N_e}) = \det \begin{pmatrix} \phi^{\uparrow}_{\vec{k}_1}(\vec{r}_1) & \phi^{\uparrow}_{\vec{k}_1}(\vec{r}_2) & \cdots & \phi^{\uparrow}_{\vec{k}_1}(\vec{r}_{N_e/2}) \\ \phi^{\uparrow}_{\vec{k}_2}(\vec{r}_1) & \phi^{\uparrow}_{\vec{k}_2}(\vec{r}_2) & \cdots & \phi^{\uparrow}_{\vec{k}_2}(\vec{r}_{N_e/2}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi^{\uparrow}_{\vec{k}_{N_e/2}}(\vec{r}_1) & \phi^{\uparrow}_{\vec{k}_{N_e/2}}(\vec{r}_2) & & \phi^{\uparrow}_{\vec{k}_{N_e/2}}(\vec{r}_{\vec{k}_{N_e/2}}) \end{pmatrix}$$

$\times$ (spin-$\downarrow$ part)

More convenient approach : second quantization

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- Second quantization:

electron / fermion creation & annihilation operators

$$c^{\dagger}_{\vec{k},\sigma} \qquad\qquad c_{\vec{k},\sigma}$$

spin

wave vector

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

$$\{c_{\vec{k},\sigma}, c_{\vec{k}',\sigma'}\} = \{c^{\dagger}_{\vec{k},\sigma}, c^{\dagger}_{\vec{k}',\sigma'}\} = 0$$

$$\{c_{\vec{k},\sigma}, c^{\dagger}_{\vec{k}',\sigma'}\} = \delta_{\vec{k},\vec{k}'}\,\delta_{\sigma\sigma'}$$

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- Second quantization:

Hilbert space :

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

single-electron state : $c^{\dagger}_{\vec{k},\sigma}|0\rangle$

two-electron state :

$$c^{\dagger}_{\vec{k}_1,\sigma_1} c^{\dagger}_{\vec{k}_2,\sigma_2}|0\rangle = - c^{\dagger}_{\vec{k}_2,\sigma_2} c^{\dagger}_{\vec{k}_1,\sigma_1}|0\rangle$$

use anticommutation relations !

§ 2.1 Free electron gas

- Second quantization:

$$C^{\dagger}_{\vec{k}_1,\sigma_1} C^{\dagger}_{\vec{k}_1,\sigma_1} |0\rangle = \left(C^{\dagger}_{\vec{k}_1,\sigma_1} \right)^2 |0\rangle = 0$$

Pauli's exclusion principle is encoded automatically!

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

$$|FS\rangle = \prod_{|\vec{k}|<k_F} \prod_{\sigma=\uparrow,\downarrow} C^{\dagger}_{\vec{k},\sigma} |0\rangle$$

§ 2.1 Free electron gas

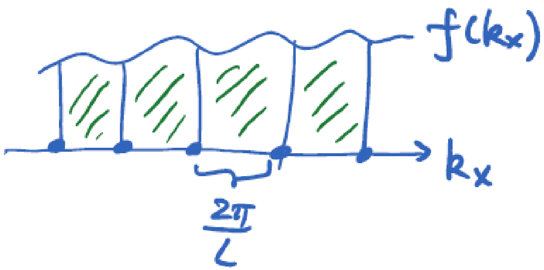
- Ground-state energy of the Fermi sphere:

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

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

1D:

$$\frac{2\pi}{L} \sum_{k_x} f(k_x) \overset{L\to\infty}{\simeq} \int dk_x\, f(k_x)$$



§ 2.1 Free electron gas

- Ground-state energy of the Fermi sphere:

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

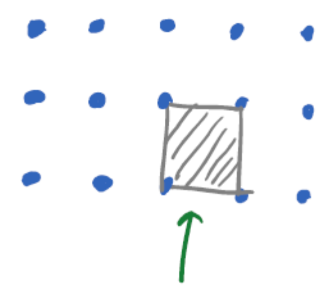
V large: sum over $\vec{k}$ becoms an integral.

3D:

$$\left(\frac{2\pi}{L}\right)^3 \sum_{\vec{k}} f(\vec{k}) \overset{L\to\infty}{\simeq} \int d\vec{k}\, f(\vec{k})$$

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

$\vec{k}$-space



volume: $\left(\frac{2\pi}{L}\right)^d$

d: dimension

§ 2.1 Free electron gas

- Ground-state energy of the Fermi sphere:

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

$$\overset{L\to\infty}{=} 2 \frac{V}{(2\pi)^3} \int_{|\vec{k}|<k_F} d\vec{k} \, \frac{\hbar^2}{2m} |\vec{k}|^2$$

$$= \frac{V}{4\pi^3} \int_0^{k_F} dk \cdot \underbrace{4\pi}_{\int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi} k^2 \cdot \frac{\hbar^2}{2m} k^2$$

$$= \frac{\hbar^2 k_F^5}{10\pi^2 m} V$$

§ 2.1 Free electron gas

- Ground-state energy of the Fermi sphere:

Energy density : $\frac{E}{V} = \frac{\hbar^2 k_F^5}{10\pi^2 m}$

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

Energy per electron :

$$\frac{E}{N_e} = \frac{\frac{E}{V}}{\frac{N_e}{V}} = \frac{3\hbar^2 k_F^2}{10 m} = \frac{3}{5} \underset{\sim}{\varepsilon_F}$$

Fermi energy

§ 2.1 Free electron gas

- Density of states (D.O.S.):

$$D(\varepsilon) = 2 \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})$$

$$\overset{L\to\infty}{=} 2 \frac{V}{(2\pi)^3} \int d\vec{k}\, \delta(\varepsilon - \varepsilon_{\vec{k}})$$

➢ It's convenient to do calculations with D.O.S..

§ 2.1 Free electron gas

- Density of states (D.O.S.):

$$D(\varepsilon) = 2 \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})$$

$$\overset{L\to\infty}{=} 2 \frac{V}{(2\pi)^3} \int d\vec{k}\, \delta(\varepsilon - \varepsilon_{\vec{k}})$$

$$\sum_{\vec{k}} f(\vec{k}) = \sum_{\vec{k}} \int d\varepsilon\, \underbrace{\delta(\varepsilon - \varepsilon_{\vec{k}})}_{=\frac{1}{2}D(\varepsilon)} f(\vec{k})$$

$$= \frac{1}{2} \int d\varepsilon\, D(\varepsilon) f(\varepsilon)$$

➢ It's convenient to do calculations with D.O.S..

§ 2.1 Free electron gas

- Density of states (D.O.S.):

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

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

§ 2.1 Free electron gas

- Density of states (D.O.S.):

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

$$D(\varepsilon) \overset{L\to\infty}{=} 2\frac{V}{(2\pi)^3}\int d\vec{k}\ \delta\left(\varepsilon - \frac{\hbar^2}{2m}|\vec{k}|^2\right)$$

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

x_n : zeros of $f(x)$

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

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

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

§ 2.1 Free electron gas

- Density of states (D.O.S.):

$$\frac{N_e}{V} = \frac{1}{3\pi^2} k_F^3$$

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

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

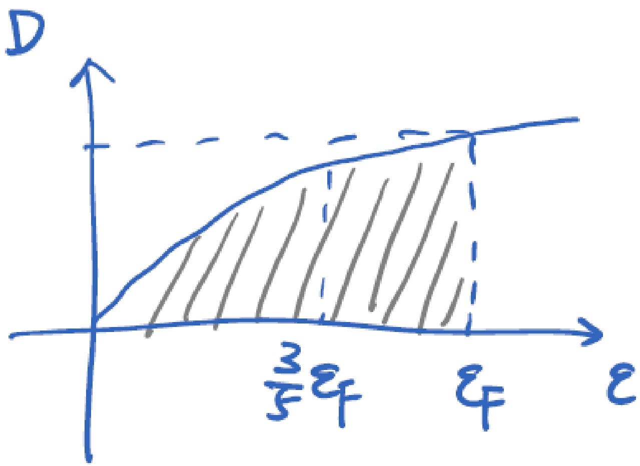
$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

$$= 3\sqrt{2}\, N_e \underbrace{\left(\frac{m}{\hbar^2 k_F^2}\right)^{3/2}}_{= \left(\frac{1}{2\varepsilon_F}\right)^{3/2}} \sqrt{\varepsilon}$$

$$= \frac{3}{2} \frac{N_e}{\varepsilon_F} \left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \quad \Rightarrow \int_0^{\varepsilon_F} d\varepsilon\, D(\varepsilon) = N_e \ \checkmark$$

§ 2.1 Free electron gas

- Density of states (D.O.S.):



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

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

2D: $D(\varepsilon) \propto$ const.