Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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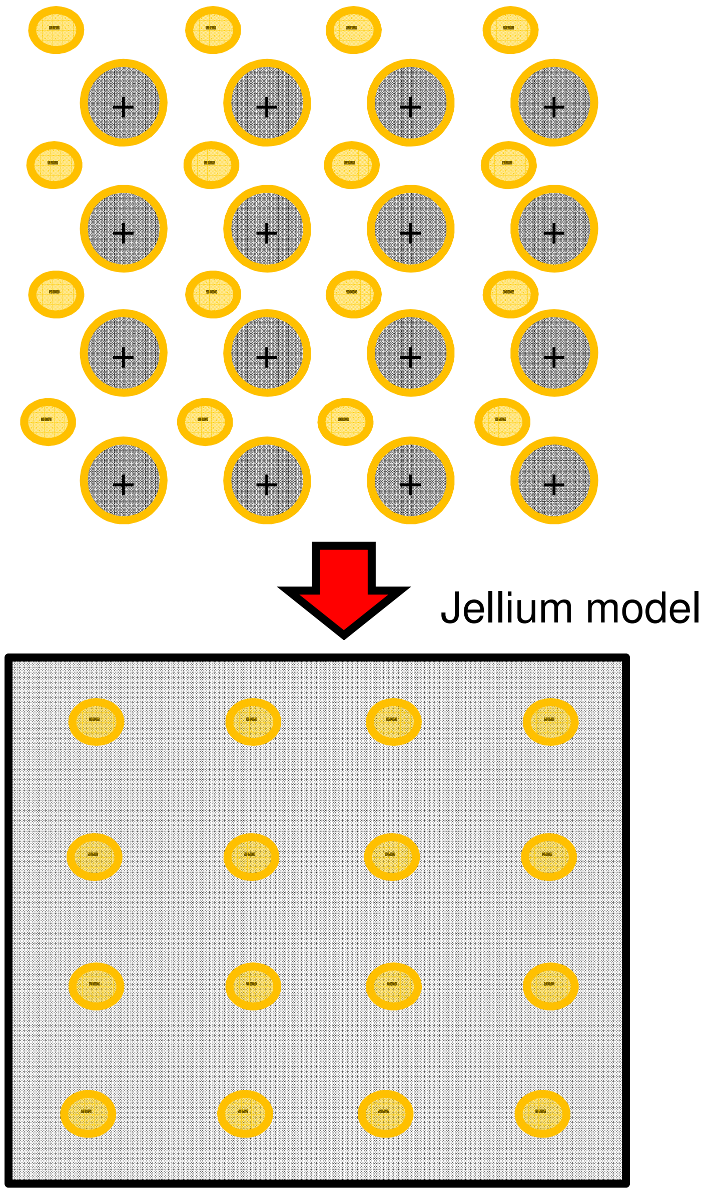
Today's class: *Non-interacting electron gas*

- Jellium model
- Non-interacting Fermi gas.
- Ground-state: Fermi energy.
- Density of states.

Electrons in a solid: the jellium model



- Model for electrons in a metal.
- “Core ions”: form a homogenous “fluid”, positively charged (positive background).
- Conduction electrons: move “freely” in this background, weakly interacting with each other.
- The whole system is charge neutral.
- Electrons behave as in a “Fermi gas”.

Free fermion "gas": single-particle picture

- Single-particle Hamiltonian: $\hat{h}|\varphi_{\mathbf{k}}\rangle = \varepsilon_{\mathbf{k}}|\varphi_{\mathbf{k}}\rangle$ $\mathbf{k} = (k_x, k_y, k_z)$
- Schrödinger's equation for a particle of mass *m**:

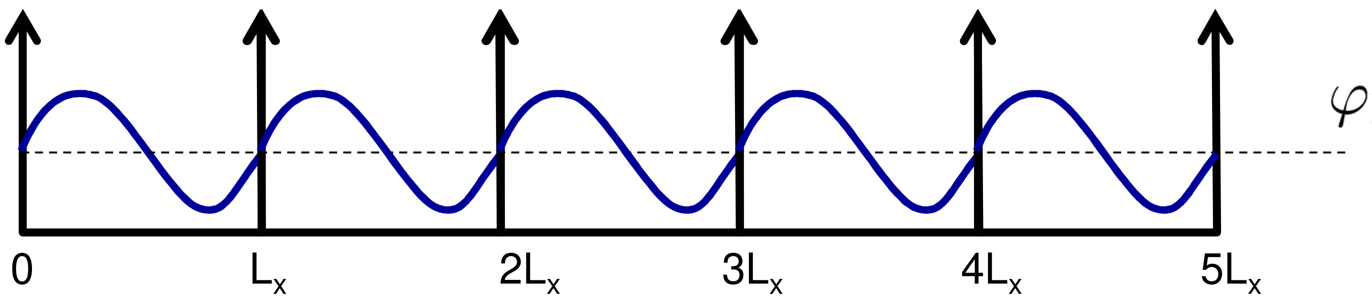
$$-\frac{\hbar^2}{2m^*}\nabla^2\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r}) \Rightarrow \nabla^2\varphi(\mathbf{r}) = -k^2\varphi(\mathbf{r})$$

Solution (plane waves):

$$\varphi_{\mathbf{k}}(\mathbf{r}) = Ae^{i\mathbf{k}\cdot\mathbf{r}} \quad |\mathbf{k}|^2 = \frac{2m^*\varepsilon}{\hbar^2}$$

- Let us consider *periodic boundary conditions*:

$$\varphi_{\mathbf{k}}(x+L_x, y, z) = \varphi_{\mathbf{k}}(x, y+L_y, z) = \varphi_{\mathbf{k}}(x, y, z+L_z) = \varphi_{\mathbf{k}}(x, y, z)$$



$$\varphi_{\mathbf{k}}(\mathbf{r}+\mathbf{L}) = Ae^{i\mathbf{k}\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{L}}$$

$$e^{i\mathbf{k}\cdot\mathbf{L}} = 1$$

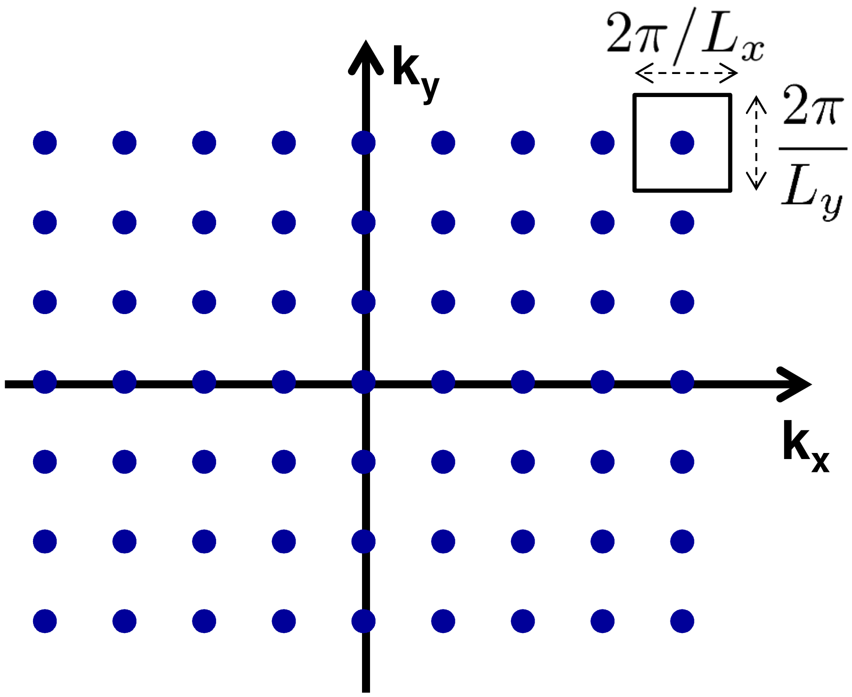
- Solution: energy quantization:

$$k_xL_x + k_yL_y + k_zL_z = 2m\pi$$

$$m = n_x + n_y + n_z = 0, \pm 1, \pm 2, ...$$

"Counting" the states.

- Possible **k** values: $$k_{x(y,z)} = \frac{2\pi n_{x(y,z)}}{L_{x(y,z)}} \text{ with } n_{x(y,z)} = 0, \pm 1, \pm 2, \ldots$$



Tip: to go from discrete → continuum!

$$\boxed{\frac{1}{V_{\mathbf{r}}}\sum_{\mathbf{k}} \rightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3}}$$

- State and energy for each **k**:

$$\varphi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{L_x L_y L_z}} e^{i\mathbf{k}\cdot\mathbf{r}} \qquad \boxed{\varepsilon_{\mathbf{k}} = \frac{\hbar^2 |\mathbf{k}|^2}{2m^*}}$$

- Number of states in **k** space (3D) :

"Volume" of each state in **k**

$$V_{\mathbf{k}}^{1\text{st}} = \left(\frac{2\pi}{L_x}\right)\left(\frac{2\pi}{L_y}\right)\left(\frac{2\pi}{L_z}\right) = \frac{(2\pi)^3}{V_{\mathbf{r}}}$$

Number of states in a given volume in **k**:

$$N_{\text{st}} = \sum_{\mathbf{k}} = \int \frac{d^3\mathbf{k}}{V_{\mathbf{k}}^{1\text{st}}} = V_{\mathbf{r}} \int \frac{d^3\mathbf{k}}{(2\pi)^3}$$

N-particle Hamiltonian

- Need to account for spin ($\sigma=\uparrow,\downarrow$). The single-particle states are then:

$$\hat{h}|\varphi_{\mathbf{k},\sigma}\rangle = \varepsilon_{\mathbf{k}}|\varphi_{\mathbf{k},\sigma}\rangle \qquad |\varphi_{\mathbf{k},\sigma}\rangle = c^{\dagger}_{\mathbf{k},\sigma}|0\rangle$$

- N-body Hamiltonian:

$$\hat{H} = \sum_{n=1}^{N} \hat{h}^{(n)} = \sum_{\mathbf{k},\sigma=\uparrow,\downarrow} \varepsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma=\uparrow,\downarrow} \varepsilon_{\mathbf{k}}\hat{n}_{\mathbf{k},\sigma} \quad \begin{cases} \varepsilon_{\mathbf{k}} = \dfrac{\hbar^2|\mathbf{k}|^2}{2m^*} \\ n_{\mathbf{k},\sigma} = 0,\ 1 \end{cases}$$

- Eigenstates and eigenenergies:

$$\hat{H}|\ldots n_{\mathbf{k},\uparrow},\ n_{\mathbf{k},\downarrow}\ldots\rangle = \left[\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}\left(n_{\mathbf{k},\uparrow} + n_{\mathbf{k},\downarrow}\right)\right]|\ldots n_{\mathbf{k},\uparrow}, n_{\mathbf{k},\downarrow}\ldots\rangle$$

- Let's consider N even (non-polarized gas): (N/2 spin $\uparrow$, N/2 spin $\downarrow$).

$$N = \sum_{\mathbf{k}} n_{\mathbf{k},\uparrow} + n_{\mathbf{k},\downarrow} \ \text{ with } \ \frac{N}{2} = \sum_{\mathbf{k}} n_{\mathbf{k},\uparrow} = \sum_{\mathbf{k}} n_{\mathbf{k},\downarrow}$$

N-particle ground state

- For a given set of occupations: $$E_{n_{\mathbf{0},\uparrow},\, n_{\mathbf{0},\downarrow}\ldots n_{\mathbf{k},\uparrow},\, n_{\mathbf{k},\downarrow}\ldots} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \left(n_{\mathbf{k},\uparrow} + n_{\mathbf{k},\downarrow}\right)$$

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 |\mathbf{k}|^2}{2m^*}$$

- Ground-state of the N-particle system:

$$\begin{cases} \hat{H}|\mathrm{GS}\rangle = \mathrm{E}_{\mathrm{GS}}|\mathrm{GS}\rangle \\ E_{\mathrm{GS}} = \langle \mathrm{GS}|\hat{H}|\mathrm{GS}\rangle \end{cases}$$

$$\langle \mathrm{GS}|\hat{N}|\mathrm{GS}\rangle = \left\langle \mathrm{GS} \left| \sum_{\mathbf{k},\sigma} \hat{n}_{\mathbf{k},\sigma} \right| \mathrm{GS} \right\rangle = N$$

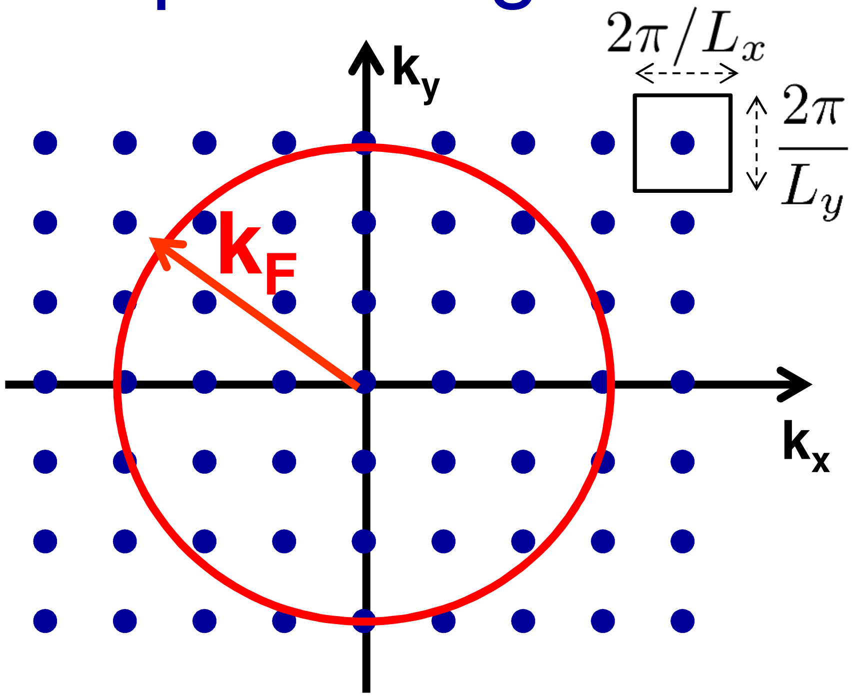
- Ground state energy :

$$E_{\mathrm{GS}} = \sum_{|\mathbf{k}|<|\mathbf{k}_F|} \varepsilon_{\mathbf{k}} \left(n_{\mathbf{k},\uparrow} + n_{\mathbf{k},\downarrow}\right)$$

$$\begin{cases} n_{|\mathbf{k}|\leq|\mathbf{k}_F|,\sigma=\uparrow,\downarrow} = 1 \\ n_{|\mathbf{k}|>|\mathbf{k}_F|,\sigma=\uparrow,\downarrow} = 0 \\ \frac{N}{2} = \sum_{|\mathbf{k}|\leq|\mathbf{k}_F|} \langle \mathrm{GS}|\hat{n}_{\mathbf{k},\uparrow}|\mathrm{GS}\rangle = \sum_{|\mathbf{k}|\leq|\mathbf{k}_F|} \langle \mathrm{GS}|\hat{n}_{\mathbf{k},\downarrow}|\mathrm{GS}\rangle\ . \end{cases}$$

$\mathbf{k}_F$: Fermi wave vector

N-particle ground state: Fermi Energy.



- In each occupied state ($k \leq k_F$) there are 2 Fermions (Pauli).
- For N fermions:

$$N = 2\sum_{|\mathbf{k}|\leq|\mathbf{k}_F|}\langle \mathrm{GS}|\hat{n}_{\mathbf{k},\uparrow}|\mathrm{GS}\rangle = 2\sum_{|\mathbf{k}|<k_F} = 2V_{\mathbf{r}}\int_{V_{\mathbf{k}}}\frac{d^3\mathbf{k}}{(2\pi)^3}$$

Integrating over the Fermi sphere in k space:

$$\frac{N}{V_{\mathbf{r}}} = \frac{2}{8\pi^3}\frac{4}{3}\pi k_F^3 = \frac{k_F^3}{3\pi^2}$$

- In terms of the density n=N/V_r :

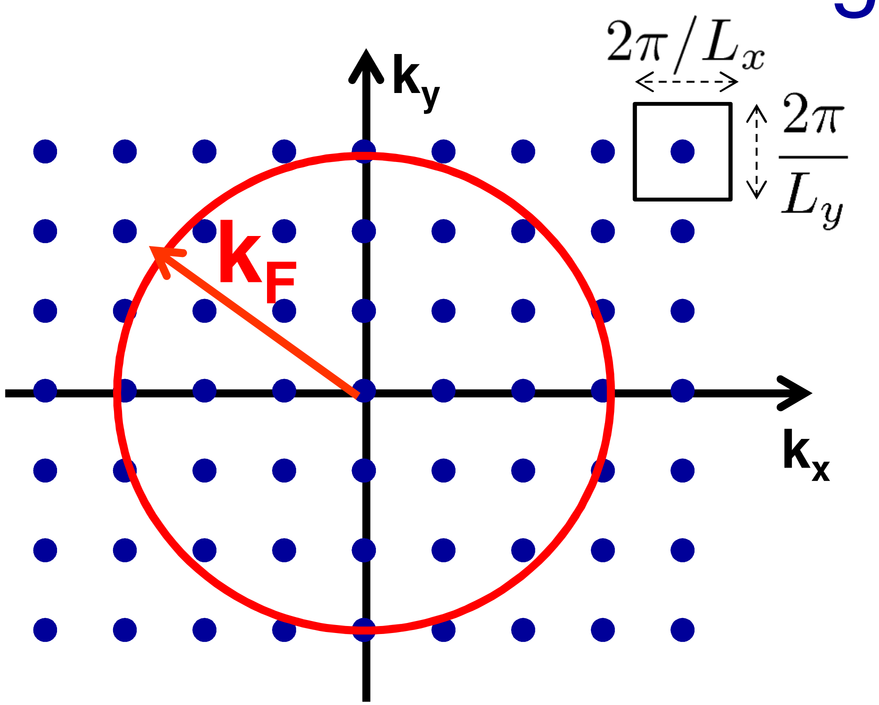
$$\varepsilon_F = \left(\frac{\hbar^2(3\pi^2)^{\frac{2}{3}}}{2m^*}\right)n^{\frac{2}{3}}$$

In 3D, $\varepsilon_F \sim n^{2/3}$!

- Fermi energy ε_F: single-particle energy of the latest occupied states.
- $\varepsilon = \varepsilon_F$: **sphere in k space**.
- The radius of this sphere is k_F

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

Ground-state energy of the N-particle state.



- Integrating e rearranging:

$$E = \frac{3}{5} V_{\mathbf{r}} n \varepsilon_F \Rightarrow \frac{E}{N} = \frac{3}{5}\varepsilon_F$$

Energy *per particle* in a Fermion gas.

- Typical values in metals (Copper) :

$$\varepsilon_F \approx 7.03 \text{ eV} = 81600 \text{ K/k}_B$$

$$\lambda_F = \frac{2\pi}{k_F} \approx 4.6 \text{Å}$$

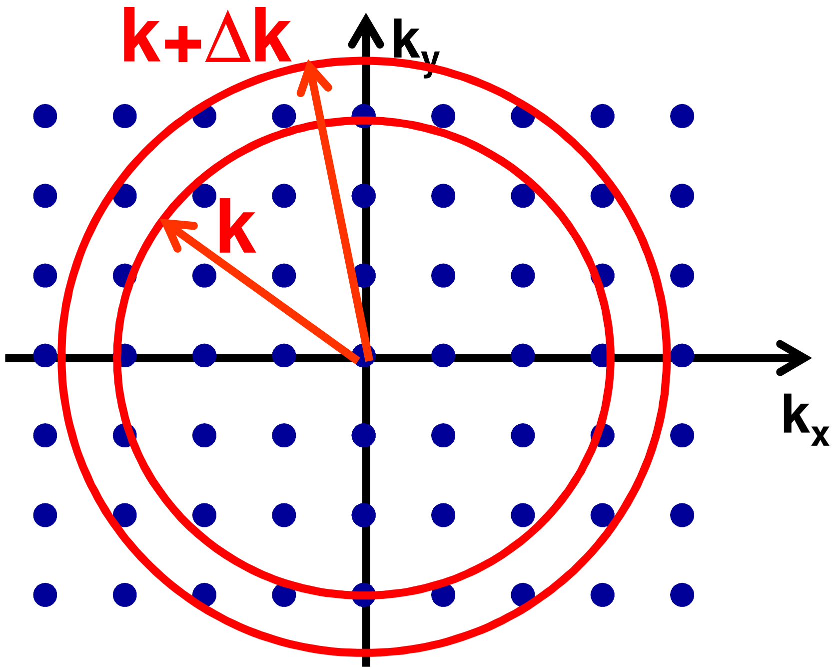
$$v_F = \frac{\hbar k_F}{m^*} \approx 1.57 \times 10^6 \text{ m/s} \approx 0.005c$$

- Useful! $(1 \text{ meV} = 11.6 \text{ K/k}_B)$

- Adding the energies of each occupied state:

$$E_{\text{GS}} = 2 \sum_{|\mathbf{k}|<|\mathbf{k}_F|} \varepsilon_{\mathbf{k}} n_{\mathbf{k},\uparrow} = 2 \sum_{|\mathbf{k}|<k_F} \varepsilon_k = 2V_{\mathbf{r}} \int_{V_{\mathbf{k}}} \frac{\hbar^2 k^2}{2m^*} \frac{d^3\mathbf{k}}{(2\pi)^3}$$

Density of states.



- No of states between k and k+Δk (3D):

$$\Delta N_{\text{st}}^{\Delta \mathbf{k}} = 2\frac{\Delta V_{\mathbf{k}}}{V_{\mathbf{k}}^{1\text{st}}} = V_{\mathbf{r}}\frac{8\pi k^2 dk}{(2\pi)^3}$$

$$\boxed{\Delta N_{\text{st}}^{\Delta \mathbf{k}} = V_{\mathbf{r}}\frac{k^2 dk}{\pi^2}}$$

- No. of states between ε and ε+Δε :

$$\Delta N_{\text{st}}^{\Delta \varepsilon} = \rho(\varepsilon) d\varepsilon$$

where ρ(ε) is the density of states:

- Converting from k to ε:

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m^*} \Rightarrow d\varepsilon = \frac{\hbar^2 k dk}{m^*}$$

Since the number of states is the same:

$$\Delta N_{\text{st}}^{\Delta \mathbf{k}} = \Delta N_{\text{st}}^{\Delta \varepsilon} = \frac{V_{\mathbf{r}}}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} \varepsilon^{\frac{1}{2}} d\varepsilon$$

- Density of states in 3D:

$$\boxed{\rho_{3\text{D}}(\varepsilon) = \frac{V_{\mathbf{r}}}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} \varepsilon^{\frac{1}{2}}}$$