

**Summary Sec. 1.2.1:**  
**The non-interacting Green's function**

Starting point: the general electron Green's function (1.1):

$$iG_{\alpha,\beta}(\mathbf{r}t, \mathbf{r}'t') = \langle \Psi_0^{(N)} | \hat{T} \left[ \hat{\psi}_{H\alpha}(\mathbf{r}t) \hat{\psi}_{H\beta}^\dagger(\mathbf{r}'t') \right] | \Psi_0^{(N)} \rangle$$

A **perturbation** calculation:

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

Operator transformation: Schrödinger → **Heisenberg**  
Schrödinger → **Interaction**

$$\hat{O}_H(t) = e^{i\hat{H}t/\hbar} \hat{O} e^{-i\hat{H}t/\hbar}$$

$$\hat{O}_I(t) = e^{i\hat{H}_0t/\hbar} \hat{O} e^{-i\hat{H}_0t/\hbar}$$

**Equation of motion** of an Interaction Operator:

$$i\hbar \frac{\partial}{\partial t} \hat{O}_I(t) = e^{i\hat{H}_0t/\hbar} \left[ \hat{O}, \hat{H}_0 \right] e^{-i\hat{H}_0t/\hbar}$$

The non-interacting Hamiltonian in the **particle number representation**

$$\hat{H}_0 = \sum_{i,j} \langle i | \hat{h} | j \rangle \hat{c}_i^\dagger \hat{c}_j$$

is diagonal in its **eigenbasis**  $\hat{h} | i \rangle = \hbar\omega_i^0 | i \rangle$

$$\hat{H}_0 = \sum_i \hbar\omega_i^0 \hat{c}_i^\dagger \hat{c}_i$$

Equation of motion of the **annihilation operator**:

$$i\hbar \frac{\partial}{\partial t} \hat{c}_{jI}(t) = e^{i\hat{H}_0t/\hbar} \left[ \hat{c}_j, \hat{H}_0 \right] e^{-i\hat{H}_0t/\hbar},$$

and with respect of  $\left[ \hat{c}_j, \hat{H}_0 \right] = \hbar\omega_j^0 \hat{c}_j$  :

$$i\hbar \frac{\partial}{\partial t} \hat{c}_{jI}(t) = \hbar\omega_j^0 \hat{c}_{jI}(t)$$

Solution of this differential equation:

$$\hat{c}_{jI}(t) = \hat{c}_j e^{-i\omega_j^0 t}$$

and -correspondingly- for the **creation operator**:

$$\hat{c}_{jI}^\dagger(t) = \hat{c}_j^\dagger e^{+i\omega_j^0 t}$$

Now back to the Green's function of the **non-interacting** electron:

$$iG_{\alpha,\beta}^0(\mathbf{r}t, \mathbf{r}'t') = \langle \Phi_0 | \hat{T} \left[ \hat{\psi}_{H\alpha}(\mathbf{r}t) \hat{\psi}_{H\beta}^\dagger(\mathbf{r}'t') \right] | \Phi_0 \rangle$$

with

$$\hat{H} = \hat{H}_0 \quad \text{and} \quad \hat{H}_0 | \Phi_0 \rangle = E_0 | \Phi_0 \rangle$$

Important consequence: **"Heisenberg = Interaction"**:

$$\hat{O}_H(t) = \hat{O}_I(t)$$

Therefore one gets

$$iG_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') = \langle \Phi_0 | \hat{T} \left[ \hat{\psi}_{\alpha I}(\mathbf{r}t) \hat{\psi}_{\beta I}^\dagger(\mathbf{r}'t') \right] | \Phi_0 \rangle .$$

Expansion of the **field operators** with respect of the **annihilation and creation operators**:

$$\hat{\psi}_{\alpha I}(\mathbf{r}t) = \sum_{\mathbf{k}\lambda} \psi_{\mathbf{k}}(\mathbf{r}) \chi_\lambda(\alpha) \hat{c}_{\mathbf{k}\lambda, I}(t) = \sum_{\mathbf{k}\lambda} \psi_{\mathbf{k}}(\mathbf{r}) \chi_\lambda(\alpha) e^{-i\omega_{\mathbf{k}}^0 t} \hat{c}_{\mathbf{k}\lambda}$$

and

$$\hat{\psi}_{\beta I}^\dagger(\mathbf{r}'t') = \sum_{\mathbf{k}\lambda} \psi_{\mathbf{k}}^*(\mathbf{r}') \chi_\lambda^\dagger(\beta) \hat{c}_{\mathbf{k}\lambda, I}^\dagger(t) = \sum_{\mathbf{k}\lambda} \psi_{\mathbf{k}}^*(\mathbf{r}') \chi_\lambda^\dagger(\beta) e^{+i\omega_{\mathbf{k}}^0 t'} \hat{c}_{\mathbf{k}\lambda}^\dagger .$$

For  $T \rightarrow 0$  K, the ground state of a system of non-interacting electrons is given by a completely filled **Fermi sphere** with radius  $k_F$ .

**For practical reasons**, the operator  $\hat{c}$  is re-defined by the following **canonical transformation**:

$$\hat{c}_{\mathbf{k}\lambda} = \begin{cases} \hat{a}_{\mathbf{k}\lambda} & \text{"annihilation of a particle state" for } |\mathbf{k}| > k_F \\ \hat{b}_{-\mathbf{k}\lambda}^\dagger & \text{"creation of a hole state" for } |\mathbf{k}| < k_F \end{cases}$$

Including this definition into the formula for the field operator  $\hat{\psi}_{\alpha I}$  leads to

$$\hat{\psi}_{\alpha I}(\mathbf{r}t) = \sum_{|\mathbf{k}| > k_F} \sum_{\lambda} \psi_{\mathbf{k}}(\mathbf{r}) \chi_{\lambda}(\alpha) e^{-i\omega_{\mathbf{k}}^0 t} \hat{a}_{\mathbf{k}\lambda} + \sum_{|\mathbf{k}| < k_F} \sum_{\lambda} \psi_{\mathbf{k}}(\mathbf{r}) \chi_{\lambda}(\alpha) e^{-i\omega_{\mathbf{k}}^0 t} \hat{b}_{-\mathbf{k}\lambda}^{\dagger}.$$

Now such equations for  $\hat{\psi}_{\alpha I}$  and  $\hat{\psi}_{\beta I}^{\dagger}$  are used in the expression of  $G_{\alpha\beta}^0$ . In case of  $t > t'$ , one gets the following four matrix elements:

1.  $\langle \Phi_0 | \hat{a}_{\mathbf{k}\lambda} \hat{a}_{\mathbf{k}'\lambda'}^{\dagger} | \Phi_0 \rangle = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\lambda,\lambda'}$
2.  $\langle \Phi_0 | \hat{a}_{\mathbf{k}\lambda} \hat{b}_{-\mathbf{k}'\lambda'} | \Phi_0 \rangle = 0$
3.  $\langle \Phi_0 | \hat{b}_{-\mathbf{k}\lambda}^{\dagger} \hat{a}_{\mathbf{k}'\lambda'}^{\dagger} | \Phi_0 \rangle = 0$
4.  $\langle \Phi_0 | \hat{b}_{-\mathbf{k}\lambda}^{\dagger} \hat{b}_{-\mathbf{k}'\lambda'} | \Phi_0 \rangle = 0$

and

$$\begin{aligned} iG_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') &= \sum_{|\mathbf{k}| > k_F} \psi_{\mathbf{k}}(\mathbf{r}) \psi_{\mathbf{k}}^*(\mathbf{r}') e^{-i\omega_{\mathbf{k}}^0(t-t')} \underbrace{\sum_{\lambda} \chi_{\lambda}(\alpha) \chi_{\lambda}^{\dagger}(\beta)}_{\delta_{\alpha,\beta}} \\ &= \delta_{\alpha,\beta} \sum_{|\mathbf{k}| > k_F} \psi_{\mathbf{k}}(\mathbf{r}) \psi_{\mathbf{k}}^*(\mathbf{r}') e^{-i\omega_{\mathbf{k}}^0(t-t')} \end{aligned}$$

The correspondent result for  $t < t'$  reads

$$iG_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') = -\delta_{\alpha,\beta} \sum_{|\mathbf{k}| < k_F} \psi_{\mathbf{k}}(\mathbf{r}) \psi_{\mathbf{k}}^*(\mathbf{r}') e^{-i\omega_{\mathbf{k}}^0(t-t')}$$

leading to

$$\begin{aligned} iG_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') &= \delta_{\alpha\beta} \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) \psi_{\mathbf{k}}^*(\mathbf{r}') e^{-i\omega_{\mathbf{k}}^0(t-t')} \\ &\times \{ \Theta(t-t') \Theta(|\mathbf{k}| - k_F) - \Theta(t'-t) \Theta(k_F - |\mathbf{k}|) \}. \end{aligned}$$

By using the **integral representation**

$$\Theta(t - t') = - \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} \frac{e^{-i\omega(t-t')}}{\omega + i\eta}$$

for the time-dependent Heaviside function, one finally gets (see pp. 8 and 9 of my lecture notes)

$$G_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') = \delta_{\alpha\beta} \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) \psi_{\mathbf{k}}^*(\mathbf{r}') \int \frac{d\sigma}{2\pi} e^{-i\sigma(t-t')} \left\{ \frac{\Theta(k - k_F)}{\sigma - \omega_{\mathbf{k}}^0 + i\eta} + \frac{\Theta(k_F - k)}{\sigma - \omega_{\mathbf{k}}^0 - i\eta} \right\}.$$

Choice of the **one-particle eigenbasis**:

$$\hat{h}|i\rangle = \hbar\omega_i^0|i\rangle \quad \rightarrow \quad \left[ -\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r}) \right] \psi_{\mathbf{k}}(\mathbf{r}) = \hbar\omega_{\mathbf{k}}^0 \psi_{\mathbf{k}}(\mathbf{r})$$

with  $v(\mathbf{r})$  as a **local, external potential energy** that acts on the electron.

**The special choice:**

**homogeneous electron gas (jellium)**  $\rightarrow v(\mathbf{r}) \equiv 0$ :

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{with} \quad \omega_{\mathbf{k}}^0 = \frac{\hbar k^2}{2m}$$

leads to the **non-interacting Green's function**

$$G_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') = \frac{\delta_{\alpha\beta}}{\Omega} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \left\{ \frac{\Theta(k - k_F)}{\omega - \omega_{\mathbf{k}}^0 + i\eta} + \frac{\Theta(k_F - k)}{\omega - \omega_{\mathbf{k}}^0 - i\eta} \right\}.$$

Obviously, this result is

- **diagonal in spin space** (because of  $\delta_{\alpha,\beta}$ )
- **homogeneous in space and time:**

$$G_{\alpha\beta}^0(\mathbf{r}t; \mathbf{r}'t') = \delta_{\alpha\beta} G^0(\mathbf{r} - \mathbf{r}'; t - t').$$

An enormous advantage of this homogeneity is that one can easily change from the  $\{\mathbf{r}; t\}$  space to the  $\{\mathbf{k}; \omega\}$  space by applying the **Fourier transform**

$$G_{\alpha\beta}^0(\mathbf{r} - \mathbf{r}'; t - t') = \frac{1}{\Omega} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G_{\alpha\beta}^0(\mathbf{k}, \omega)$$

with

$$G_{\alpha\beta}^0(\mathbf{k}, \omega) = \delta_{\alpha\beta} G^0(\mathbf{k}, \omega)$$

and

$$G^0(\mathbf{k}, \omega) = \frac{\Theta(k - k_F)}{\omega - \omega_{\mathbf{k}}^0 + i\eta} + \frac{\Theta(k_F - k)}{\omega - \omega_{\mathbf{k}}^0 - i\eta}.$$