Summary Sec. 1.4: The concept of quasiparticles

<u>From Sec. 1.2.1</u>: Remember the Fourier coefficient of the non-interacting Green's function:

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

Starting from this, one can prove the following statement: The singularities of $G(\mathbf{k}, \omega)$ determine the energies and the decay rates (= lifetimes) of the corresponding electron states.

In case of $G^0(\mathbf{k}, \omega)$, one gets

$$\left[G^{0}(\mathbf{k},\omega)\right]^{-1} = \omega - \omega_{\mathbf{k}}^{0} + i\eta \quad \operatorname{sign}(k-k_{F}) = 0.$$

Here, the limitation $\eta \to 0$ is trivial, and one obtains

$$\omega = \omega_{\mathbf{k}}^0 \quad \to \quad \hbar\omega = \epsilon_{\mathbf{k}}^0 = \frac{\hbar^2 k^2}{2m}$$

 $[G^0(\mathbf{k},\omega)]^{-1}$ leads to the $\epsilon(\mathbf{k})$ dispersion of a free particle.

In case of an interacting electron, the Green's function looks like

$$G(\mathbf{k},\omega) = \frac{1}{\left[G^0(\mathbf{k},\omega)\right]^{-1} - \Sigma^{pr}(\mathbf{k},\omega)},$$

giving the singularity condition

$$\left[G^{0}(\mathbf{k},\omega)\right]^{-1} - \Sigma^{pr}(\mathbf{k},\omega) \stackrel{!}{=} 0 \quad \rightarrow \quad \omega - \omega_{\mathbf{k}}^{0} - \Sigma^{pr}(\mathbf{k},\omega) \stackrel{!}{=} 0.$$

Taking into account that the solutions of the above equation will generally lie on the complex ω plane ($\omega = \nu - i\gamma$), one obtains

$$\nu - i\gamma - \omega_{\mathbf{k}}^0 - \Sigma^{pr}(\mathbf{k}, \omega = \nu - i\gamma) \stackrel{!}{=} 0.$$

"Experience teaches us" that - in most cases - the zeros lie close to the real ω axis, i.e.

$$|\gamma| << |\nu|,$$

and the selfenergy function can be linearly Taylor-expanded:

$$\nu - i\gamma - \omega_{\mathbf{k}}^{0} - \Sigma^{pr}(\mathbf{k},\nu) + i\frac{\partial\Sigma^{pr}}{\partial\omega}|_{\nu}\gamma = 0$$

With $\Sigma = \Re \Sigma + i \Im \Sigma$, one gets

$$\nu - i\gamma - \omega_{\mathbf{k}}^{0} - \Sigma^{pr}(\mathbf{k}, \nu) + \frac{\partial \Sigma^{pr}}{\partial \omega}|_{\nu} i\gamma = 0,$$

and a separation of this equation in its real and imaginary part yields

$$\nu - \omega_{\mathbf{k}}^{0} - \Re \Sigma^{pr}(\mathbf{k}, \nu) - \frac{\partial \Im \Sigma^{pr}}{\partial \omega} |_{\nu} \gamma \stackrel{!}{=} 0$$

and

$$\gamma + \Im \Sigma^{pr}(\mathbf{k}, \nu) - \frac{\partial \Re \Sigma^{pr}}{\partial \omega}|_{\nu} \gamma \stackrel{!}{=} 0.$$

Taking into account only the leading terms (written in red), one obtains the following important results:

• The real part of the proper selfenergy function Σ^{pr} describes the $\epsilon(\mathbf{k})$ dispersion of an interacting electron (the energy states of quasiparticles):

$$\epsilon_{\mathbf{k}} = \hbar \nu_{\mathbf{k}} = \frac{\hbar^2}{2m} k^2 + \hbar \Re \Sigma^{pr}(\mathbf{k}, \nu_{\mathbf{k}}) \approx \frac{\hbar^2}{2m} k^2 + \hbar \Re \Sigma^{pr}(\mathbf{k}, \frac{\hbar k^2}{2m}) \,.$$

Generally, this equation can only be solved iteratively. However, in many cases, it might be sufficient to perform only the first iteration step.

• The (negative of the) imaginary part of the proper selfenergy function Σ^{pr} describes the decay constant (= the inverse lifetime) of the corresponding quasiparticle state:

$$\gamma_{\mathbf{k}} = \frac{1}{\tau_{\mathbf{k}}} = -\Im \Sigma^{pr}(\mathbf{k}, \nu_{\mathbf{k}}).$$

The quasiparticle condition:

According to Heisenberg's uncertainty condition, the finite lifetime τ of a particle causes an uncertainty of its energy $\Delta \epsilon$ such that

$$\tau \Delta \epsilon \geq \hbar$$

Therefore, for a precise measurement of the energy difference between the excited electron state and the Fermi energy $\epsilon_{\mathbf{k}} - \epsilon_F$, the condition

$$\Delta \epsilon \ll \epsilon_{\mathbf{k}} - \epsilon_F$$

must be fulfilled.

Combining the last two equations, one gets the quasiparticle condition

$$\frac{\hbar}{\tau_{\mathbf{k}}} << \left|\epsilon_{\mathbf{k}} - \epsilon_{F}\right|.$$

A discussion of the simplest selfenergy function:

A numerical evaluation of the "simplest" approximation of the selfenergy function [Eq. (1.37) in my lecture notes]

$$\hbar\Sigma^{pr(c)}(k) = \frac{i}{(2\pi)^4} \int d^4q \, V(\mathbf{q}) \, \mathrm{e}^{i(\omega-\omega_1)\eta} \, G^0(k-q)$$

leads to the result (see appendix 2):

$$\Sigma^{pr(c)}\left(\mathbf{k},\omega\right) = -\frac{e^2}{2\pi^2\hbar} \int_{|\mathbf{k}'| \le k_{\rm F}} \frac{d^3k'}{|\mathbf{k} - \mathbf{k}'|^2}$$

The calculation of this integral is elementary and one gets

$$\Sigma^{pr(c)}(\mathbf{k},\omega) = \Sigma^{pr(c)}(\mathbf{k}) = -\frac{e^2 k_{\rm F}}{2\pi\hbar} \left[2 + \frac{k_{\rm F}^2 - k^2}{kk_{\rm F}} \ln \left| \frac{k_{\rm F} + k}{k_{\rm F} - k} \right| \right] \,.$$

This approximation of the selfenergy is obviously real and not dependent on ω .

The consequences:

• The $\epsilon^{(c)}(\mathbf{k})$ dispersion reads precisely

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_{\rm F}}{2\pi} \left[2 + \frac{k_{\rm F}^2 - k^2}{k k_{\rm F}} \ln \left| \frac{k_{\rm F} + k}{k_{\rm F} - k} \right| \right] \,,$$

and we learn "from earlier lectures" (...) that this result is exactly the energy dispersion of electrons including the Fock or exchange term.

• The lifetime of these "quasiparticle states" is infinite:

$$\tau_{\mathbf{k}} = \infty$$
.

The deviation of the energy function from the free-electron parabola is due to exchange interactions inside the Fermi sphere. In fact, no electrons are scattered out, and no quasiparticles outside and holes inside the Fermi sphere with finite lifetimes are created.

The calculation of the electronic selfenergy by means of Feynman diagrams of <u>first order</u> with respect to the Coulomb potential is equivalent to the (Hartree-)Fock ansatz.

Especially, for the homogeneous electron gas, one has



and

$$\iint_{HF} = 1 + \frac{1}{1} = 1 + \frac{1}{1} + \frac{1}{1} + \cdots$$

(1)

Is this the most complete Hartree-Fock representation a la Feynman? A more careful investigation, especially in connection with inhomogeneous electron gases, shows that a more realistic diagrammatic solution of the Hartree-Fock gas looks like

(In fact, you will easily find the last graph above in the list of diagrams given on page 12 of my lecture notes.)

Obviously, the HF proper selfenergy insertion is enlarged as shown in the following:

$$\Sigma^{\mathsf{pr}(\mathsf{HF})} = \left\{ \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \end{array} \right\} = \left\{ \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \end{array} \right\} + \left\{ \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \end{array} \right\} + \cdots$$

$$(2)$$

The problem is now: is the solution (2) better than the "old" solution (1)?

This is hard to believe because - as it already has been shown the solution (1) leads exactly to the correct Hartree-Fock energy dispersion of the homogeneous electron gas.

The problem's solution: For jellium - and only for jellium, the additional terms of the selfenergy (2) do not contribute, and one has

$$\begin{pmatrix} (H_F) \\ \uparrow \\ \end{pmatrix} = \begin{pmatrix} \uparrow \\ + \end{pmatrix} + \begin{pmatrix} \uparrow \\ \uparrow \\ \downarrow \\ \downarrow \end{pmatrix} = \begin{pmatrix} \uparrow \\ + \end{pmatrix} + \begin{pmatrix} \uparrow \\ \uparrow \\ \uparrow \\ \downarrow \end{pmatrix}$$

