4.) Perturbation theory and Feynman diagrams:

Explicit calculation of Green's functions: „Easy" for noninteracting systems!

For instance: $H_0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma}$, $\vec{k} \in BZ$ (Brillouinzone) ... lattice momentum
fermions $\quad \varepsilon_{\vec{k}}$ ... dispersion relation (see exercises)

$$\Rightarrow \tilde{G}^{M}_{\vec{k}}(i\nu_m) = \frac{1}{i\nu_m + \mu - \varepsilon_{\vec{k}}} \qquad \tilde{G}^{R}_{\vec{k}}(\omega) = \frac{1}{\omega + \mu - \varepsilon_{\vec{k}} + i\delta} \qquad \tilde{G}^{A}_{\vec{k}}(\omega) = \frac{1}{\omega + \mu - \varepsilon_{\vec{k}} - i\delta}$$

$$\hookrightarrow A_{\vec{k}}(\omega) = -\frac{1}{\pi} \mathrm{Im}\, \tilde{G}^{R}_{\vec{k}}(\omega) = \delta(\omega + \mu - \varepsilon_{\vec{k}}) \qquad (1)$$

$$\Rightarrow G^{(2),M}_{\vec{k}(\vec{k}+\vec{q})(\vec{k}'+\vec{q})}(i\nu, i\nu', i\Omega) = \beta\, \tilde{G}^{M}_{\vec{k}}(i\nu)\, \tilde{G}^{M}_{\vec{k}'}(i\nu')\, \delta^{(3)}(\vec{q})\, \delta_{\Omega 0} - \beta\, \tilde{G}^{M}_{\vec{k}}(i\nu)\, \tilde{G}^{M}_{\vec{k}+\vec{q}}\, \delta^{(3)}(\vec{k}-\vec{k}')\, \delta_{\nu\nu'} \qquad (2)$$

(see exercises)

How can we perform the calculations for an interacting system?

For instance: $H_I = \frac{1}{2} \sum_{\sigma\sigma'} \sum_{\vec{k}\vec{k}'\vec{q}} U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'}\, c^{\dagger}_{\vec{k}\sigma}\, c_{(\vec{k}+\vec{q})\sigma}\, c^{\dagger}_{(\vec{k}'+\vec{q})\sigma'}\, c_{\vec{k}'\sigma'}$ (in momentum representation) (3)

Coulomb interaction: $U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'} = \frac{e^2}{\varepsilon_0} \frac{1}{\vec{q}^2}$ $\quad$ Hubbard model: $U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'} = U \delta_{\sigma(-\sigma')}$

The Hamiltonian can be now written as: $H = H_0 + H_I$ (4)

⇒ Standard Ansatz to treat such problem: Perturbation Theory!

Basic idea: „Separate" H_0 and H_I in the formalism!

⇒ In our equations, H appears in the form $e^{\alpha H}$, where $\alpha = \pm\tau, \pm it$ or $-\beta$:
(Here, we will focus on perturbation theory for Matsubara Green's functions, i.e., $\alpha = \pm\tau$ or $-\beta$)

<u>Ansatz:</u> $$\boxed{e^{-(\tau-\tau')H} = e^{-\tau H_0}\, U(\tau,\tau')\, e^{\tau' H_0} \quad \text{with } \tau > \tau' \qquad (5)}$$

<u>Note:</u> $U(\tau,\tau') \neq e^{-(\tau-\tau')H_I}$ when $[H_0, H_I] \neq 0$ (which is usully the case for correlated systems)

How can we determine $U(\tau,\tau') = e^{\tau H_0} e^{-(\tau-\tau')H} e^{-\tau' H_0}$?

⇒ <u>Idea:</u> Construct a differential equation for $U(\tau,\tau')$!

$$U(\tau,\tau') = e^{\tau H_0} e^{-(\tau-\tau')H} e^{-\tau' H_0} \Rightarrow \frac{d}{d\tau} U(\tau,\tau') = e^{\tau H_0} H_0 e^{-(\tau-\tau')H} e^{-\tau' H_0} - e^{\tau H_0} \overset{H_0+H_I}{\overset{\Uparrow}{H}} e^{-(\tau-\tau')H} e^{-\tau' H_0} \quad (6)$$

$$\Rightarrow \frac{d}{d\tau} U(\tau,\tau') = \cancel{e^{\tau H_0} H_0 e^{-(\tau-\tau')H} e^{-\tau' H_0}} - \cancel{e^{\tau H_0} H_0 e^{-(\tau-\tau')H} e^{-\tau' H_0}} - e^{\tau H_0} H_I e^{-(\tau-\tau')H} e^{-\tau' H_0}$$

$$= -\underbrace{e^{\tau H_0} H_I \overbrace{e^{-\tau H_0}}^{\mathbb{I}}}_{H_I(\tau)} \underbrace{\overbrace{e^{\tau H_0}}^{} e^{-(\tau-\tau')H} e^{-\tau' H_0}}_{U(\tau,\tau')} = -H_I(\tau)\, U(\tau,\tau') \quad (7)$$

$$\Rightarrow \boxed{\frac{d}{d\tau} U(\tau,\tau') = -H_I(\tau)\, U(\tau,\tau'),\quad U(\tau',\tau') = \mathbb{I},\quad H_I(\tau) = e^{\tau H_0} H_I e^{-\tau H_0} \quad (8)}$$

→ Eq. (8) is a first order linear autonomous differential equation for $U(\tau,\tau')$ with the initial condition $U(\tau',\tau') = \mathbb{I}$, which has a unique solution.

→ $H_I(t)$ is the interaction Hamiltonian in the interaction representation where the time evolution of the operators is determined by the noninteracting part of the Hamiltonian H_0 (instead of the full Hamiltonian as in the Heisenberg picture).

→ Most important question: How can we solve Eq. (8)?

⇒ Transform differential to an *integral* equation:

$$\frac{d}{d\tau_1} U(\tau_1,\tau') = -H_I(\tau_1)\, U(\tau_1,\tau') \Big/ \int_{\tau'}^{\tau} d\tau_1 \Rightarrow U(\tau,\tau') - \underbrace{U(\tau',\tau')}_{\mathbb{1}} = -\int_{\tau'}^{\tau} d\tau_1\, H_I(\tau_1)\, U(\tau_1,\tau')$$

$$\Rightarrow \boxed{U(\tau,\tau') = \mathbb{1} - \int_{\tau'}^{\tau} d\tau_1\, H_I(\tau_1)\, U(\tau_1,\tau') \quad (10)}$$

integral equation includes already $U(\tau',\tau') = \mathbb{1}$!

This integral equation can be now solved in an *iterative* way by reinserting the equation (10) for $U(\tau,\tau')$ into $U(\tau_1,\tau')$ on the right hand side of this equation:

$$U(\tau,\tau') = \mathbb{1} - \int_{\tau'}^{\tau} d\tau_1\, H_I(\tau_1) \left[\mathbb{1} - \int_{\tau'}^{\tau_1} d\tau_2\, H_I(\tau_2)\, \overbrace{U(\tau_2,\tau')}^{\mathbb{1} - \int_{\tau'}^{\tau_2} d\tau_3\, H_I(\tau_3)\, U(\tau_3,\tau')}\right] =$$

$$= \mathbb{1} - \int_{\tau'}^{\tau} d\tau_1\, H_I(\tau_1) + \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau_1} d\tau_2\, H_I(\tau_1)\, H_I(\tau_2)\, U(\tau_2,\tau') = \ldots =$$

$$= \mathbb{1} + \sum_{n=1}^{\infty} (-1)^n \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau_1} d\tau_2 \ldots \int_{\tau'}^{\tau_{n-1}} d\tau_n\, H_I(\tau_1)\, H_I(\tau_2) \ldots H_I(\tau_n) \quad (11)$$

For $[H_0, H_I] = 0$: $H_I(\tau) = e^{\tau H_0} H_I\, e^{-\tau H_0} = H_I \Rightarrow U(\tau,\tau') = \sum_{n=0}^{\infty} (-1)^n (H_I)^n \underbrace{\int_{\tau'}^{\tau} d\tau_1 \ldots \int_{\tau'}^{\tau_{n-1}} d\tau_n}_{\frac{(\tau-\tau')^n}{n!}}$

$$\Rightarrow U(\tau,\tau') = \sum_{n=0}^{\infty} (-1)^n (H_I)^n (\tau-\tau')^n \frac{1}{n!} = e^{-(\tau-\tau') H_I}$$

But in general: $[H_0, H_I] \neq 0 \Leftrightarrow [H_I(\tau_1), H_I(\tau_2)] \neq 0$

To simplify Eq. (11), we would like to extend all upper integration limits to τ:
⇒ This, however, would lead to terms $H_I(\tau_1) \ldots H_I(\tau_n)$ where the time order $\tau_1 > \tau_2 > \ldots > \tau_n$ is violated, which is otherwise enforced by the integral limits.
⇒ The correct time order can be restored by introducing the time order operator $T_\tau(H_I(\tau_1) \ldots H_I(\tau_n))$ which then allows to extend all integral limits to τ!
⇒ Due to the time order operator, each order of the times $\tau_1, \ldots, \tau_n$ gives the same contribution leading to an additional factor $n!$, which has to be compensated.

$$\boxed{\begin{aligned} U(\tau, \tau') &= \mathbb{1} + \sum_{n=1}^{\infty} (-1)^n \frac{1}{n!} \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2 \ldots \int_{\tau'}^{\tau} d\tau_n \, T_\tau\left(H_I(\tau_1) \ldots H_I(\tau_n)\right) \\ &= T_\tau \, e^{-\int_{\tau'}^{\tau} d\bar{\tau} \, H_I(\bar{\tau})}, \quad \tau > \tau', \quad H_I(\tau) = e^{\tau H_0} H_I e^{-\tau H_0} \qquad (12) \end{aligned}}$$

The time order operator T_τ has allowed us to formally rewrite $U(\tau, \tau')$ in terms of an exponential function!

We can now express the Matsubara Green's function $G^M_{ij}(\tau)$ in the following way:

$$G^M_{ij}(\tau>0) = -\frac{1}{Z}\,\mathrm{Tr}\left(e^{-(\beta-\tau)H} c_i e^{-\tau H} c_j^+\right) \overset{\text{Eq.(5)}}{=} -\frac{1}{Z}\,\mathrm{Tr}\Big(e^{-\beta H_0}\, U(\beta,\tau) \underbrace{e^{\tau H_0} c_i e^{-\tau H_0}}_{c_i^0(\tau)} U(\tau,0)\, c_j^+\Big) \quad (13)$$

(for $\tau \geq 0$)

$$\text{Eq.(12)} \rightarrow = -\frac{1}{Z}\sum_{\ell=0}^{\infty}\sum_{m=0}^{\infty}(-1)^{\ell+m}\frac{1}{\ell!}\frac{1}{m!}\int_\tau^\beta d\tau_1 \dots d\tau_\ell \int_0^\tau d\tau_{\ell+1}\dots d\tau_{\ell+m}\,\mathrm{Tr}\Big(e^{-\beta H_0} T_\tau\big(H_I(\tau_1)\dots c_i^0(\tau)\dots H_I(\tau_{\ell+m})\big)\Big) \quad (14)$$

$\Rightarrow$ $c_i^0(\tau) = e^{\tau H_0} c_i e^{-\tau H_0}$ (15) ... Time evolution with the **noninteracting** Hamiltonian
(i.e., time evolution in the interaction picture)

$\Rightarrow$ We can now reorganize the sums over ℓ and m in the following way:

$$\boxed{\ell = N-m}: \quad \sum_{\ell=0}^{\infty}\sum_{m=0}^{\infty} = \sum_{m=0}^{\infty}\sum_{N=m}^{\infty} = \sum_{N=0}^{\infty}\sum_{m=0}^{N} \quad (16)$$

$$\Rightarrow -\frac{1}{Z}\sum_{N=0}^{\infty}(-1)^N\sum_{m=0}^{N}\frac{1}{m!}\frac{1}{(N-m)!}\int_\tau^\beta d\tau_1\dots\int_0^\tau d\tau_{N-m+1}\dots\int_0^\tau d\tau_N\,\mathrm{Tr}\Big(e^{-\beta H_0} T_\tau\big(H_I(\tau_1)\dots c_i^0(\tau)\dots H_I(\tau_N)\big)\Big) \quad (17)$$

Note: For a fixed N, there are always N $H_I(\tau_i)$ operators in the trace, independent of the number m, which indicates the fraction of H_I's with $\tau_i \leq \tau$!

Let us now extend one of the integrals $\int_0^\tau d\tau_i$ to the full interval $(0,\beta)$:

$\int_0^\beta d\tau_i = \int_0^\tau d\tau_i + \int_\tau^\beta d\tau_i$: Due to the time ordering operator T_τ, the corresponding $H(\tau_i)$ are moved in front of $c_i^0(\tau)$ in the $\int_\tau^\beta d\tau_i$ integral!

⇒ The resulting term is then equal to the contribution for $m-1$ in the $\sum_{m=0}^{N}$. → The same is true for $\int_\tau^\beta \to \int_0^\beta$

⇒ extending $\int_0^\tau d\tau_i \to \int_0^\beta d\tau_i$ yields just an additional factor 2!

⇒ When we extend all N integrals to the interval $(0,\beta)$, we have an additional factor 2^N!

$$G_{ij}^M(\tau) = -\frac{1}{Z}\sum_{N=0}^{\infty}(-1)^N \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_N \, \mathrm{Tr}\left(e^{-\beta H_0} T_\tau\left[H_I(\tau_1)\ldots H_I(\tau_N)\, c_i^0(\tau) c_j^{+}\right]\right) \frac{1}{2^N} \underbrace{\sum_{m=0}^{N}\frac{1}{m!}\frac{1}{(N-m)!}}_{\frac{2^N}{N!}}$$

$$= -\frac{1}{Z}\sum_{N=0}^{\infty}(-1)^N \frac{1}{N!}\int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_N \, \mathrm{Tr}\left(e^{-\beta H_0} T_\tau\left[H_I(\tau_1)\ldots H_I(\tau_N)\, c_i^0(\tau) c_j^{+}\right]\right)$$

$$= -\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H_0} T_\tau\left[U(\beta,0)\, c_i(\tau) c_j^{+}\right]\right) \qquad (18)$$

Note: The simple form of Eq. (18) could be only achieved, since the „original" operators in $G^M_{ij}(\tau)$, $c_i(\tau)$ and c_j^+, where already time-ordered. In fact, a compact form of perturbation theory can be constructed ONLY for the time ordered Green's functions $G^c_{ij}(t)$ and $G^M_{ij}(\tau)$, but NOT for $G^R_{ij}(t)$ and $G^A_{ij}(t)$, due to the time ordered form of $U(\tau,\tau')$!

To further improve Eq. (18), we consider the noninteracting expectation values:

$$\boxed{\langle \ldots \rangle_0 = \frac{1}{Z_0}\,\mathrm{Tr}\left(e^{-\beta H_0}\ldots\right), \quad Z_0 = \mathrm{Tr}\left(e^{-\beta H_0}\right) \qquad (19)}$$

- $Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \mathrm{Tr}\left(e^{-\beta H_0}\,U(\beta,0)\right) = Z_0 \cdot \langle U(\beta,0)\rangle_0$
- $G^M_{ij}(\tau) = \frac{-1}{\langle T_\tau U(\beta,0)\rangle_0}\,\frac{1}{Z_0}\,\mathrm{Tr}\left(e^{-\beta H_0}\,T_\tau\left[U(\beta,0)\,c_i^0(\tau)\,c_j^+\right]\right)$

$$\Rightarrow \boxed{G^M_{ij}(\tau) = \frac{\langle T_\tau\left(U(\beta,0)\,c_i^0(\tau)\,c_j^+\right)\rangle_0}{\langle T_\tau U(\beta,0)\rangle_0}, \quad c_i^0(\tau) = e^{\tau H_0}\,c_i\,e^{-\tau H_0} \qquad (20)}$$

Eq. (20) can be, in principle, evaluated for any single particle basis i, however, it is most convenient to use a basis in which H_0 is diagonal, which is typically the (lattice) momentum-spin basis, i.e.: $i \hat{=} (\vec{k}, \sigma)$, for (lattice) translational invarian systems:

- $H_0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}$ (21), with $\sum_{\vec{k}} = \frac{1}{(2\pi)^3} \int d^3k$ for free electrons and $\sum_{\vec{k}} = \frac{1}{V_{BZ}} \int_{BZ} d^3k$ for lattice electrons in a periodic potential. (1st Brillouin zone)

The free time evolution of $c^{(+)}_{\vec{k}\sigma}$ becomes particularly simple: $\boxed{c^{(+),0}_{\vec{k}\sigma}(\tau) = e^{\pm\varepsilon_{\vec{k}}\tau} c^{(+)}_{\vec{k}\sigma} \text{ (22)}}$

(To see this, consider $\frac{d}{d\tau} c^{(+),0}_{\vec{k}\sigma}(\tau) = \underbrace{[H_0, c^{(+)}_{\vec{k}\sigma}]}_{\mathrm{II}} = \pm \varepsilon_{\vec{k}} c^{(+),0}_{\vec{k}\sigma}(\tau)$, see Eqs. (28)-(33))

- $H_I(\tau) = \frac{1}{2} \sum_{\vec{k}\vec{k}'\vec{q}} U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'} \underbrace{e^{\tau H_0} c^+_{\vec{k}\sigma} e^{-\tau H_0}}_{c^{+,0}_{\vec{k}\sigma}(\tau) = e^{\varepsilon_{\vec{k}}\tau} c^+_{\vec{k}\sigma}} \overbrace{e^{\tau H_0} c_{(\vec{k}+\vec{q})\sigma} e^{-\tau H_0}} e^{\tau H_0} c^+_{(\vec{k}'+\vec{q})\sigma'} e^{-\tau H_0} e^{\tau H_0} c_{\vec{k}'\sigma'} e^{-\tau H_0}$ (23)

[see Eqs. (3), (8)]

$$\Rightarrow \boxed{H_I(\tau) = \frac{1}{2} \sum_{\vec{k}\vec{k}'\vec{q}} U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'} c^{+,0}_{\vec{k}\sigma}(\tau)\, c^{0}_{(\vec{k}+\vec{q})\sigma}(\tau)\, c^{+,0}_{(\vec{k}'+\vec{q})\sigma'}(\tau)\, c^{0}_{\vec{k}'\sigma'}(\tau) \quad (24)}$$

Next, we evaluate the expression for $G^{M}_{ij}(\tau)$ in Eq. (20) for $i = j \hat{=} (\vec{k},\sigma)$:

$$G^{M}_{\vec{k}\sigma}(\tau) = \frac{1}{\langle U(\beta,0)\rangle_0} \langle T_\tau [U(\beta,0)\, c^{0}_{\vec{k}\sigma}(\tau)\, c^{+}_{\vec{k}\sigma}]\rangle_0 \quad (25)$$

($G^{M}_{\vec{k}\sigma}(\tau)$ is diagonal in momentum space!)

↳ for $SU(2)$ symmetry $G_{\vec{k}\sigma} = G_{\vec{k}}$!

Let us first concentrate on the numerator and discuss the denominator later:

$$\langle T_\tau [U(\beta,0)\, c^{0}_{\vec{k}\sigma}(\tau)\, c^{+}_{\vec{k}\sigma}]\rangle_0 = \sum_{N=0}^{\infty} (-1)^N \frac{1}{N!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_N \, \frac{1}{2}\sum_{\vec{k}_1 \vec{k}_1' \vec{q}_1} \sum_{\sigma_1 \sigma_1'} \ldots \frac{1}{2}\sum_{\vec{k}_N \vec{k}_N' \vec{q}_N} \sum_{\sigma_N \sigma_N'}$$

$$\times\, U^{\vec{k}_1 \vec{k}_1' \vec{q}_1}_{\sigma_1 \sigma_1'} \cdot \ldots \cdot U^{\vec{k}_N \vec{k}_N' \vec{q}_N}_{\sigma_N \sigma_N'} \underbrace{\langle T_\tau [c^{+,0}_{\vec{k}_1 \sigma_1}(\tau_1)\, c^{0}_{(\vec{k}_1+\vec{q}_1)\sigma_1}(\tau_1)\, c^{+,0}_{(\vec{k}_1'+\vec{q}_1)\sigma_1'}(\tau_1)\, c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1) \cdots c^{0}_{\vec{k}\sigma}(\tau)\, c^{+}_{\vec{k}j}]\rangle_0} \quad (26)$$

The N^{th} term in this sum is proportional to U^N and contains all contributions from N^{th} order perturbation theory to $G^{M}_{\vec{k}}(\tau)$!

The matrix element $\langle T_\tau [\ldots]\rangle$ corresponds to a noninteracting $(2N+1)$ particle Green's function $G_0^{M,(2N+1)}$. As for the two-particle case (see exercise 3), this corresponds to all possible products of $(2N+1)$ noninteracting one-particle Green's functions which arise from all possible contraction of c^+'s and c's in the trace. This procedure can be formalized by means of the following theorem:

Wick's theorem (for finite temperatures):

We consider a generic matrix element with n creation and n annihilation operators:

$$\langle T_\tau \left(c^{+,0}_{k_1\sigma_1}(\tau_1) \ldots c^{+,0}_{\vec{k}_n\sigma_n}(\tau_n)\, c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1') \ldots c^{0}_{\vec{k}_n'\sigma_n'}(\tau_n') \right)\rangle_0 \quad (27)$$

(1) Time evolution $\quad c^{(+),0}_{\vec{k}\sigma}(\tau) = e^{\tau H_0}\, c^{(+)}_{\vec{k}\sigma}\, e^{-\tau H_0} \Leftrightarrow \frac{d}{d\tau} c^{(+),0}_{\vec{k}\sigma}(\tau) = [H, c^{(+)}_{\vec{k}\sigma}](\tau)$ (28)

$$H_0 = \sum_{\vec{k}'\sigma'} \varepsilon_{\vec{k}'}\, c^{+}_{\vec{k}'\sigma'} c_{\vec{k}'\sigma'} \Rightarrow [\underset{0}{H}, c^{(+)}_{\vec{k}\sigma}] = \sum_{\vec{k}'\sigma'} \varepsilon_{\vec{k}'} [c^{+}_{\vec{k}'\sigma'} c_{\vec{k}'\sigma'}, c^{(+)}_{\vec{k}\sigma}] \quad (29)$$

- $[c^{+}_{\vec{k}'\sigma'} c_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}] = c^{+}_{\vec{k}'\sigma'} \underbrace{\{c_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}\}}_{0} - \{c^{+}_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}\} c_{\vec{k}'\sigma'} = -\delta^{(3)}(\vec{k}-\vec{k}')\,\delta_{\sigma\sigma'}\, c_{\vec{k}\sigma}$ (30)
- $[c^{+}_{\vec{k}'\sigma'} c_{\vec{k}'\sigma'}, c^{+}_{\vec{k}\sigma}] = \ldots = \delta^{(3)}(\vec{k}-\vec{k}')\,\delta_{\sigma\sigma'}\, c^{+}_{\vec{k}\sigma}$ (31)

$\Rightarrow \frac{d}{d\tau} c^{0}_{\vec{k}\sigma}(\tau) = -\varepsilon_{\vec{k}}\, c^{0}_{\vec{k}\sigma}(\tau) \Leftrightarrow \boxed{c^{0}_{\vec{k}\sigma}(\tau) = e^{-\tau\varepsilon_{\vec{k}}}\, c^{0}_{\vec{k}\sigma}} \quad (32)$

$\Rightarrow \frac{d}{d\tau} c^{+,0}_{\vec{k}\sigma}(\tau) = \varepsilon_{\vec{k}}\, c^{+,0}_{\vec{k}\sigma}(\tau) \Leftrightarrow \boxed{c^{+,0}_{\vec{k}\sigma}(\tau) = e^{\tau\varepsilon_{\vec{k}}}\, c^{+,0}_{\vec{k}\sigma}} \quad (33)$

$$\Rightarrow \quad \langle T_\tau (c^{+,0}_{\vec{k}_1\sigma_1}(\tau_1) \ldots c^0_{\vec{k}'_n\sigma'_n}(\tau'_n)) \rangle_0 = e^{\tau_1 \varepsilon_{\vec{k}_1}} \ldots e^{\tau_n \varepsilon_{\vec{k}_n}} e^{-\tau'_1 \varepsilon_{\vec{k}'_1}} \ldots e^{-\tau'_n \varepsilon_{\vec{k}'_n}} \tag{34}$$
$$\times \langle T_\tau (\underbrace{c^+_{\vec{k}_1\sigma_1} \ldots c_{\vec{k}'_n\sigma'_n}}_{\text{time independent!}}) \rangle_0$$

(In the second line, the time order operator sets the order of the now time independent creation and annihilation operators according to the order of their previous time arguments).

(2) Matrix element: $\langle T_\tau (c^+_{\vec{k}_1\sigma_1} \ldots c_{\vec{k}'_n\sigma'_n}) \rangle_0$

Let us first assume, that all momenta or spins of the creation operators are different from the corresponding momenta or spins of the anihilation operat.

$$(\vec{k}_i, \sigma_i) \neq (\vec{k}'_j, \sigma'_j) \quad \forall i, j = 1 \ldots n \tag{35}$$

$\Rightarrow$ All operators in the Trace anticommute with each other $\left(\{ c^{(+)(0)}_{\vec{k}_i\sigma_i}, c^{(+)(0)}_{\vec{k}'_j\sigma'_j} \} = 0 \right)$

$\Rightarrow$ We can rearrange all possible time orders in the form $\langle c^+_{\vec{k}_1\sigma_1} \ldots c_{\vec{k}'_n\sigma'_n} \rangle_0$ where for odd time orders an additional minus sign occurs!

$$\Rightarrow \underbrace{\langle c^+_{\vec{k}_1\sigma_1} \dots c_{\vec{k}'_n\sigma'_n}\rangle_0} = \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H_0} c^+_{\vec{k}_1\sigma_1} \dots c_{\vec{k}'_n\sigma_n}\right) = \left| \begin{array}{l} \text{bring } c^+_{\vec{k}_1\sigma_1} \text{ to the} \\ \text{end} \to 2n-1 \text{ exchanges} \\ \to (-1)^{2n-1} = -1 \end{array} \right|$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H_0} c^+_{\vec{k}_2\sigma_2} \dots c_{\vec{k}'_n\sigma_n} c^+_{\vec{k}_1\sigma_1}\right) = -\frac{1}{Z}\,\mathrm{Tr}\left(c^+_{\vec{k}_1\sigma_1} e^{-\beta H_0} c^+_{\vec{k}_2\sigma_2} \dots c_{\vec{k}'_n\sigma'_n}\right) \quad (36)$$

↳ cyclicity of Tr!

Now, we use again the equation of motion for $c^{+,0}_{\vec{k}_1\sigma_1}(\tau)$:

$$c^{+,0}_{\vec{k}_1\sigma_1}(\tau) = e^{\tau H_0} c^+_{\vec{k}_1\sigma_1} e^{-\tau H_0} = e^{\tau\varepsilon_{\vec{k}_1}} c^+_{\vec{k}_1\sigma_1} \Leftrightarrow \boxed{c^+_{\vec{k}_1\sigma_1} e^{-\tau H_0} = e^{\tau\varepsilon_{\vec{k}_1}} e^{\tau H_0} c^+_{\vec{k}_1\sigma_1} \quad (37)}$$

⇒ Setting $\tau = \beta$, we can use Eq. (37) to further rewrite our Trace:

$$\Rightarrow \langle c^+_{\vec{k}_1\sigma_1} \dots c_{\vec{k}'_n\sigma_n}\rangle_0 = \dots = -\frac{1}{Z} e^{\tau\varepsilon_{\vec{k}_1}}\,\mathrm{Tr}\left(e^{-\beta H_0} c^+_{\vec{k}_1\sigma_1} \dots c_{\vec{k}'_n\sigma'_n}\right)$$

$$= -e^{\tau\varepsilon_{\vec{k}_1}} \langle c^+_{\vec{k}_1\sigma_1} \dots c_{\vec{k}'_n\sigma'_n}\rangle_0 \quad (38)$$

$$\Rightarrow \text{Since } -e^{\tau\varepsilon_{\vec{k}_1}} \neq 1 \Rightarrow \boxed{\langle c^+_{\vec{k}_1\sigma_1} \dots c_{\vec{k}'_n\sigma'_n}\rangle_0 = 0,\ \text{if } (\vec{k}_i,\sigma_i) \neq (\vec{k}'_j,\sigma'_j)\ \forall i,j = 1..n \quad (39)}$$

⇒ To obtain a finite value, we must have pairs of creation and annihilation operators with the same quantum numbers $(\vec{k},\sigma)$!

⇒ W.l.o.g. we assume: $\boxed{(\vec{k}_1,\sigma_1) = (\vec{k}_1',\sigma_1') = (\vec{k},\sigma) \text{ and } (\vec{k},\sigma) \neq (\vec{k}_i^{(\prime)},\sigma_i^{(\prime)}),\ i=2\dots n}$

⇒ Then, all possible time orders of the operators $c^+_{\vec{k}_1\sigma_1} \dots c^+_{\vec{k}_n'\sigma_n'}$ can be decomposed into two classes: In the first one $c_{\vec{k}\sigma}$ is left from $c^+_{\vec{k}\sigma}$, in the other it is right from $c^+_{\vec{k}\sigma}$. Since $c^{(+)}_{\vec{k}\sigma}$ anticommute with all other operators in the trace, we have to consider only the two following generic matrix elements:

$\langle c_{\vec{k}\sigma}\, c^+_{\vec{k}\sigma}\, c^+_{\vec{k}_2\sigma_2} \dots c_{\vec{k}_n'\sigma_n'}\rangle_0$ and $\langle c^+_{\vec{k}\sigma}\, c_{\vec{k}\sigma}\, c^+_{\vec{k}_2\sigma_2} \dots c_{\vec{k}_n'\sigma_n'}\rangle_0$, where the order of the operators after $c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}$ or $c_{\vec{k}\sigma} c^+_{\vec{k}\sigma}$ can be arbitrary! Note, that there is always a relative sign between the above matrix elements.

⇒ For the evaluation of these matrix elements, we apply the same technique as above:

$$\odot \quad \langle c_{\vec{k}\sigma} c^+_{\vec{k}\sigma} \ldots \rangle_0 = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H_0} c_{\vec{k}\sigma} c^+_{\vec{k}\sigma} c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \right) =$$

$$= \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H_0} c_{\vec{k}\sigma} c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} c^+_{\vec{k}\sigma} \right) =$$

$$= \frac{1}{Z} \mathrm{Tr}\left(c^+_{\vec{k}\sigma} e^{-\beta H_0} c_{\vec{k}\sigma} c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \right) =$$

$$\overset{\text{Eq. (37)}}{=} e^{\beta \varepsilon_{\vec{k}}} \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H_0} c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \right) = \left| c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} = 1 - c_{\vec{k}\sigma} c^+_{\vec{k}\sigma} \right.$$

$$= e^{\beta \varepsilon_{\vec{k}}} \langle c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \rangle_0 - e^{\beta \varepsilon_{\vec{k}}} \langle c_{\vec{k}\sigma} c^+_{\vec{k}\sigma} \ldots \rangle_0 \quad (40)$$

$$\Rightarrow \langle c_{\vec{k}\sigma} c^+_{\vec{k}\sigma} c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \rangle_0 = \frac{e^{\beta \varepsilon_k}}{1 + e^{\beta \varepsilon_k}} \langle c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \rangle_0 \quad (41)$$

in this matrix element are $2(n-1)$ operators

$$\odot \quad \langle c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \rangle_0 = \frac{e^{-\beta \varepsilon_{\vec{k}}}}{1 + e^{-\beta \varepsilon_{\vec{k}}}} \langle c^+_{\vec{k}_2\sigma_2} \ldots c_{\vec{k}_n'\sigma_n'} \rangle_0 \quad (42)$$

With the Fermi function $f(x) = \frac{1}{1+e^{\beta x}}$, we can write: $\frac{e^{\pm\beta\varepsilon_{\vec{k}}}}{1+e^{\pm\beta\varepsilon_{\vec{k}}}} = f(\mp \varepsilon_{\vec{k}})$

We can now combine this result with the time dependent terms which yields (remember, $(\vec{k}, \sigma) \triangleq (\vec{k}_1^{(1)}, \sigma_1^{(1)}) \Rightarrow$ the relevant times are τ_1, τ_1'):

$$\underbrace{\left[- e^{-(\tau_1'-\tau_1)\varepsilon_{\vec{k}_1}} f(-\varepsilon_{\vec{k}_1}) \Theta(\tau_1'-\tau_1) + e^{-(\tau_1'-\tau_1)} \cdot f(\varepsilon_{\vec{k}_1}) \Theta(\tau_1-\tau_1') \right]}_{\text{NONINTERACTING ONE-PARTICLE GF: } G^{M,0}_{\vec{k}_1}(\tau_1'-\tau_1)} \cdot \underbrace{\langle T (c^+_{\vec{k}_2\sigma_2} \dots c_{\vec{k}_n'\sigma_n'}) \rangle_0}_{\text{Same as at the beginning, but with 2 operators less}} \quad (43)$$

$\Rightarrow$ We can now iterate this procedure for the remaining matrix element, which has two operators less

$\Rightarrow$ Product of n noninteracting one-particle Green's function!

$$\boxed{\begin{aligned} \langle T (c^+_{\vec{k}_1\sigma_1}(\tau_1) \dots c^+_{\vec{k}_n\sigma_n}(\tau_n) c_{\vec{k}_1'\sigma_1'}(\tau_1') \dots c_{\vec{k}_n'\sigma_n'}(\tau_n')) \rangle_0 &= \sum_{\pi \in S_n} (-1)^{\pi} \delta_{\vec{k}_{\pi(1)}\vec{k}_1'} \dots \delta_{\vec{k}_{\pi(n)}\vec{k}_n'} \\ &\times \delta_{\sigma_{\pi(1)}\sigma_1'} \dots \delta_{\sigma_{\pi(n)}\sigma_n'} \quad G^{M,0}_{\vec{k}_1}(\tau_1'-\tau_{\pi(1)}) \cdot \dots \cdot G^{M,0}_{\vec{k}_n}(\tau_n'-\tau_{\pi(n)}) \qquad (44) \end{aligned}}$$

$\hookrightarrow$ WICK'S THEOREM

In a more pictorial way: $\langle T_\tau (c^{+,0}_{\vec{k}_1\sigma_1}(\tau_1) \dots c^{+,0}_{\vec{k}_n\sigma_n}(\tau_n) c^{0}_{\vec{k}'_1\sigma'_1}(\tau'_1) \dots c^{0}_{\vec{k}'_n\sigma'_n}(\tau'_n)) \rangle_0$ (45)

⇒ We have to consider all contractions of creation and annihilation operators, each of which gives a noninteracting one-particle Green's functions!

Let us go back to Eq. (26), i.e., the perturbation expansion for $G^M_{\vec{k}}(\tau)$:

⇒ In the N^{th} order: we have $2N$ creation and $2N$ annihilation operators from $U(\beta,0)$ and one „external" creation and annihilation operator ($c_{\vec{k}\sigma}(\tau)$ and $c^\dagger_{\vec{k}\sigma}$) from the definition of $G^M_{\vec{k}}(\tau)$.

⇒ The $2N$ „internal" creation operators come from N copies of $H_I(\tau)$; The $N!$ permutations of these N copies lead to $N!$ times the same contribution to $G^M_{\vec{k}}(\tau)$ ⇒ Cancellation of the factor $\frac{1}{N!}$ if we consider each of these expressions only once!

⇒ As an example, we consider a 2nd order term :

$$\sum_{\vec{k}_1\vec{k}_1'\vec{q}}\ \sum_{\vec{k}_2\vec{k}_2'\vec{q}}\ \sum_{\sigma_1\sigma_1'}\sum_{\sigma_2\sigma_2'} U^{\vec{k}_1\vec{k}_1'\vec{q}_1}_{\sigma_1\sigma_1'}\, U^{\vec{k}_2\vec{k}_2'\vec{q}_2}_{\sigma_2\sigma_2'} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \ \times \tag{46}$$

$$\times \left\langle T\Big(\overbrace{c^{+,0}_{\vec{k}_1\sigma_1}(\tau_1)\, c^{0}_{(\vec{k}_1+\vec{q}_1)\sigma_1}(\tau_1)\, c^{+,0}_{(\vec{k}_1'+\vec{q}_1)\sigma_1'}(\tau_1)\, c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1)}^{H_I(\tau_1)}\ \overbrace{c^{+,0}_{\vec{k}_2\sigma_2}(\tau_2)\, c^{0}_{(\vec{k}_2+\vec{q}_2)\sigma_2}(\tau_2)\, c^{+,0}_{(\vec{k}_2'+\vec{q}_2)\sigma_2'}(\tau_2)\, c^{0}_{\vec{k}_2'\sigma_2'}(\tau_2)}^{H_I(\tau_2)}\ \overbrace{c^{0}_{\vec{k}\sigma}(\tau)\, c^{+}_{\vec{k}\sigma}}^{\text{"external"}} \Big) \right\rangle_0$$

⇒ Under an exchange of the integration/summation varibles $1 \Leftrightarrow 2$ the blue contractions become equivalent to the brown contractions!

⇒ This yields a factor of 2 for this term, which cancels $\frac{1}{2!} = \frac{1}{2}$ from the definition of the perturbation series!

<u>Question</u>: What is the meaning of the denominator $\langle U(\beta,0)\rangle_0$ in Eq. (20)?

Unconnected vaccum terms:

$$\langle T_\tau \left(H_I(\tau_1)\, H_I(\tau_2)\ H_I(\tau_3)\, H_I(\tau_4)\ c^0_{\vec{k}6}(\tau)\, c^+_{\vec{k}6} \right)\rangle_0 \quad (47)$$

4x (3x)

$\Rightarrow$ The interaction operators

$\Rightarrow$ $H_I(\tau_1)$ and $H_I(\tau_2)$ are NOT connected to the real physical particles $c_{\vec{k}6}(\tau)$ and $c^+_{\vec{k}6}$ $\Rightarrow$ UNCONNECTED VACUUM CONTRIBUTIONS

$\Rightarrow$ The other factor is called CONNECTD.

$\Rightarrow$ Going to higher orders in perturbation theory, keeping the connected contribution fixed, we can generate ALL unconnected contributions.

$\Rightarrow$ The total expression for $G^M_{\vec{k}}(\tau)$ in terms of perturbation theory can be written as a product of all connected and all unconnected terms:

$$\langle T_\tau \left(U(\beta,0)\, c^0_{\vec{k}6}(\tau)\, c^+_{\vec{k}6} \right)\rangle_0 = \langle T_\tau \left(U(\beta,0)\, c^0_{\vec{k}6}(\tau)\, c^+_{\vec{k}6} \right)\rangle_0^{\text{connected}(c)} \cdot \langle T_\tau \left(U(\beta,0) \right)\rangle_0^{\text{unconnected}(u)} \quad (48)$$

⇒ Obviously, the term which is unconnected from the external $c^{0}_{\vec{k}\sigma}(\tau)$ and $c^{+}_{\vec{k}\sigma}$ is just given by the expectation value of the operator $U(\beta,0)$, which exactly cancels the denominator in Eq. (20)

⇒ In practice: If we discard all unconnected terms in our perturbation expansion, we can „neglect" the denominator in Eq. (20).

⇒ This is known as: LINKED CLUSTER THEOREM!

Fourier transform: It is usully easier to work in (Matsubara) frequency than in (imaginary) time representation!

⇒ We express all „internal" Green's function $G^{M,0}_{\vec{k}_i}(\tau_i - \tau_j')$ in Fourier space:

$$G^{M,0}_{\vec{k}_i}(\tau_i - \tau_j') = \frac{1}{\beta} \sum_{\nu_i} e^{-i\nu_i(\tau_i - \tau_j')} \tilde{G}^{M,0}_{\vec{k}_i}(i\nu_i) \quad (49)$$

⇒ We Fourier transform $G^{M}_{\vec{k}}(\tau)$ in its perturbative representation by applying $\int_0^\beta d\tau\, e^{i\nu\tau}$:

$\Rightarrow$ The N^{th}-order term corresponds to a sum of products of $2N+1$ non-interacting Green's functions. Each internal time $\tau_1 \dots \tau_N$ appears 4 times (there are four operators in $H_I(\tau_i)$, each of which depends on τ_i)!

$\Rightarrow$ $\int_0^\beta d\tau_i \, e^{i(\nu_1+\nu_2-\nu_3-\nu_4)\tau_i} = \beta \, \delta_{(\nu_1+\nu_2-\nu_3-\nu_4)0}$ $\Rightarrow$ Frequency (energy) conservation at each interaction $H_I(\tau_i)$

(Momentum conservation is implemented already right from the beginning)!

$\Rightarrow$ All τ_i-integrals are carried out explicitly $\rightarrow$ Only sums over Matsubara frequencies remain.

To get a better „feeling" for these terms, we consider $N=1$ (first) order terms:
(For simplicity, we assume the Coulomb interaction $U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'} = U_{\vec{q}} - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{\vec{q}^2}$)

$$\tilde{G}^{M,1}_{\vec{k}}(i\nu) = -\int_0^\beta d\tau \, e^{i\nu\tau} \cdot (-1)\frac{1}{2} \sum_{\vec{k}_1\vec{k}_1'\vec{q}_1} \sum_{\sigma_1\sigma_1'} U_{\vec{q}_1} \int_0^\beta d\tau_1 \tag{48}$$

$$\times \left\langle T_\tau \left(c^{+,0}_{\vec{k}_1\sigma_1}(\tau_1)\, c^{0}_{(\vec{k}_1+\vec{q}_1)\sigma_1}(\tau_1)\, c^{+,0}_{(\vec{k}_1'+\vec{q}_1)\sigma_1'}(\tau_1)\, c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1)\, c^{0}_{\vec{k}\sigma}(\tau)\, c^{+}_{\vec{k}\sigma}\right)\right\rangle_0^{c}$$

$c \rightarrow$ only CONNECTED contribut.

<u>Note:</u> The other two possible contractions, where $c^{+}_{\vec{k}\sigma}$ is connected to $c^{0}_{(\vec{k}_1+\vec{q}_1)\sigma}(\tau_1)$ instead of $c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1)$ give the same result as it can be easily seen by the coordinate transformation $\vec{k}_1+\vec{q}_1=\vec{k}_2'$, $\vec{k}_1=\vec{k}_2'+\vec{q}_2$, $\vec{k}_1'=\vec{k}_2+\vec{q}_2$ as well as $\sigma_1=\sigma_2'$ and $\sigma_1'=\sigma_2$. Under this transformation of summation variables, $\vec{q}_1=-\vec{q}_2 \Rightarrow U_{\vec{q}_1}=U_{-\vec{q}_2}=U_{\vec{q}_2}$ since $U_{\vec{q}}$ depends only on $\vec{q}^{\,2}$. The factor $\frac{1}{2}$, already present in the definition of H_I, removes the factor of 2 due to this „double counting" of the contractions marked in Eq. (48)!

<u>Signs:</u> $G^{M}_{\vec{k}}(\tau_1-\tau_2)\sim-\langle c_{\vec{k}\sigma}(\tau_1)\,c^{+}_{\vec{k}\sigma}(\tau_2)\rangle \Rightarrow$ We have to count the number of transposit. to bring the operators from it's original order into the form $\langle c c^{+} c c^{+} \dots\rangle$! (For an odd number of transpositions, an additional minus sign occurs.)

Contractions 1: $$+^{\circledast}\langle T_\tau\big(\overbrace{c^{+,0}_{\vec{k}_1\sigma_1}(\tau_1)\,c^{0}_{(\vec{k}_1+\vec{q}_1)\sigma_1}(\tau_1)}^{1}\;\overbrace{c^{0}_{\vec{k}\sigma}(\tau)\,c^{+,0}_{(\vec{k}_1'+\vec{q}_1)\sigma_1'}(\tau_1)}^{2}\;\overbrace{c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1)\,c^{+}_{\vec{k}\sigma}}^{3}\big)\rangle_0 \quad (49)$$

$$\Rightarrow \underbrace{\oplus\, G^{M,0}_{\vec{k}_1}(0-)\,\delta_{\vec{q}_1,0}}_{1}\;\underbrace{G^{M,0}_{\vec{k}}(\tau-\tau_1)\,\delta_{\sigma\sigma_1'}\,\delta_{(\vec{k}_1'+\vec{q}_1)\vec{k}}}_{2}\;\underbrace{G^{M,0}_{\vec{k}}(\tau_1)\,\delta_{\sigma\sigma_1'}\,\delta_{\vec{k}_1'\vec{k}}}_{3} \quad (50)$$

$\hookrightarrow \tau_1-\tau_1$

since $c^{0}c^{+,0}\sim-G^{M,0}$! and $c^{+,0}c^{0}\sim+G^{M,0}$

$\circledast$ One „−" from the definition of G^{M}, One „−" from perturb. theory $[(-1)^{\nu=1}]$ $\Rightarrow (-1)^2=+1$

$$\tilde{G}^{M,1a}_{\vec{k}}(i\nu) = \int_0^\beta d\tau\, e^{i\nu\tau} \int_0^\beta d\tau_1 \sum_{\substack{\vec{k}_1,\vec{k}_1',\vec{q}_1\\ \sigma_1\sigma_1'}} U_{\vec{q}_1}\, \overbrace{G^{M,0}_{\vec{k}_1}(0-)}^{\lim_{\tau\to 0,\,\tau<0} G^{M,0}_{\vec{k}}(\tau)}\, \delta_{\vec{q}_1,0}\, G^{M,0}_{\vec{k}}(\tau-\tau_1)\, \delta_{\sigma\sigma_1'}\, \delta_{(\vec{k}_1'+\vec{q}),\vec{k}}$$
$$\times\, G^{M,0}_{\vec{k}}(\tau_1)\, \delta_{\sigma\sigma_1'}\, \delta_{\vec{k}_1',\vec{k}} \qquad (51)$$

$$\left\{\begin{array}{ll} G^{M,0}_{\vec{k}_1}(0^-) = \frac{1}{\beta}\sum_{\nu_1} e^{-i\nu_1 0-}\, \tilde{G}^{M,0}_{\vec{k}_1}(i\nu_1) & G^{M,0}_{\vec{k}}(\tau-\tau_1) = \frac{1}{\beta}\sum_{\nu_2} e^{-i\nu_2(\tau-\tau_1)}\, \tilde{G}^{M,0}_{\vec{k}}(i\nu_2) \\ G^{M,0}_{\vec{k}}(\tau_1) = \frac{1}{\beta}\sum_{\nu_3} e^{-i\nu_3\tau_1}\, \tilde{G}^{M,0}_{\vec{k}}(i\nu_3) & \qquad (52) \end{array}\right\}$$

$$\Rightarrow \tilde{G}^{M,1a}_{\vec{k}}(i\nu) = \frac{1}{\beta^3}\sum_{\nu_1,\nu_2,\nu_3} U_{\vec{q}=0} \sum_{\vec{k}_1\sigma_1} \tilde{G}^{M,0}_{\vec{k}_1}(i\nu_1)\, \tilde{G}^{M,0}_{\vec{k}}(i\nu_2)\, \tilde{G}^{M,0}_{\vec{k}}(i\nu_3) \underbrace{\int_0^\beta d\tau\, e^{i(\nu-\nu_2)\tau}}_{\beta\delta_{\nu\nu_2}} \underbrace{\int_0^\beta d\tau_1\, e^{i(\nu_2-\nu_3)\tau_1}}_{\beta\delta_{\nu_2\nu_3}}$$

$$\sum_{\sigma_1} \Rightarrow 2\,\frac{1}{\beta}\sum_{\nu_1,\vec{k}_1} \tilde{G}^{M,0}_{\vec{k}_1}(i\nu_1)\, e^{-i\nu_1 0-}\, U_{\vec{q}=0} \left[G^{M,0}_{\vec{k}}(i\nu)\right]^2 \qquad (53)$$

$$\left(\frac{1}{\beta}\sum_{\nu_1} e^{-i\nu_1 0-}\, \tilde{G}^{M,0}_{\vec{k}_1}(i\nu_1) = G^{M,0}_{\vec{k}}(\tau\to 0-) = \langle c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}\rangle = n_{\vec{k}\sigma} = \frac{1}{2} n_{\vec{k}} \ \ldots \text{particle density!} \qquad (54)\right)$$

$$\boxed{\tilde{G}^{M,1a}_{\vec{k}}(i\nu) = U_{\vec{q}=0}\, \frac{1}{\beta}\sum_{\nu_1\vec{k}_1\sigma_1} e^{-i\nu_1 0-}\, \tilde{G}^{M,0}_{\vec{k}_1}(i\nu_1) \left[\tilde{G}^{M,0}_{\vec{k}}(i\nu)\right]^2 = U_{\vec{q}=0} \sum_{\vec{k}_1} n_{\vec{k}_1} \left[\tilde{G}^{M,0}_{\vec{k}}(i\nu)\right]^2 \quad (55)}$$

... Interaction of "target" particle $(i\nu, \vec{k})$ with the density $n_{\vec{k}}$ of the "other" particles

⇒ HARTREE TERM (Problem: $U_{\vec{q}=0} \sim \frac{1}{\vec{q}^2}\Big|_{\vec{q}=0} \sim \infty$ for bare Coulomb interaction ⇒ $U^{TF}_{\vec{q}} \sim \frac{1}{\vec{q}^2+\lambda_{TF}^{-2}}$)

$$\text{Contraction 2: } + \langle T_\tau \big(\overbrace{c^{0}_{(\vec{k}_1+\vec{q}_1)\sigma_1}(\tau_1)\, c^{+,0}_{(\vec{k}_1'+\vec{q}_1')\sigma_1'}}^{1}(\tau_1)\, \overbrace{c^{0}_{\vec{k}\sigma}(\tau)\, c^{+,0}_{\vec{k}_1\sigma_1}}^{2}(\tau_1)\, \overbrace{c^{0}_{\vec{k}_1'\sigma_1'}(\tau_1)\, c^{+,0}_{\vec{k}\sigma}}^{3} \big) \rangle_0 \quad (56)$$

$$\Rightarrow - G^{M,0}_{(\vec{k}_1+\vec{q}_1)}(0+)\, \delta_{\sigma_1\sigma_1'}\, \delta_{\vec{k}_1\vec{k}_1'} \quad G^{M,0}_{\vec{k}}(\tau-\tau_1)\, \delta_{\sigma\sigma_1}\, \delta_{\vec{k}\vec{k}_1} \quad G^{M,0}_{\vec{k}}(\tau_1)\, \delta_{\sigma\sigma_1'}\, \delta_{\vec{k}\vec{k}_1'} \quad (57)$$

$$\tilde{G}^{M,1b}_{\vec{k}}(i\nu) = - \int_0^\beta d\tau\, e^{i\nu\tau} \int_0^\beta d\tau_1 \sum_{\substack{\vec{k}_1\vec{k}_1'\vec{q}_1 \\ \sigma_1\sigma_1'}} U_{\vec{q}_1}\, G^{M,0}_{(\vec{k}_1+\vec{q}_1)}(0+)\, \delta_{\sigma_1\sigma_1'}\, \delta_{\vec{k}_1\vec{k}_1'}\, G^{M,0}_{\vec{k}}(\tau-\tau_1)\, \delta_{\sigma\sigma_1}\, \delta_{\vec{k}\vec{k}_1}$$

$$\times\, G^{M,0}_{\vec{k}}(\tau_1)\, \delta_{\sigma\sigma_1'}\, \delta_{\vec{k}\vec{k}_1'} \quad (58)$$

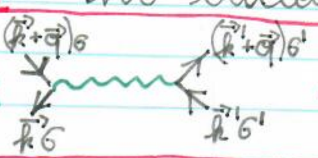
Fourier transform as in Eq. (52)

$$(\vec{q}_1 \to \vec{q}) \overset{\uparrow}{=} -\frac{1}{\beta^3} \sum_{\nu_1\nu_2\nu_3} \sum_{\vec{q}} U_{\vec{q}}\, \tilde{G}^{M,0}_{\vec{k}+\vec{q}}(i\nu_1)\, \tilde{G}^{M,0}_{\vec{k}}(i\nu_2)\, \tilde{G}^{M,0}_{\vec{k}}(i\nu_3) \underbrace{\int_0^\beta d\tau\, e^{i(\nu-\nu_2)\tau}}_{\beta\,\delta_{\nu\nu_2}} \underbrace{\int_0^\beta d\tau_1\, e^{i(\nu_3-\nu_2)\tau_1}}_{\beta\,\delta_{\nu_2\nu_3}} \quad (59)$$

$$\Rightarrow \boxed{\tilde{G}^{M,1b}_{\vec{k}}(i\nu) = -\frac{1}{\beta} \sum_{\nu_1\vec{q}} U_{\vec{q}}\, \tilde{G}^{M,0}_{\vec{k}+\vec{q}}(i\nu_1)\, \big[\tilde{G}^{M,0}_{\vec{k}}(\nu)\big]^2 \quad \text{... EXCHANGE (FOCK) TERM}} \quad (60)$$

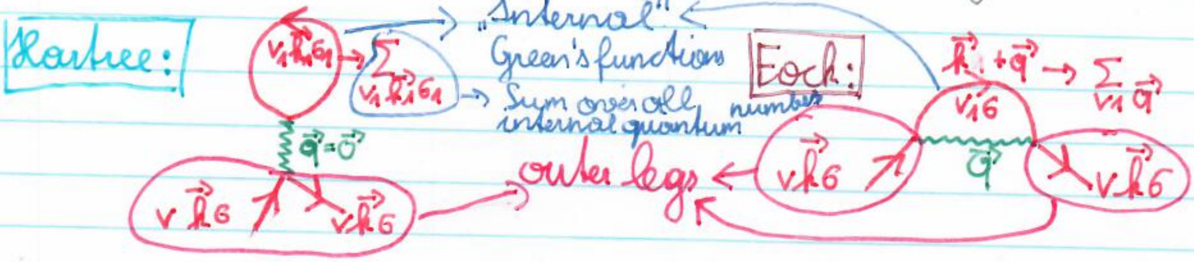
For higher orders, the evaluation of the perturbation theory becomes very „confusing" ⇒ R. Feynman realized, that each contraction corresponds to a scattering diagram, which leads to a graphical representation of perturbation theory in terms of so called Feynman diagrams!

FEYNMAN DIAGRAMS: Two building blocks:

- Interaction $U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'}$: 

- Noninteracting GF $\tilde{G}^{M,0}_{\vec{k}\sigma}(i\nu)$: $\xrightarrow{\nu\vec{k}\sigma}$

E.g.: Hartree and Fock diagrams for 1^{st} order perturbation theory:



The N^{th} order perturbation theory corresponds to all topologically different, connected, diagrams with N vertices (interactions) and $2(N+1)$ free propagators (noninteracting Green's function lines), two of which correspond to the so-called „outer lines" $\tilde{G}^{M,0}_{\vec{k}}(i\nu)$.

⇒ We can draw an N^{th}-order diagram and obtain the corresponding mathematical expression by means of the Feynman rules!

Feynman rules

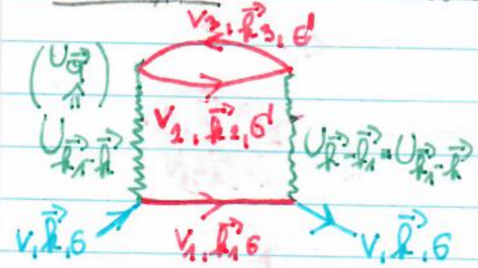
1) Draw a diagram with N interaction vertices $U^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'}$ (〰〰) and $2N+2$ non-interacting Green's function lines $\tilde{G}^{\mu,0}_{\vec{k}}(i\nu)$ ($\longrightarrow$), two of which are the so-called „outer legs" with a fixed frequency ν, momentum $\vec{k}$ and spin σ.

2) Associate frequencies ν_i, momenta $\vec{k}_i$ and spins σ_i with all $2N$ internal lines so that at each of the N vertices frequency-, momentum- and spin conservation are fulfilled (and, of course, particle conservation).

3) Sum (Integrate) over all internal degrees of freedom, i.e. ν_i, $\vec{k}_i$ and σ_i, where each frequency sum contains a prefactor $\frac{1}{\beta}$ and each momentum integral a prefactor $\frac{1}{V_{BZ}}$. Each frequency conservation comes with $\beta \cdot \delta_{(\nu_1+\nu_2+\nu_3+\nu_4),0}$

4) Multiply the final expression with $(-1)^N (-1)^F$, where F is the number of closed loops formed by the Green's function lines. (A closed loop consists in the contractions $c_1^+ c_1 c_2^+ c_2 \dots c_{n-1} c_n^+ c_n = - c_n c_1^+ c_1 c_2^+ \dots c_n^+ c_n$, see Hartree term)
$\hookrightarrow$ $2n-1$ transpositions

Example: 2^{nd} order diagram (with an interaction $U^{\vec k \vec k' \vec q}_{\sigma\sigma'} = U_{\vec q} = U_{-\vec q}$):



$$\Rightarrow \overset{2^{nd}\text{order}}{(-1)^2}\ \overset{1\ \text{fermionic loop}}{(-1)^1}\ \frac{1}{\beta^3} \sum_{\nu_1\nu_2\nu_3}\ \overset{\text{includes } \frac{1}{V_{BZ}}}{\sum_{\vec k_1 \vec k_2 \vec k_3}} \sum_{\sigma'} (U_{\vec k_1 - \vec k})^2\, \tilde G^{M,0}_{\vec k_1}(i\nu_1)\, \tilde G^{M,0}_{\vec k_2}(i\nu_2)\, \tilde G^{M,0}_{\vec k_3}(i\nu_3)$$

$$\times\, \beta\,\delta_{(\nu+\nu_3)(\nu_1+\nu_2)}\ \delta_{(\vec k+\vec k_3)(\vec k_1+\vec k_2)}\ [\tilde G^{M,0}_{\vec k}(i\nu)]^2$$

$$\overset{\sum_{\sigma'}}{=} -2\,\frac{1}{\beta^2} \sum_{\nu_1\nu_2} \sum_{\vec k_1 \vec k_2} (U_{\vec k_1 - \vec k})^2\, \tilde G^{M,0}_{\vec k_1}(i\nu_1)\, \tilde G^{M,0}_{\vec k_2}(i\nu_2)\, \tilde G^{M,0}_{\vec k_1+\vec k_2-\vec k}(i(\nu_1+\nu_2-\nu)) \times (\tilde G^{M,0}_{\vec k}(i\nu))^2$$

$$\left\{\begin{matrix} \nu_1 = \nu+\Omega & \vec k_1 = \vec k + \vec q \\ \nu_2 = \nu' & \vec k_2 = \vec k' \end{matrix}\right\}$$

$$= \boxed{-2\,\frac{1}{\beta^2} \sum_{\nu'\Omega} \sum_{\vec k' \vec q} (U_{\vec q})^2\, \tilde G^{M,0}_{\vec k+\vec q}(i(\nu_1+\Omega))\, \tilde G^{M,0}_{\vec k'+\vec q}(i(\nu'+\Omega))\, \tilde G^{M,0}_{\vec k'}(i\nu')\, [\tilde G^{M,0}_{\vec k}(i\nu)]^2 \quad (62)}$$

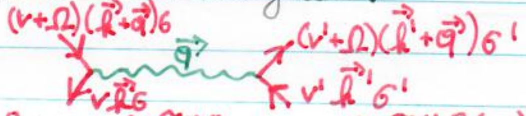
Perturbation Theory for the the two-particle Green's function:

$$\boxed{G^{(2),M}_{\vec k \vec k' \vec q,\sigma\sigma'}(\tau_1,\tau_2,\tau_3) = \langle T_\tau \big(U(\beta,0)\, c^{\dagger,0}_{\vec k\sigma}(\tau_1)\, c^{0}_{(\vec k+\vec q)\sigma}(\tau_2)\, c^{\dagger,0}_{(\vec k'+\vec q)\sigma'}(\tau_3)\, c^{0}_{\vec k'\sigma'}\big)\rangle_0 \big/ \langle T_\tau (U(\beta,0))\rangle_0 \quad (63)}$$

⇒ can be also expanded in terms of (2-particle) Feynman diagrams.

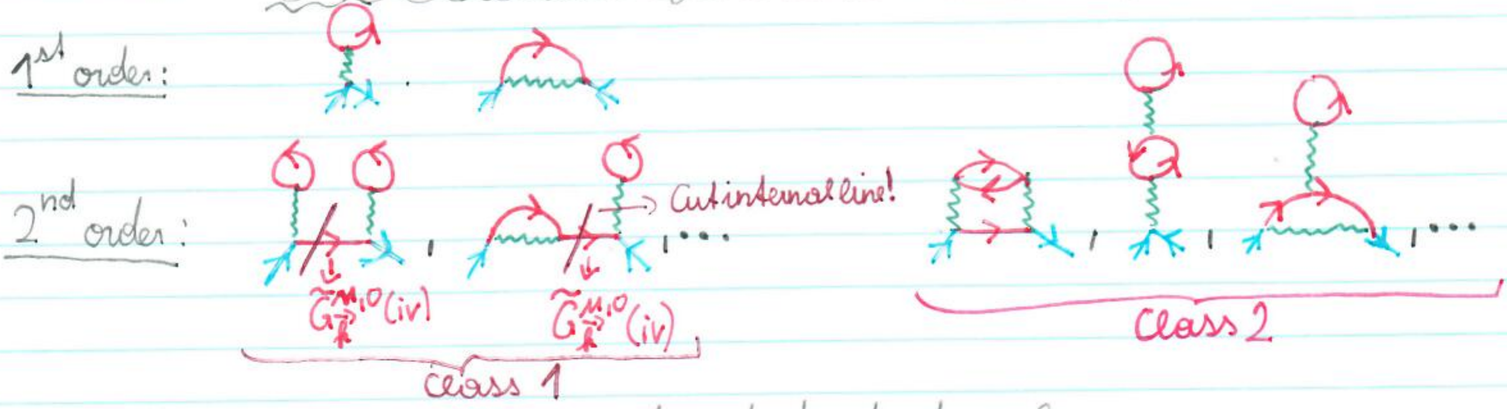
⇒ Analogous Feynman rules!

E.g.: 1^{st} order diagram:



$$= \overset{1^{st}\text{order}}{-} U_{\vec q}\, \tilde G^{M,0}_{\vec k}(i\nu)\, \tilde G^{M,0}_{\vec k+\vec q}(i(\nu+\Omega))\, \tilde G^{M,0}_{\vec k'+\vec q}(i(\nu'+\Omega))\, \tilde G^{M,0}_{\vec k'}(i\nu') \quad (64)$$

General structure of diagrammatic perturbation theory



The set of all diagrams can be divided into two classes:

Class 1: ONE-PARTICLE REDUCIBLE diagrams: Such diagrams can be split into two parts by cutting one internal Green's function line.

Class 2: ONE-PARTICLE IRREDUCIBLE diagrams: Such diagrams CANNOT be split into two parts by cutting one internal Green's function line.

⇒ Diagrams of Class 1 are just „repetitions" of diagrams of Class 2 connected with a non-interacting Green's function $\tilde{G}^{M,0}_{\vec{k}}(i\nu)$!

⇒ The sum of all diagrams of Class 2 without the outer legs $[\tilde{G}^{M,0}_{\vec{k}}(i\nu)]$ is called

SELF-ENERGY $\Sigma_{\vec{k}}(i\nu)$

⇒ Class 1 (without outer legs): $\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu) + \Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu) + \ldots$ (65)

⇒ Since $\tilde{G}^{M}_{\vec{k}}(i\nu) = \tilde{G}^{M,0}_{\vec{k}}(i\nu)$ + Class 1 + Class 2 (with outer legs), we have:

$$\begin{aligned}
\tilde{G}^{M}_{\vec{k}}(i\nu) &= \tilde{G}^{M,0}_{\vec{k}}(i\nu) + \tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu) + \tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu) + \ldots \\
&= \tilde{G}^{M,0}_{\vec{k}}(i\nu) + \tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\underbrace{\left[\tilde{G}^{M,0}_{\vec{k}}(i\nu) + \tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M,0}_{\vec{k}}(i\nu) + \ldots\right]}_{\tilde{G}^{M}_{\vec{k}}(i\nu)} \\
&= \tilde{G}^{M,0}_{\vec{k}}(i\nu) + \tilde{G}^{M,0}_{\vec{k}}(i\nu)\,\Sigma_{\vec{k}}(i\nu)\,\tilde{G}^{M}_{\vec{k}}(i\nu) \qquad (66)
\end{aligned}$$

(corresponds to a geometric series)

⇒ This equation can be solved for $\tilde{G}^{M}_{\vec{k}}(i\nu)$:

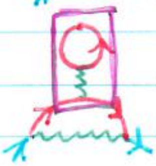
$$\boxed{\text{DYSON EQUATION:} \quad \tilde{G}^{M}_{\vec{k}}(i\nu) = \frac{1}{[G^{M,0}_{\vec{k}}(i\nu)]^{-1} - \Sigma_{\vec{k}}(i\nu)} = \frac{1}{i\nu + \mu - \varepsilon_{\vec{k}} - \Sigma_{\vec{k}}(i\nu)} \quad (67)}$$

In practice: We calculate only **one-particle irreducible diagrams** for $\Sigma_{\vec{k}}(i\nu)$ and obtain $\tilde{G}^{M}_{\vec{k}}(i\nu)$ via the Dyson equation!

⇒ In this way, we generate an INFINITE number of (reducible) diagrams for $G^{M}_{\vec{k}}(i\nu)$ from a SINGLE **irreducible** diagram for $\Sigma_{\vec{k}}(i\nu)$!

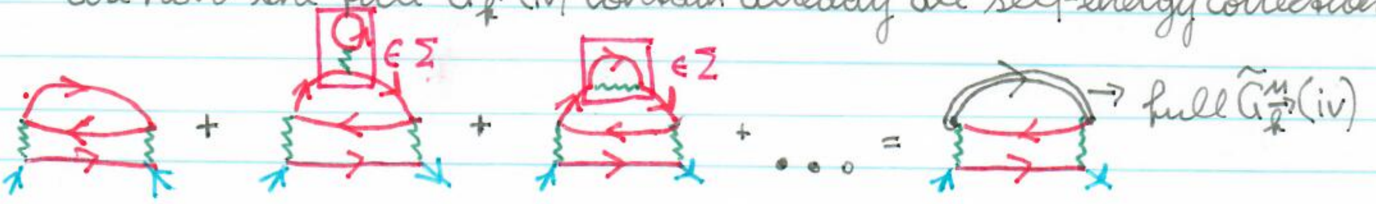
Further classification of irreducible diagrams for $\Sigma_{\vec{k}}(i\nu)$:


... SKELETON DIAGRAM: No self-energy corrections of internal lines!


... NON-SKELETON DIAGRAM: Internal lines contain selfenergy corrections.

⇒ If we consider ALL self-energy corrections for all internal lines, we can replace the internal non-interacting Green's functions by the interacting ones.

But: Then we should consider only skeleton diagrams since the lines which are now the full $\tilde{G}^{\mu}_{\vec{k}}(i\nu)$ contain already all self-energy corrections!



⇒ If we consider only Skeleton diagrams, we can replace all non-interacting Greensfunctions by fully interacting („bold") ones: $\tilde{G}^{\mu,0}_{\vec{k}}(i\nu) \rightarrow G^{\mu}_{\vec{k}}(i\nu)$

⇒ This is often called „BOLD" diagrammatic perturbation theory, which leads to the following self-consistent (fixed point) equations:

(68) $\Sigma = \Sigma[G] \qquad G = \dfrac{1}{G_0^{-1} - \Sigma}$ ... Iteration until convergence!

↓ Self-energy is a Functional of the full („bold") Green's function, which is defined by the Seleton diagrams which are used to calculate Σ from G!

Caveat: For large U, iteration (68) can lead to a wrong fix point!

Approximations for the self-energ:

⇒ We assume, that for low frequencies, a Taylor expansion of $\Sigma_{\vec{k}}(i\nu)$ is possible:

$$\Sigma_{\vec{k}}(i\nu) = -i\gamma_{\vec{k}} - \alpha_{\vec{k}}\cdot(i\nu) + O((i\nu)^2), \quad \text{for } \nu > 0 \qquad (68)$$

(For simplicity we assume: $\alpha_{\vec{k}}, \gamma_{\vec{k}} \in \mathbb{R}$, i.e. $\mathrm{Im}\{\alpha_{\vec{k}}, \gamma_{\vec{k}}\} = 0$)

$$\Rightarrow \tilde{G}^{\mu}_{\vec{k}}(i\nu) = \frac{1}{i\nu + \mu - \varepsilon_{\vec{k}} + \alpha_{\vec{k}} i\nu + \gamma_{\vec{k}}} = \frac{1}{(1+\alpha_{\vec{k}})i\nu + \mu - \varepsilon_{\vec{k}} + i\gamma_{\vec{k}}}$$

$$= \frac{Z_{\vec{k}}}{i\nu + \tilde{\varepsilon}_{\vec{k}} + i\tilde{\gamma}_{\vec{k}}}, \quad Z_{\vec{k}} = \frac{1}{1+\alpha_{\vec{k}}}, \quad \tilde{\varepsilon}_{\vec{k}} = Z_{\vec{k}}(\varepsilon_{\vec{k}} - \mu), \quad \tilde{\gamma}_{\vec{k}} = Z_{\vec{k}}\gamma_{\vec{k}} \qquad (69)$$

(1) For $\gamma_{\vec{k}} = 0$, we find a Green's function for a non-interacting system with a renormalized dispersion relation $\tilde{\varepsilon}_{\vec{k}}$: $\varepsilon_{\vec{k}} = \frac{\vec{k}^2}{2m} \rightarrow \tilde{\varepsilon}_{\vec{k}} \sim \frac{\vec{k}^2}{2m^*}$

⇒ New effective mass $\boxed{m^* = \frac{m}{Z_{\vec{k}}} > m}$ if $Z_{\vec{k}} < 1$ ($\hat{=}\ \alpha_{\vec{k}} > 0$)

$\hat{=}$ non-interacting electrons, with a larger effective mass: FERMI LIQUID.

(2) For $\gamma_{\vec{k}} \neq 0$: $\tilde{G}^R_{\vec{k}}(\omega) = \frac{Z_{\vec{k}}}{\omega - \tilde{\varepsilon}_{\vec{k}} + i\tilde{\gamma}_{\vec{k}}}$, $\tilde{\gamma}_{\vec{k}} > 0$ ⇒ $G^R_{\vec{k}}(t) = -i Z_{\vec{k}}\, e^{-i\tilde{\varepsilon}_{\vec{k}} t} \boxed{e^{-\tilde{\gamma}_{\vec{k}} t}}$ ... damping

⇒ $\tilde{\gamma}_{\vec{k}}$ is the inverse lifetime of the renormalized particle!

⇒ These considerations are the starting point of the Fermi liquid theory!

Diagrammatic structure of $G^{(2)}$

$$G^{(2),M}_{\vec{k}\vec{k}'\vec{q},\sigma\sigma'}(\tau_1,\tau_2,\tau_3) = \langle T_\tau \big(U(\beta,0)\; c^{+,0}_{\vec{k}\sigma}(\tau_1)\, c^{0}_{(\vec{k}+\vec{q})\sigma}(\tau_2)\, c^{+,0}_{(\vec{k}'+\vec{q})\sigma'}(\tau_3)\, c^{0}_{\vec{k}'\sigma'}(\tau_4) \big\rangle_0 \big/ \langle T_\tau (U(\beta,0))\rangle \qquad (70)$$

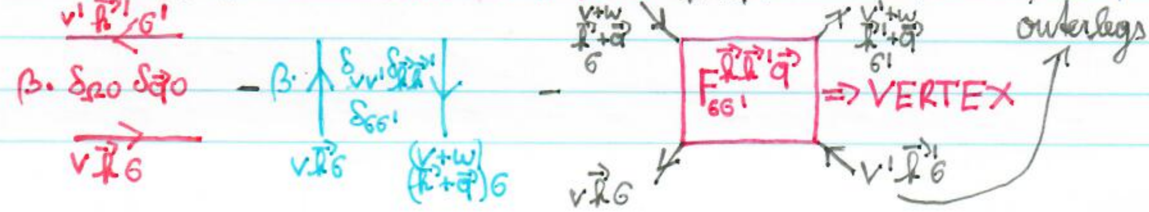
⇒ For $G^{(2)}$, we will always consider Skeleton diagrams, where internal lines correspond to the <u>full</u> one-particle Green's functions!

⇒ The full $G^{(2)}$ contains DISCONNECTED contributions, for which we consider only separate contractions for the two pairs of external operators and a CONNECTED contribution:

$$\tilde{G}^{(2),M}_{\vec{k}\vec{k}'\vec{q},\sigma\sigma'}(i\nu,i\nu',i\Omega) = \beta\, \tilde{G}^{M}_{\vec{k}}(i\nu)\,\tilde{G}^{M}_{\vec{k}'}(i\nu')\,\delta_{\vec{q}0}\,\delta_{\Omega 0} - \beta\, \tilde{G}_{\vec{k}}(i\nu)\,\tilde{G}_{\vec{k}+\vec{q}}(i\nu+i\Omega)\,\delta_{\vec{k}\vec{k}'}\,\delta_{\nu\nu'}\,\delta_{\sigma\sigma'}$$

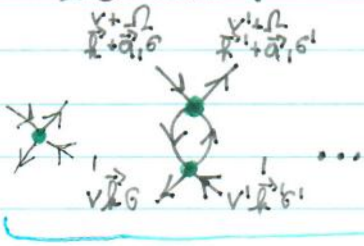
$$- \tilde{G}^{M}_{\vec{k}}(i\nu)\,\tilde{G}_{\vec{k}+\vec{q}}(i\nu+i\Omega)\; F^{\vec{k}\vec{k}'\vec{q}}_{\sigma\sigma'}(i\nu,i\nu',i\Omega)\; \tilde{G}^{M}_{\vec{k}'+\vec{q}}(i\nu'+i\Omega)\,\tilde{G}^{M}_{\vec{k}'}(i\nu') \qquad (71)$$

⇒ diagrammatic representation =



⇒ The fully connected part of $G^{(2)}$ (after removing the outer legs), i.e., the vertex F is the SCATTERING AMPLITUDE for a two-particle scattering process!

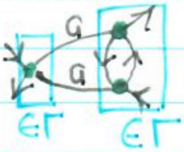
Classification of diagrams for F ⇒ 2 classes:



(for simplicity, we have replaced "〰" by "•")

2-PARTICLE REDUCIBLE diagrams Φ in the particle-hole channel $(\nu\vec{k}\sigma, (\nu+\Omega)(\vec{k}+\vec{q})\sigma) \leftrightarrow (\nu'\vec{k}'\sigma', (\nu'+\Omega)(\vec{k}'+\vec{q})\sigma')$

2-PARTICLE IRREDUCIBLE diagrams Γ_{PH} in the particle-hole channel.

⇒ Construct Φ from Γ and 2 Green's functions: $\Phi =$ 

⇒ Similar to Dyson Equation: $\Phi = \Gamma\tilde{G}\tilde{G}\Gamma + \Gamma\tilde{G}\tilde{G}\Gamma\tilde{G}\tilde{G}\Gamma + \dots$

$F = \Gamma + \Phi = \Gamma + \Gamma GG\Gamma + \dots = \Gamma + \Gamma GG(\underbrace{\Gamma + \Gamma GG\Gamma + \dots}_{F}) \Rightarrow \boxed{F = \Gamma + \Gamma GG F \text{ ... Bethe-Salpeter Eq.}}$

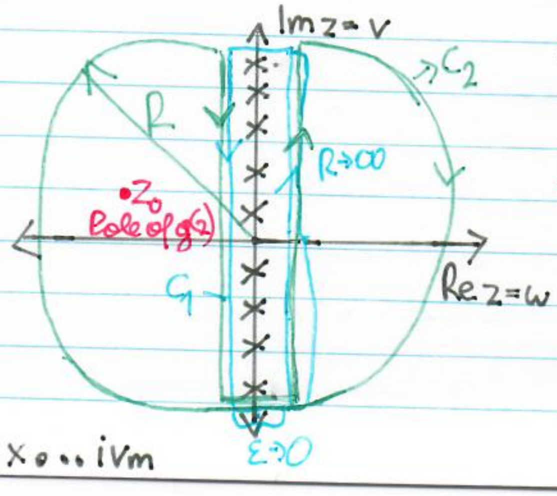
(integral equation)

Technical aspects – summations over Matsubara frequencies

For the evaluation of Feynman diagrams, we are typically concerned with the evaluation of sums over Matsubara frequencies:

$\frac{1}{\beta}\sum_{\nu_m} g(i\nu_m)$, where $g(i\nu_m)$ is a function which should decay for $\nu_m \to \infty$ at least as $\left(\frac{1}{\nu_m}\right)^{1+\varepsilon}$, $\varepsilon > 0$ (otherwise the sum does not converge.)

$\Rightarrow$ Such sums can be evaluated by means of the following „trick":



We consider the following complex function:

$$f(z) = \frac{1}{e^{\beta z} \mp 1} \quad \begin{cases} - \Rightarrow \text{Bose function} \\ + \Rightarrow \text{Fermi function} \end{cases}$$

The Matsubara frequencies are poles of $f(z)$, e.g. for the fermionic case:

$z = i\frac{\pi}{\beta}(2n+1) \Rightarrow e^{z\beta} = e^{i\pi(2n+1)} = -1 \Rightarrow \frac{1}{e^{\beta z}+1} = \frac{1}{-1+1}$ "

Function which should be summed!

Residue theorem for closed path C_1: $\oint_{C_1} dz\, f(z) \cdot g(z) = 2\pi i \sum \mathrm{Res}\, f(z) \cdot g(z)$

Typical situation: $g(z)$ has no poles on the imaginary axis
$\Rightarrow$ only the poles of $f(z)$ at the Matsubara frequencies contrib.

Residua of $f(z)$ at $z = i\frac{\pi}{\beta}\cdot\begin{Bmatrix}(2m)\\(2m+1)\end{Bmatrix} = i\nu_m$: $\lim\limits_{z\to i\nu_m} (z-i\nu_m) f(z) = \frac{z-i\nu_m}{e^{\beta z}\mp 1}\Big|_{z\to i\nu_m} = \pm\frac{1}{\beta}$

$\Rightarrow \oint_{C_1} dz\, f(z)\cdot g(z) = \pm\frac{1}{\beta}\, 2\pi i \sum_{\nu_m} g(i\nu_m) \Rightarrow$ $\boxed{\frac{1}{\beta}\sum_{\nu_m} g(i\nu_m) = \pm\frac{1}{2\pi i}\oint_{C_1} dz\, f(z)\cdot g(z)}$

For C_1, only the vertical parts contribute since the length of the horizontal parts $\varepsilon \to 0$ $\Rightarrow$ The integral over C_1 is the same as over C_2 if the integral over the two half-circles with radius $R\to\infty$ vanishes!

Circle: $z = R\cdot e^{i\varphi}$: $\begin{cases} \varphi \in [-\frac{\pi}{2}, \frac{\pi}{2}] \to \mathrm{Re}\, z = R\cdot\cos\varphi \geq 0 \to f(R\cdot e^{i\varphi}) \xrightarrow{R\to\infty} 0 \\ \varphi \in [-\pi, -\frac{\pi}{2}] \cup [\frac{\pi}{2}, \pi] \to \mathrm{Re}\, z \leq 0 \to f(Re^{i\varphi}) \to \mp 1 \text{ but } g(Re^{i\varphi}) \to \frac{1}{R^2} \to 0 \end{cases}$

$$\boxed{\frac{1}{\beta}\sum_{\nu_m} g(i\nu_m) = \pm\frac{1}{2\pi i}\oint_{C_1} dz\, f(z)\, g(z) = \pm\oint_{C_2} dz\, f(z)\, g(z) = \mp\sum_{\mathrm{Res}\ z=z_0 \text{ inside } C_2} f(z)\cdot g(z)}$$