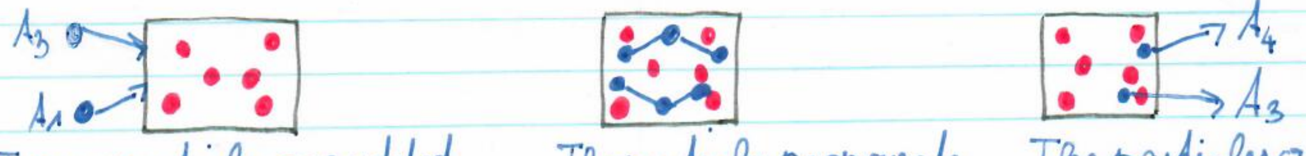
Two-particle Green's functions

Two-particle processes:



Two particles are added to the system at times t_1 and t_3. The particles propagate through the system. The particles are removed at the times t_2 and t_4.

⇒ Analogous processes, where one particle and one hole or two holes propagate through the system also have to be considered!

⇒ Such processes can be described by the the causal (time ordered) two-particle Green's function $G^{(2),c}_{ijlm}(t_1,t_2,t_3,t_4)$:

$$\boxed{G^{(2),c}_{ijlm}(t_1,t_2,t_3,t_4) = \langle T\left(c_i^{+}(t_1)\, c_j(t_2)\, c_l^{+}(t_3)\, c_m(t_4)\right)\rangle \quad (111)}$$

↳ Time order operator

- The time-ordering operator T orders the operators $c_i^+(t_1)$, $c_j(t_2)$, $c_l^+(t_3)$ and $c_m(t_4)$ according to the order of their time arguments; For fermions an additional minus sign has to be added if the final order is reached from the original order by an odd number of transpositions!

- For a time-translational invariant system, $G^{(2),c}_{ijlm}$ depends only on time differences, e.g., t_1-t_4, t_2-t_4 and t_3-t_4
  $\rightarrow$ w.l.o.g. we can $\boxed{\text{set } t_4=0}$

- The letters i, j, l, m again are multi-indices which contain all quantum numbers which define the corresponding single-particle state, e.g., $i \hat{=} (\vec{r},\sigma)$ or $i \hat{=} (\vec{R}_i,\sigma)$ or $i \hat{=} (\vec{k},\sigma)$, ...

- Remark: The definition of the two-particle Green's function is not unique in the literature as the overall sign depends on the starting order of the operators. However, two different definitions differ typically only by a sign.

As for the one-particle Green's function, it is advantageous to work with imaginary times (and Matsubara frequencies)!

$$\boxed{G^{(2),M}_{ijem}(\tau_1,\tau_2,\tau_3) = \langle T_\tau\left(c_i^+(\tau_1)\,c_j(\tau_2)\,c_\ell^+(\tau_3)\,c_m\right)\rangle \quad (112)}$$

(where we have already set $\tau_4=0$).

⊙ Domain of definition: Let us evalute $G^{(2),M}_{ijem}(\tau_1,\tau_2,\tau_3)$ explicitly for $\tau_1>\tau_2>0>\tau_3$:

$$G^{(2),M}_{ijem}(\tau_1,\tau_2,\tau_3) = \overset{\to \text{Bosons}}{\underset{\to \text{Fermions}}{\pm}}\frac{1}{Z}\sum_N \langle N|e^{-\beta H}e^{\tau_1 H}c_i^+e^{-\tau_1 H}e^{\tau_2 H}c_j e^{-\tau_2 H}c_m e^{\tau_3 H}c_\ell^+ e^{-\tau_3 H}|N\rangle$$

$$= \pm\frac{1}{Z}\sum_N e^{-(\beta-\tau_1+\tau_3)E_N}\langle N|c_i^+e^{-(\tau_1-\tau_2)H}c_j e^{-\tau_2 H}c_m e^{\tau_3 H}c_\ell^+|N\rangle \quad (113)$$

To ensure convergence of $\sum_N\ldots$, the exponential term $e^{-(\beta-\tau_1+\tau_3)}$ should correspond to a damping factor for $E_N\to\infty$!

$\Rightarrow \quad \beta - \tau_1 + \tau_3 > 0 \quad \Rightarrow \quad \boxed{\underbrace{\tau_1 > \tau_2 > 0 > \tau_3}_{\text{that was our assumption!}} > \tau_1 - \beta \quad (114)}$

$\Rightarrow \quad \tau_1 - \beta < 0 \rightarrow \boxed{\tau_1 < \beta} \quad$ and $\quad \tau_1 > 0 \rightarrow \boxed{\tau_3 > -\beta} \qquad (115)$

$\Rightarrow$ From these inequalities we can draw two conclusions:

- $\boxed{\tau_1, \tau_2, \tau_3 \in [-\beta, \beta] \quad (116)}$
- For a given choice of times τ_1, τ_2, τ_3 (and 0) the difference between the largest and the smallest time is at most β:
  $\boxed{\tau_{MAX} - \tau_{MIN} \leq \beta \quad (117)}$

$\Rightarrow$ These conditions guarantee the convergence of the matrix elements for all time orders!

- **(Anti) periodicity** Let us again consider $\tau_1 > \tau_2 > 0 > \tau_3$:

$$\boxed{G^{(2),M}_{ij\ell m}(\tau_1, \tau_2, \tau_3)} = \pm\frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} e^{\tau_1 H} c_i^+ e^{-\tau_1 H} e^{\tau_2 H} c_j e^{-\tau_2 H} c_m e^{\tau_3 H} c_\ell^+ e^{-\tau_3 H}\right)$$

(→ cyclicity of Tr)
$$= \pm\frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} e^{(\tau_3+\beta)H} c_\ell^+ e^{-(\tau_3+\beta)H} e^{\tau_1 H} c_i^+ e^{-\tau_1 H} e^{\tau_2 H} c_j e^{-\tau_2 H} c_m\right)$$

$$= \boxed{\pm\, G^{(2),M}_{ij\ell m}(\tau_1, \tau_2, \tau_3+\beta) \quad (118)}$$

(Note: Since $\tau_3 > \tau_1 - \beta \Rightarrow \tau_3 + \beta > \tau_1$!)

$G^{(2),M}_{ij\ell m}(\tau_1, \tau_2, \tau_3)$ is (anti) periodic under a shift of the smallest (largest) time argument by $+\beta$ ($-\beta$) !

Remark: Corresponding shifts of the other time arguments (i.e., not the smallest or largest) lead to a set of time variables which do not fulfill Eq. (117) !

● Fourier transform: As for the one-particle Green's function, we can define the Fourier transform as:

$$\boxed{\tilde{G}^{(2),M}_{ijlm}(i\nu_1, i\nu_2, i\nu_3) = \int_0^\beta d\tau_1 d\tau_2 d\tau_3 \, e^{-i\nu_1\tau_1} e^{+i\nu_2\tau_2} e^{-i\nu_3\tau_3} \, G^{(2),M}_{ijlm}(\tau_1,\tau_2,\tau_3)} \quad (119)$$

where ν_1, ν_2, ν_3 are $\left\{\begin{matrix}\text{bosonic}\\ \text{fermionic}\end{matrix}\right\}$ Matsubara frequencies: $\left\{\begin{matrix}\nu_i = \frac{2m_i\pi}{\beta}\\ \nu_i = \frac{(2m_i+1)\pi}{\beta}\end{matrix}\right\} m_i \in \mathbb{Z}$

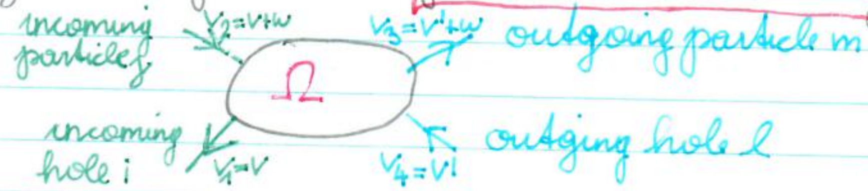
Often, it is advantageous to use other frequency representations:

$\Omega = \frac{\pi}{\beta}(2m_2+1-2m_1-1) = \frac{2(m_2-m_1)\pi}{\beta}$

$$\left\{\begin{matrix}\nu_1 = \nu\\ \nu_2 = \nu+\Omega\\ \nu_3 = \nu'+\Omega\end{matrix}\right\} \Rightarrow \boxed{\Omega = \nu_2 - \nu_1} \text{ is } \boxed{\text{always bosonic}}$$

also for fermionic ν_1 and ν_2!

Physical interpretation: **particle-hole scattering:**



The total transferred energy (frequency) is given by the bosonic transfer frequency Ω.

Representing $G^{(2),M}_{ij\ell m}(i\nu, i\nu', i\Omega)$ in terms of the fermionic frequencies ν, ν' and the bosonic transfer frequency Ω is sometimes refered to as particle-hole frequency notation.

Representing $G^{(2),M}_{ij\ell m}(i\nu_1, i\nu_2, i\nu_3)$ from the view point of a particle-particle scattering event is achieved by the particle-particle frequency notation: $\nu_1 = \nu$, $\nu_2 = \Omega - \nu'$, $\nu_3 = \Omega - \nu$, with the fermionic frequencies ν, ν' and the bosonic frequency Ω.

- Analytic structure of $\tilde{G}^{(2),M}_{ij\ell m}(i\nu, i\nu', i\Omega)$: NOT understood so far!

  $\Rightarrow$ This would require multi-dimensional complex analysis!

- Physical content of $\tilde{G}^{(2),M}_{ij\ell m}(i\nu, i\nu', i\Omega)$:

  $\Rightarrow$ In high-energy physics: $\tilde{G}^{(2),c}_{ij\ell m}(\omega_1, \omega_2, \omega_3) \sim$ scattering cross-section of two coliding particles!

$\Rightarrow$ In many-body physics: NO direct experimental access to two-particle Green's functions so far!

$\Rightarrow$ But: „Reduced" two-particle Green's functions play an important role:
We set: $j=i$, $m=l$, $\tau_2=\tau_1=\tau$, $\tau_3=0 \Rightarrow \chi^M_{il}(\tau) = G^{(2),M}_{iill}(\tau,\tau,0) = \langle T_\tau(\underbrace{c_i^+(\tau)c_i(\tau)}_{n_i(\tau)}\underbrace{c_l^+c_l}_{n_l})\rangle$

$$\tilde{\chi}^M_{il}(i\Omega) = \frac{1}{\beta^2}\sum_{\nu\nu'} G^{(2),M}_{iill}(i\nu, i\nu', i\Omega) = \int_0^\beta d\tau_1 d\tau_2 d\tau_3 \underbrace{\left(\frac{1}{\beta}\sum_\nu e^{-i\nu(\tau_1-\tau_2)}\right)}_{\delta(\tau_1-\tau_2)}\underbrace{\left(\frac{1}{\beta}\sum_{\nu'} e^{-i\nu'\tau_3}\right)}_{\delta(\tau_3)} e^{i\Omega(\tau_2-\tau_3)} \times G^{(2),M}_{iill}(\tau_1,\tau_2,\tau_3)$$

$$\stackrel{\tau_1=\tau}{=} \int_0^\beta d\tau\, e^{i\Omega\tau} G^{(2),M}_{iill}(\tau,\tau,0) = \int_0^\beta d\tau\, e^{i\Omega\tau}\langle n_i(\tau) n_l\rangle = \int_0^\beta d\tau\, e^{i\Omega\tau}\chi^M_{il}(\tau) \quad (120)$$

$\tilde{\chi}^M_{il}(i\Omega)$ ... Susceptibility $\Rightarrow$ See chapter 5 about „Linear response theory"!

Note: $\chi^M_{il}(\tau) = \langle n_i(\tau) n_l\rangle$ can be also interpreted as one-particle Green's function for the (bosonic) particle number operators $n_i = c_i^+ c_i$ and $n_l = c_l^+ c_l$.
$\Rightarrow$ Theory of one-particle Green's function is applicable with some modifications, since $n_i^+ = (c_i^+ c_i)^+ = n_i \Rightarrow [n_i, n_j^+] \equiv 0$ $(\neq \delta_{ij})$!

The equation of motion

Let us consider the time derivative of $G^M_{ij}(\tau) = -\langle c_i(\tau) c_j^+ \rangle \Theta(\tau) \mp \langle c_j^+ c_i(\tau) \rangle \Theta(-\tau)$:

$$\frac{d}{d\tau} G^M_{ij}(\tau) = -\langle c_i(\tau) c_j^+ \rangle \delta(\tau) \pm \langle c_j^+ c_i(\tau) \rangle \delta(\tau) - \langle \frac{dc_i(\tau)}{d\tau} c_j^+ \rangle \Theta(\tau) \mp \langle c_j^+ \frac{dc_i(\tau)}{d\tau} \rangle \Theta(-\tau)$$

$$= -\langle \underbrace{c_i c_j^+ \mp c_j^+ c_i}_{\text{(Anti) commutator: } \delta_{ij}} \rangle \delta(\tau) - \langle \frac{dc_i(\tau)}{d\tau} c_j^+ \rangle \Theta(\tau) \mp \langle c_j^+ \frac{dc_i(\tau)}{d\tau} \rangle \Theta(-\tau) \quad (121)$$

Heisenberg equation of motion for $c_i(\tau)$: $\frac{dc_i(\tau)}{d\tau} = [H, c_i](\tau) \quad (122)$

$\Rightarrow$ To further evaluate this expression, we have to specify the Hamiltonian:

$$H = \sum_{lm} t_{lm} c_l^+ c_m + \frac{1}{2} \sum_{lmno} U_{lmno} c_l^+ c_m c_n^+ c_o \quad (123)$$ (see chapter 2 on second quantization)

For simplicity, we restrict ourselves to the fermionic case!

We have the operator identities : $[AB, C] = A[B, C] + [A, C]B$ and (124a)
$[AB, C] = A\{B, C\} - \{A, C\}B$ (124b)

With this, we can evaluate $[H, c_i]$:

- $\left[\sum_{lm} A_{lm} c_l^\dagger c_m, c_i\right]$: $= \sum_{lm} A_{lm} [c_l^\dagger c_m, c_i] = \sum_{lm} c_l^\dagger \underbrace{\{c_m, c_i\}}_{0} - \underbrace{\{c_l^\dagger, c_i\}}_{\delta_{li}} c_m$

$$= -\sum_m A_{im} c_m \quad (125)$$

- $\left[\frac{1}{2}\sum_{lmno} U_{lmno} c_l^\dagger c_m c_n^\dagger c_o, c_i\right]$: $= \frac{1}{2}\sum_{lmno} U_{lmno}\, c_l^\dagger c_m \underbrace{[c_n^\dagger c_o, c_i]}_{-\delta_{ni} c_o} + \underbrace{[c_l^\dagger c_m, c_i]}_{-\delta_{li} c_m} c_n^\dagger c_o$

$$= -\frac{1}{2}\sum_{lmio}\left(U_{lmio}\, c_l^\dagger c_m c_o + U_{imno}\, c_m c_n^\dagger c_o\right) = \sum_{lmn} \underbrace{\frac{1}{2}\left(U_{lmin} - U_{imln}\right)}_{= -U_{imln} \text{ since for fermions}} c_m c_l^\dagger c_n$$

$U_{lmin} = -U_{imln}$

$$= -\sum_{lmn} U_{imln}\, c_m c_l^\dagger c_n \quad (126)$$

$$\Rightarrow \frac{d}{d\tau} G^M_{ij}(\tau) = -\delta_{ij}\,\delta(\tau) - \sum_m A_{im} \underbrace{\left[-\langle c_m(\tau) c_j^\dagger\rangle \Theta(\tau) + \langle c_j^\dagger c_m(\tau)\rangle \Theta(-\tau)\right]}_{G^M_{mj}(\tau)} \quad (127)$$
$$- \sum_{lmn} U_{imln}\left[-\langle c_m(\tau) c_l^\dagger(\tau) c_n(\tau) c_j^\dagger\rangle \Theta(\tau) + \langle c_j^\dagger c_m(\tau) c_l^\dagger(\tau) c_n(\tau)\rangle \Theta(-\tau)\right]$$

$\Rightarrow$ The term in the second line can be rewritten, using the cyclic property of the Tr:

$$-\langle c_m(\tau)\, c_e^+(\tau)\, c_n(\tau)\, c_j^+ \rangle \Theta(\tau) + \langle c_j^+\, c_m(\tau)\, c_e^+(\tau)\, c_n(\tau) \rangle \Theta(-\tau)$$

$$= \langle c_j^+(-\tau)\, c_m\, c_e^+\, c_n \rangle \Theta(-\tau) - \langle c_m\, c_e^+\, c_n\, c_j^+(-\tau) \rangle \Theta(\tau) = G^{(2),M}_{jmen}(-\tau, 0, 0) \quad (128)$$

$$\Rightarrow \boxed{\frac{d}{d\tau} G^M_{ij}(\tau) = -\delta_{ij}\,\delta(\tau) - \sum_m A_{im}\, G^M_{mj}(\tau) - \sum_{men} U_{imen}\, G^{(2),M}_{jmen}(-\tau, 0, 0) \quad (129)}$$

or in the frequency domain: $G^M_{ij}(\tau) = \frac{1}{\beta}\sum_\nu e^{-i\nu\tau}\, \tilde{G}^M_{ij}(i\nu)$ and $G^{(2),M}_{jmen}(-\tau,0,0) = \frac{1}{\beta^3}\sum_{\nu\nu'\Omega} e^{-i\nu\tau}\, \tilde{G}^{(2),M}_{jmen}(i\nu, i\nu', i\Omega)$

$$\Rightarrow \frac{1}{\beta}\sum_\nu (-i\nu)\, \tilde{G}^M_{ij}(i\nu)\, e^{-i\nu\tau} = -\delta_{ij} \underbrace{\frac{1}{\beta}\sum_\nu e^{-i\nu\tau}}_{\delta(\tau)} - \frac{1}{\beta}\sum_\nu e^{-i\nu\tau} \sum_m A_{im}\, \tilde{G}^M_{mj}(i\nu) - \frac{1}{\beta}\sum_\nu e^{-i\nu\tau} \quad (130)$$

$$\times \sum_{men} U_{imen} \frac{1}{\beta^2} \sum_{\nu'\Omega} \tilde{G}^{(2),M}_{jmen}(i\nu, i\nu', i\Omega)$$

$\Rightarrow$ Comparing the terms inside $\frac{1}{\beta}\sum_\nu e^{-i\nu\tau}$, and reshuffeling the terms, leads to:

$$\boxed{\sum_m (i\nu\, \delta_{im} - A_{im})\, \tilde{G}^M_{mj}(i\nu) = \delta_{ij} + \sum_{men} U_{imen} \frac{1}{\beta^2} \sum_{\nu'\Omega} \tilde{G}^{(2),M}_{jmen}(i\nu, i\nu', i\Omega) \quad (131)}$$

Discussion:

- For the $\boxed{\text{noninteracting}}$ case $U_{imen}=0$, the equation of motion is a closed equation for calculating the one-particle Green's function:

$\Rightarrow$ $\left(-\frac{d}{d\tau} - H_0\right) G^M_{mj}(\tau) = \delta_{ij}\,\delta(\tau)$ (132)
$\hookrightarrow = \sum_m t_{im} \ldots$ for $U=0$

$\Rightarrow$ Let us define the index $x = (i\text{-}j,\tau)$ and the operator $L = \frac{\partial}{\partial\tau} - H_0$

$\Rightarrow$ We can formally write: $L\,G^M(x) = \delta(x)$ (133)

$\Rightarrow$ This is exactly the mathematical definition of a Green's function for a (differential) operator L!

- The interaction term couples the one- and the two-particle Green's function!
$\Rightarrow$ Going further, the Equation of motion for $G^{(2),M}$ couples to $G^{(3),M}$ and so on

$\Rightarrow$ Infinite hierarchy of coupled equations for the n-particle Green's function!