3. Green's functions and Matsubara formalism

How can we describe quantum many-body systems?

- Many-body wavefunction $\psi(\vec{r}_1, \dots, \vec{r}_N, t)$:

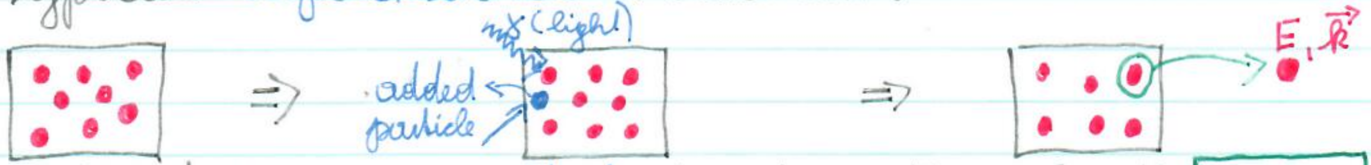
Problems for a very large number of particles (e.g.: $N \sim 10^{23}$ electrons in a solid)

→ No analytical solution is possible for interacting particles (see first chapter of the lecture)

→ Numerical calculation of $\psi(\vec{r}_1, \dots, \vec{r}_N, t)$ is very difficult:
e.g.: if we discretize the $\vec{r}$-space into 10 grid points in each direction
⇒ we have to calculate and store 10^{69} values for $\psi \triangleq 10^{60}$ GByte!!

→ A lot of information in $\psi(\vec{r}_1, \dots, \vec{r}_N, t)$ is NOT useful:
⇒ NO experiment can measure the positions of 10^{23} particles!

⇒ Typical experimental situation:



System of particles in equilibrium ⇒ We perturb the system (e.g.: add/excite particles) at time t_1 ⇒ We analyse the $\boxed{\text{response}}$ of the system to the perturbation (e.g. measure energy E and momentum $\vec{k}$ of emitted particle(s)) at time t_2.

⇒ This situation is formally described by the:

⊙ n-particle GREEN'S FUNCTION:

$$G^{(n)}_{i_1 \dots i_n; i_1' \dots i_n'} \sim \langle c_{i_1}(t_1) \dots c_{i_n}(t_n)\, c^\dagger_{i_1'}(t_1') \dots c^\dagger_{i_n'}(t_n') \rangle \quad (1)$$

→ $\langle \dots \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta(H-\mu N)} \dots\right),\ Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right)$ (2)... grand-canonical expectation value!

→ $c_i^{(\dagger)}(t) = e^{iHt} c_i^{(\dagger)} e^{-iHt} \Leftrightarrow \frac{dc_i^{(\dagger)}}{dt} = i[H, c_i^{(\dagger)}(t)]$ (3)... annihilation operator in Heisenberg picture!

$\Rightarrow i_j^{(1)}$ ... Quantum number(s) of single-particle state,
e.g.: $i_j^{(1)} \hat{=} (\vec{r}_j^{(1)} \sigma_j^{(1)})$ or $i_j^{(1)} \hat{=} (R_j^{(1)} \sigma_j^{(1)})$ or $i_j^{(1)} \hat{=} (\vec{k}_j^{(1)} \sigma_j^{(1)})$ or .....
↳ position ↳ lattice vector ↳ (lattice) momentum

Most important cases:

$\Rightarrow n=1$ ... $G^{(1)} = G_{i_1 i_2}(t_1, t_2) \sim \langle c_{i_1}(t_1)\, c_{i_2}^{+}(t_2) \rangle$ ... one-particle Green's function (4)

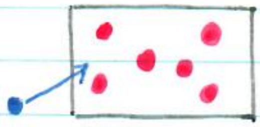
$\Rightarrow n=2$ ... $G^{(2)} \sim \langle c_{i_1}(t_1)\, c_{i_2}(t_2)\, c_{i_1'}^{+}(t_1')\, c_{i_2'}^{+}(t_2') \rangle$ ... two-particle Green's functions (5)

One-particle operator: $\langle O_1 \rangle = \sum_{i_1 i_2} \underbrace{\langle \varphi_{i_1} | O_1^{(1)} | \varphi_{i_2} \rangle}_{O_{i_1 i_2}} \langle c_{i_1}^{+} c_{i_2} \rangle \sim \sum_{i_1 i_2} O_{i_1 i_2}\, G_{i_1 i_2}(0,0)$ (6)

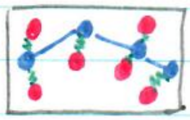
$\Rightarrow$ <u>Any</u> expectation value of a n-particle operator can be expressed through the n-particle Green's function!!

One-particle Green's functions

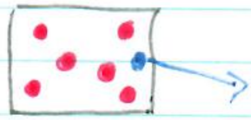
We have to consider two processes:



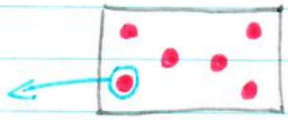
A particle is added to the system at time t'



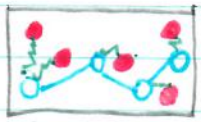
The particle propagates through the system



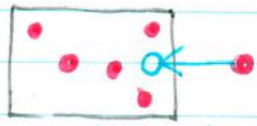
The particle is removed at time $t > t'$



A particle is removed from the system at time t



The hole propagates through the system



A particle is added at time $t' > t$

This processes are described by the $\boxed{\text{causal}}$ or $\boxed{\text{time-ordered}}$ GF:

$$G^{C}_{ij}(t',t) = -i\,\langle c_i(t)\, c_j^{\dagger}(t')\rangle\, \Theta(t-t') \overset{\text{Bosons}}{\underset{\text{Fermions}}{\mp}} i\,\langle c_j^{\dagger}(t')\, c_i(t)\rangle\, \Theta(t'-t) \tag{7}$$

Define: Time order operator T: $T(A(t)B(t')) = A(t)B(t')\Theta(t-t') \pm B(t')A(t)\Theta(t'-t)$ (8)

(+ → Bosonic operator, − → Fermionic operator)

$\Rightarrow G^c_{ij}(t',t) = -i\langle T(c_i(t)\, c_j^\dagger(t'))\rangle$ (9). also called „timeordered" Green's function!

Multiindices i and j $\left\{\begin{matrix} i \,\hat{=}\, (\vec{r}, \sigma) \\ j \,\hat{=}\, (\vec{r}\,', \sigma') \end{matrix}\right\}$ $\left\{\begin{matrix} i \,\hat{=}\, (\vec{R}_i, \sigma) \\ j \,\hat{=}\, (\vec{R}_j, \sigma') \end{matrix}\right\}$ $\left\{\begin{matrix} i \,\hat{=}\, (\vec{k}, \sigma) \\ j \,\hat{=}\, (\vec{k}\,', \sigma') \end{matrix}\right\}$ (10)

Coordinate, $\in \mathbb{R}^3$ — Lattice vector — (lattice) momentum

Typical simplifications due to symmetries:

→ (Lattice) translational symmetry:
- $\Rightarrow$ G^c depends only on $(\vec{R}_i - \vec{R}_j)$ / $\vec{r} - \vec{r}\,'$
- $\Rightarrow$ $\vec{k} = \vec{k}\,'$ (momentum conservation)

→ SU(2) rotational symmetry:
- $\Rightarrow$ $\sigma = \sigma'$

→ For a time independent Hamiltonian $H \Rightarrow$ time translational invariance:

$$\langle c_i(t)\, c_j^+(t')\rangle = \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} e^{itH} c_i e^{-itH} e^{it'H} c_j^+ e^{-it'H}\right)$$

(Here, we have redefined: $H-\mu N = H$)

$$= \frac{1}{Z}\,\mathrm{Tr}\left(e^{-it'H} e^{-\beta H} e^{itH} c_i e^{-i(t-t')H} c_j^+\right)$$

Cyclic property of the trace: $\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$

$$= \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} e^{i(t-t')H} c_i e^{-i(t-t')H} c_j^+\right) = \langle c_i(t-t')\, c_j^+(0)\rangle \quad (11)$$

... and analogous for $\langle c_i^+(t')\, c_j(t)\rangle$!

$$\Rightarrow G_{ij}^c(t',t) = G_{ij}^c(0,t-t') =: G_{ij}^c(t) \quad (12)$$

$\Rightarrow$ we can always assume $t'=0$!

Remark: For $T=0$ $(\beta = \infty)$, $\rho = \frac{e^{-\beta H}}{Z} = |\psi_0\rangle\langle\psi_0|$, i.e. ρ becomes the projection operator on the ground state $|\psi_0\rangle$, $H|\psi_0\rangle = E_0|\psi_0\rangle$

$$\Rightarrow \langle c_j(t)\, c_j^+(t')\rangle = \langle\psi_0| e^{itH} c_j e^{-i(t-t')H} c_i^+ e^{-it'H}|\psi_0\rangle = e^{i\boxed{(t-t')}E_0}\langle\psi_0| c_j e^{i\boxed{(t-t')}H} c_i^+|\psi_0\rangle \quad (13)$$

Matsubara Formalism

Let us have a closer look at the matrix element

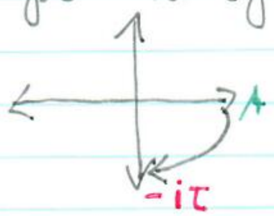
$$\langle c_i(t)\, c_j^+ \rangle = \frac{1}{Z}\,\mathrm{Tr}\Big(e^{\overset{\in\mathbb{R}}{-\beta H}}\, e^{\overset{\in\mathbb{I}}{itH}}\, c_i\, e^{-itH}\, c_j^+\Big) = \frac{1}{Z}\,\mathrm{Tr}\Big(e^{\overset{\in\mathbb{C}}{-(\beta-it)H}}\, c_i\, e^{-itH}\, c_j^+\Big) \quad (14)$$

⇒ we have the complex factor $\beta - it$ in the exponent

- Theory would be „easier", if we have only real numbers in the exponent.
- A Fourier transform $\int_{-\infty}^{+\infty} dt\, e^{i\omega t} \dots$ can lead to convergence problems due to the oscillating factors $e^{\pm itH}$
  ⇒ a suppressing prefactor e^{-tH} (i.e. without imaginary unit in the exponent) would be „better."

⇒ This can be achieved by going from real times t to imaginary times τ:

Complex time plane:



i.e., we perform the replacement $\boxed{t \to -i\tau}$

⇒ We can now define the Matsubara Green's function:

$$G_{ij}^{M}(\tau) = -\langle T_\tau \left(c_i(\tau)\, c_j^\dagger \right) \rangle = -\langle c_i(\tau) c_j^\dagger \rangle \Theta(\tau) \underset{\text{Fermions}}{\overset{\text{Bosons}}{\mp}} \langle c_j^\dagger\, c_i(\tau) \rangle \Theta(-\tau) \quad (15)$$

→ T_τ ... time ordering operator for imaginary times

→ $c_i(\tau) = e^{\tau H}\, c_i\, e^{-\tau H}$ (16) *Note:* $c_i^\dagger(\tau) = e^{\tau H} c_i^\dagger e^{-\tau H} \Rightarrow [c_i(\tau)]^\dagger = e^{-\tau H} c_i e^{\tau H} \neq c_i^\dagger(\tau)$!!
$c_i(\tau)$ and $c_i^\dagger(\tau)$ not Hermitian conjugates!!

→ $\langle \ldots \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} \ldots\right)$, $Z = \mathrm{Tr}\left(e^{-\beta H}\right)$ (17) as usual
The chemical potential is again included in H $(H \to H - \mu N)$!

In which interval can τ vary?

$\Rightarrow$ Evaluate $G^M_{ij}(\tau)$ for an Eigenbasis of H: $H|N\rangle = E_N|N\rangle$ (18)

$|N\rangle$ ... many-body eigenstate of H to the eigenvalue E_N
(in contrast to the single particle states $i, j, \ldots, m, n, \ldots$!)

$$\Rightarrow G^M_{ij}(\tau) = \frac{1}{Z}\left[-\mathrm{Tr}\left(e^{-\beta H} e^{\tau H} c_i e^{-\tau H} c_j^+\right)\Theta(\tau) \mp \mathrm{Tr}\left(e^{-\beta H} c_j^+ e^{\tau H} c_i e^{-\tau H}\right)\Theta(-\tau)\right]$$

$$= \frac{1}{Z}\sum_N \langle N|e^{-\beta H} e^{\tau H} c_i e^{-\tau H} c_j^+|N\rangle\Theta(\tau) \mp \langle N|e^{-\beta H} c_j^+ e^{\tau H} c_i e^{-\tau H}|N\rangle\Theta(-\tau)$$

$$= \frac{1}{Z}\sum_N \bar{e}^{(\beta-\tau)E_N}\langle N|c_i e^{-\tau H} c_j^+|N\rangle\Theta(\tau) \mp \bar{e}^{(\beta+\tau)E_N}\langle N|c_j^+ e^{\tau H} c_i|N\rangle\Theta(-\tau) \quad (19)$$

$\Rightarrow$ To guarantee the convergence of the $\sum_N$, the exponential functions should exponentially damp the contributions for $E_N \to \infty$:

$\Rightarrow$ $\beta-\tau > 0$ and $\beta+\tau > 0$ $\Rightarrow$ $\boxed{-\beta < \tau < +\beta}$ $\left[\tau \in (-\beta, \beta)\right]$ (20)

For $0 < \tau < \beta$, let us now consider $G^M_{ij}(\tau-\beta)$:

$$G^M_{ij}(\tau-\beta) = \mp \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} c_j^+ e^{(\tau-\beta)H} c_i e^{-(\tau-\beta)H}\right)$$

cyclic property of the trace

$$= \mp \frac{1}{Z}\,\mathrm{Tr}\left(e^{(\tau-\beta)H} c_i \overbrace{e^{-\beta H} e^{-(\tau-\beta)H}}^{e^{-\tau H}} c_j^+\right)$$

$$= \mp \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} e^{\tau H} c_i e^{-\tau H} c_j^+\right) = \underset{\text{Fermions}}{\overset{\text{Bosons}}{\pm}} G^M_{ij}(\tau) \quad (21)$$

(In particular: $G^M_{ij}(-\beta) = G^M_{ij}(+\beta) = \pm G^M_{ij}(0) \Rightarrow \tau = \pm\beta$ can be included!)

<u>Summary:</u>

$$\boxed{G^M_{ij}(\tau) = -\langle T_\tau(c_i(\tau)c_j^+)\rangle,\quad \tau\in[-\beta,\beta],\quad G^M_{ij}(\tau-\beta) = \pm G^M_{ij}(\tau) \text{ for } 0\leq\tau\leq\beta} \quad (22)$$

$\Rightarrow$ The Matsubara Green's function is periodic (bosons) or antiperiodic (fermions) in the interval $[-\beta, +\beta]$ with periodicity β!

Remarks:

→ For $T=0$ ($\beta=\infty$), the $\mathrm{Tr}(\ldots)$ is replaced by the expectation value $\langle\psi_0|\ldots|\psi_0\rangle$ of the ground state $|\psi_0\rangle$
⇒ no cyclicity ⇒ no (anti)periodicity for $\tau\in(-\beta=-\infty, +\beta=+\infty)$!

→ Outside the interval $[-\beta,\beta]$, $G^M_{ij}(\tau)$ is not defined.
⇒ One can extend the domain of definition, by continuing $G^M_{ij}(\tau)$ (anti)periodically to $\tau\in\mathbb{R}$:

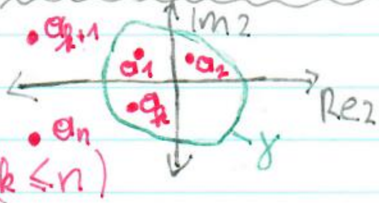
For $\tau>\beta$: $G^M_{ij}(\tau) := (\pm 1)^{\frac{\tau}{\beta}} \cdot G^M_{ij}(\tau \bmod \beta)$ (23) (and analogous for $\tau<-\beta$)

⇒ This (anti)periodization of the Green's function will be further discussed later in the section on the Fourier transform!

Fourier transform and analytical properties of the one-particle Green's functions

Reminder: Useful mathematical relations and theorems

1) Residue Theorem:



$f: \mathbb{C} \to \mathbb{C}$ ... complex function, which is analytic
$z \to f(z)$ on $\mathbb{C}$ except for the points $a_1, \dots, a_n$

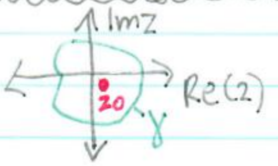
$$\Rightarrow \oint_\gamma dz\, f(z) = 2\pi i \sum_{j=1}^{k} \mathrm{Res}(f, a_j) \quad (24)$$

$\mathrm{Res}(f, a_j)$ ... Residue of f at a_j

If a_j is a pole of n^{th} order of $f(z)$:

$$\mathrm{Res}(f, a_j) = \frac{1}{(n-1)!} \lim_{z \to a_j} \frac{d^{n-1}}{dz^{n-1}} \left((z-a_j)^n f(z) \right) \quad (25)$$

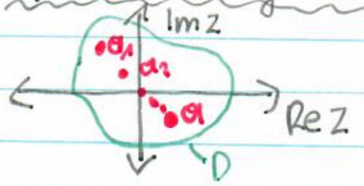
2) Cauchy's integral formula: ($\Rightarrow$ follows from residue theorem)



$f: \mathbb{C} \to \mathbb{C}$ ... analytic
$z \to f(z)$ on $\mathbb{C}$

$$\Rightarrow f(z_0) = \frac{1}{2\pi i} \oint_\gamma dz \frac{f(z)}{z - z_0} \quad (26)$$

3) Identity theorem for complex functions:



$f, g : D \to \mathbb{C}$ are two complex analytic functions
$z \to f(z), g(z)$ on the domain $D \subseteq \mathbb{C}$.

$a_n \in D$ ... Series of complex numbers with $\lim_{n\to\infty} a_n = a$

Theorem: If $f(a_n) = g(a_n)$ $\forall n \in \mathbb{N}$: $f(z) = g(z)$ $\forall z \in D$

In words: Two complex analytic functions are equivalent on a domain D, when they are equivalent for a series of complex numbers $a_n \in D$ with an accumulation point $a \in D$

Practical Relevance: If we know a function $f(z)$ for a series of points $z_1, z_2, \ldots$, we can continue it analytically larger region of the complex plane in a unique way!

4) Convolution Theorem:

Consider two function $f(t), g(t)$ with the Fourier transforms $\tilde{f}(\omega), \tilde{g}(\omega)$:

$$\tilde{f}(\omega) \,|\, \tilde{g}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t} f(t) \,|\, g(t) \Rightarrow \text{For the product } f(t)\cdot g(t) \text{ we have:}$$

$$F(f(t)\cdot g(t)) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t} f(t)\, g(t) = \frac{1}{2\pi} \underbrace{\int d\omega'\, \tilde{f}(\omega')\, \tilde{g}(\omega-\omega')}_{\text{convolution of } \tilde{f}(\omega) \text{ and } \tilde{g}(\omega)} \quad (27)$$

5) Fourier transform of the Θ function:

convergence factor $\delta > 0$

$$F[\Theta(t)] = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, \Theta(t) = \lim_{\delta\to 0+} \int_0^{\infty} dt\, e^{i\omega t - \delta t}$$

$$= \lim_{\delta\to 0+} -\frac{1}{i\omega-\delta} = \lim_{\delta\to 0+} \frac{i\omega+\delta}{\omega^2+\delta^2} = i \underbrace{\lim_{\delta\to 0+} \frac{\omega}{\omega^2+\delta^2}}_{P\frac{1}{\omega}} + \underbrace{\lim_{\delta\to 0+} \frac{\delta}{\omega^2+\delta^2}}_{\pi\,\delta(\omega)}$$

$$\Rightarrow \quad F[\Theta(t)] = \int_{-\infty}^{+\infty} dt\, \Theta(t)\, e^{i\omega t} = \pi\,\delta(\omega) + i\,P\frac{1}{\omega} \quad (28)$$

Principal value!

Fourier transforms of $G_{ij}^{c}(t)$ and $G_{ij}^{M}(\tau)$:

$$\boxed{\tilde{G}_{ij}^{c}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, G_{ij}^{c}(t) \iff G_{ij}^{c}(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega\, e^{-i\omega t}\, \tilde{G}_{ij}^{c}(\omega) \quad (29)}$$

⇒ Fourier integral for function defined on $(-\infty, +\infty)$ without periodicity!

The Matsubara Green's function is defined on the finite interval $[-\beta, \beta]$

⇒ If we continue $G_{ij}^{M}(\tau)$ to a periodic function outside this interval, i.e., $G_{ij}^{M}(\tau + 2\beta) = G_{ij}^{M}(\tau)$, we can represent it as Fourier series:

$$g_{ij}(n) = \frac{1}{2\beta}\int_{-\beta}^{\beta} d\tau\, e^{i\frac{2\pi n \tau}{2\beta}}\, G_{ij}^{M}(\tau) \iff G_{ij}^{M}(\tau) = \sum_{n=-\infty}^{+\infty} e^{-i\frac{2\pi n\tau}{2\beta}}\, g_{ij}(n) \quad (30)$$

↳ Fourier coefficient with $n \in \mathbb{Z}$!

How can we implement the constraint (21): $G_{ij}^{M}(\tau + \beta) = \pm G_{ij}^{M}(\tau)$?

$$\Rightarrow \quad G^M_{ij}(\tau+\beta) = \sum_{n=-\infty}^{+\infty} \underbrace{e^{-i\pi n}}_{(-1)^n} e^{-i\frac{2\pi n \tau}{2\beta}} g_{ij}(n) \overset{!}{=} \pm \sum_{n=-\infty}^{+\infty} e^{-i\frac{2\pi n\tau}{2\beta}} g_{ij}(n) \quad (31)$$

$$\text{i.e.:} \quad \begin{cases} \text{For bosons: } (-1)^n \overset{!}{=} +1 \ \ldots \text{ only even } n = 2m,\ m \in \mathbb{Z} \\ \text{For fermions: } (-1)^n \overset{!}{=} -1 \ \ldots \text{ only odd } n = 2m+1,\ m \in \mathbb{Z}. \end{cases} \quad (32)$$

We define the following quantities:

$$\rightarrow \quad \nu_m = \begin{cases} \frac{2m\pi}{\beta},\ m \in \mathbb{Z} \ \ldots \text{ BOSONIC MATSUBARA FREQUENCY} \\ \frac{(2m+1)\pi}{\beta},\ m \in \mathbb{Z} \ \ldots \text{ FERMIONIC MATSUBARA FREQUENCY} \end{cases} \quad (33)$$

$$\rightarrow \quad \tilde{G}^M_{ij}(i\nu_m) = \beta \cdot \begin{cases} g_{ij}(2m) \ldots \text{Bosons} \\ g_{ij}(2m+1) \ldots \text{Fermions} \end{cases} \quad (34)$$

$$\boxed{\tilde{G}^M_{ij}(i\nu_m) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau\, e^{i\nu_m \tau} G^M_{ij}(\tau) \iff G^M_{ij}(\tau) = \frac{1}{\beta} \sum_{\nu_m} e^{-i\nu_m \tau} \tilde{G}_{ij}(i\nu_m) \quad (35)}$$

imaginary unit indicates that this is an imaginary frequency!

<u>Note</u>: For $T=0$, the Matsubara frequencies become continuous and the difference between bosonic and fermionic frequencies is lost!

Simplification due to (anti) periodicity:

$$\tilde{G}^M_{ij}(i\nu_m) = \frac{1}{2}\int_{-\beta}^{0} d\tau\, e^{i\nu_m\tau} G^M_{ij}(\tau) + \frac{1}{2}\int_0^\beta d\tau\, e^{i\nu_m\tau} G^M_{ij}(\tau)$$

$\hookrightarrow \tau = \tau' - \beta$

$$= \frac{1}{2}\int_0^\beta d\tau'\, e^{i\nu_m\tau'} e^{-i\nu_m\beta} G^M_{ij}(\tau'-\beta) + \frac{1}{2}\int_0^\beta d\tau\, e^{i\nu_m\tau} G^M_{ij}(\tau) \quad (36)$$

We have: $G^M_{ij}(\tau'-\beta) = \pm G^M_{ij}(\tau)$ and $e^{-i\nu_m\beta} = \begin{cases} e^{-i2m\pi} = +1 \text{ (Bosons)} \\ e^{-i(2m+1)\pi} = -1 \text{ (Fermion)} \end{cases}$

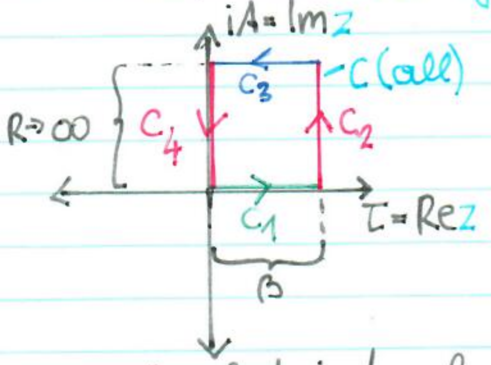
$\Rightarrow e^{-i\nu_m\beta} G^M_{ij}(\tau'-\beta) = + G^M_{ij}(\tau')$ (37) (for bosons and fermions!)

$$\Rightarrow \boxed{\tilde{G}^M_{ij}(i\nu_m) = \int_0^\beta d\tau\, e^{i\nu_m\tau} G^M_{ij}(\tau) \iff G^M_{ij}(\tau) = \frac{1}{\beta}\sum_{\nu_m} e^{-i\nu_m\tau}\tilde{G}^M_{ij}(i\nu_m) \quad (38)}$$

Important question: How are $G^C_{ij}(t)$ and $G^M_{ij}(\tau)$ as well as $\tilde{G}^C_{ij}(\omega)$ and $\tilde{G}^M_{ij}(i\nu_m)$ related?

$\Rightarrow$ The answer should also unravel the physical meaning of G^M_{ij}!

⇒ Consider the complex time variable $z = \tau + it$ (unpublished work from G.R. et al)



We consider the contour integral along the closed path C (consisting of C_1, C_2, C_3, C_4):

$$\oint_C dz\, e^{i\nu_m \cdot z} G^M_{ij}(z) = \left[\int_{C_1} dz + \int_{C_2} dz + \int_{C_3} dz + \int_{C_4} dz \right] e^{i\nu_m z} G^M_{ij}(z) \tag{39}$$

$= 0$! ($e^{i\nu_m z} G^M_{ij}(z)$ has no singularities inside C)

⇒ Calculate integrals for C_1, C_2, C_3 and C_4:

• C_1: $z = \tau$, $\tau \in [0, \beta]$, $dz = d\tau$

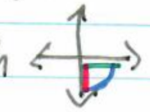
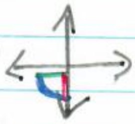
$$\Rightarrow \boxed{\int_{C_1} dz\, e^{i\nu_m z} G^M_{ij}(z) =} -\frac{1}{Z} \int_0^\beta d\tau\, e^{i\nu_m \tau} \mathrm{Tr}\left(e^{-\beta H} e^{\tau H} c_i e^{-\tau H} c_j^+ \right) = \boxed{\tilde{G}^M_{ij}(i\nu_m)} \tag{40}$$

⇒ This integral gives us the Matsubara Green's function in Fourier representation $\tilde{G}^M_{ij}(i\nu_m)$!

$\Rightarrow$ $\boxed{\nu > 0:}$

$$\tilde{G}^M_{ij}(i\nu) = -i \int_0^\infty dt\, e^{-\nu t} \langle 0 | c_i(t) c_j^\dagger \mp c_j^\dagger c_i(t) | 0 \rangle$$
$$= \int_{-\infty}^{\infty} dt\, e^{-\nu t}\, G^R_{ij}(t)$$

where: $G^R_{ij}(t) = -i \langle 0 | c_i(t) c_j^\dagger \mp c_j^\dagger c_i(t) | 0 \rangle$

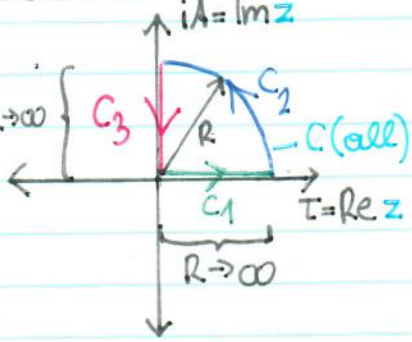
$\Rightarrow$ $\boxed{\nu < 0:}$ Analogous procedure with  and 

$$\tilde{G}^M_{ij}(\nu) = +i \int_{-\infty}^{0} dt\, e^{\nu t} \langle 0 | c_i(t) c_j^\dagger \mp c_j^\dagger c_i(t) | 0 \rangle$$
$$= \int_{-\infty}^{+\infty} e^{\nu t}\, G^A_{ij}(t)$$

where: $G^A_{ij}(t) = i \langle 0 | c_i(t) c_j^\dagger \mp c_j^\dagger c_i(t) | 0 \rangle$

The definition and properties of $\tilde{G}^R_{ij}(\omega)$ and $\tilde{G}^A_{ij}(\omega)$ are the same as for $T \neq 0$ $(\beta < \infty)$!

$\Rightarrow g^{(1)}_{ij}(v)$: $\int_0^\infty d\tau\, e^{iv\tau} \langle 0| e^{\tau H} c_i e^{-\tau H} c_j^\dagger |0\rangle$, $\boxed{v>0}$



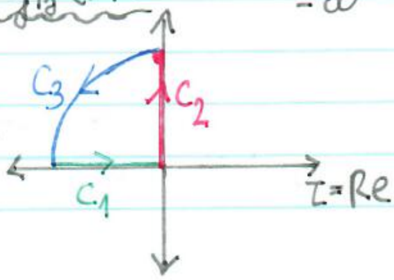
$$\oint_C dz\, e^{ivz} \langle 0| e^{zH} c_i e^{-zH} c_j^\dagger |0\rangle = 2\pi i \,\mathrm{Res}(\;) = 0$$

$$\Rightarrow \underbrace{\int_0^\infty d\tau\, e^{iv\tau} \langle 0| e^{\tau H} c_i e^{-\tau H} c_j^\dagger |0\rangle}_{C_1} + \underbrace{iR \int_0^{\pi/2} d\varphi\, e^{i\varphi} e^{ivR\cos\varphi} \boxed{e^{-vR\sin\varphi}} \times \langle 0| \dots |0\rangle}_{C_2,\ \Rightarrow 0 \text{ for } R\to\infty}$$

$$+ \underbrace{i \int_\infty^0 d\lambda\, e^{-v\lambda} \langle 0| e^{i\lambda H} c_i e^{-i\lambda H} c_j^\dagger |0\rangle}_{C_3} = 0!$$

$$\Rightarrow \boxed{g^{(1)}_{ij}(v) = \int_0^\infty d\tau\, e^{iv\tau} \langle 0| e^{\tau H} c_i e^{-\tau H} c_j^\dagger |0\rangle = i \int_0^\infty d\lambda\, e^{-v\lambda} \langle 0| e^{i\lambda H} c_i e^{-i\lambda H} c_j^\dagger |0\rangle}$$

$\Rightarrow g^{(2)}_{ij}(v)$: $\int_{-\infty}^0 d\tau\, e^{iv\tau} \langle 0| c_j^\dagger e^{\tau H} c_i e^{-\tau H} |0\rangle$



$$\boxed{\begin{aligned} g^{(2)}_{ij}(v) &= \int_0^\infty d\tau\, e^{iv\tau} \langle 0| c_j^\dagger e^{\tau H} c_i e^{-\tau H} |0\rangle \\ &= -i \int_0^\infty d\lambda\, e^{-v\lambda} \langle 0| c_j^\dagger e^{i\lambda H} c_i e^{-i\lambda H} |0\rangle \end{aligned}}$$

⊙ Fourier transform: $G^M_{ij}(\tau) = -\langle c_i(\tau) c^+_j \rangle \Theta(\tau) \mp \langle c^+_j c_i(\tau) \rangle \Theta(-\tau)$

$\tau \in (-\beta, \beta) \rightarrow \tau \in (-\infty, +\infty)$, NO (anti) periodicity!

$$\Rightarrow \tilde{G}^M_{ij}(i\nu) = \int_{-\infty}^{+\infty} d\tau \, e^{i\nu\tau} G^M_{ij}(\tau) \Leftrightarrow G^M_{ij}(\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\nu \, e^{-i\nu\tau} \tilde{G}^M_{ij}(i\nu)$$

Note: The Matsubara frequency ν is now a continuous variable!

$$\tilde{G}^M_{ij}(i\nu) = \underbrace{-\int_0^{\infty} d\tau \, e^{i\nu\tau} \langle 0 | e^{\tau H} c_i e^{-\tau H} c^+_j | 0 \rangle}_{g^{(1)}_{ij}(\nu)} \mp \underbrace{\int_{-\infty}^{0} d\tau \, e^{i\nu\tau} \langle 0 | c^+_j e^{\tau H} c_i e^{-\tau H} | 0 \rangle}_{g^{(2)}_{ij}(\nu)}$$

$\Rightarrow$ Here, both time orders give different contributions to $\tilde{G}^M_{ij}(i\nu)$ and, hence, have to be treated explicitly!

$\Rightarrow$ There is no relation which allows to express $\int_{-\infty}^{0}$ in terms of $\int_0^{\infty}$!

$\tilde{G}^M_{ij}(i\nu_m)$ at $T=0$ ($\beta=0$):

⊙ $\langle \ldots \rangle = \frac{1}{Z}\,\mathrm{Tr}(e^{-\beta H}\ldots)$, $Z = \mathrm{Tr}(e^{-\beta H})$

⇒ Evaluate $\frac{1}{Z}\mathrm{Tr}(e^{-\beta H}\ldots)$ using an eigenbasis of H: $H|E_N\rangle = E_N|N\rangle$

$$\Rightarrow \langle \ldots \rangle = \frac{1}{\sum_N e^{-\beta E_N}} \sum_N e^{-\beta E_N} \langle N|\ldots|N\rangle =$$

$$= \frac{1}{e^{-\beta E_0}} \frac{1}{1+\sum_{N\neq 0} e^{-\beta(E_N-E_0)}} \cdot e^{-\beta E_0}\left(\langle 0|\ldots|0\rangle + \sum_{N\neq 0} e^{-\beta(E_N-E_0)}\langle N|\ldots|N\rangle\right)$$

$|0\rangle$ ... ground state with ground state energy $E_0 < E_{N\neq 0}$!

⇒ for $\beta\to\infty$ we have: $\lim_{\beta\to\infty} e^{-\beta\underbrace{(E_N-E_0)}_{>0}} = 0$!

$\boxed{\langle \ldots \rangle = \langle 0|\ldots|0\rangle}$, i.e., the expectation value of any operator (indicated by ...) is the expectation value for the ground state!

• C_2 : $z = \beta + i\lambda$, $\lambda \in [0, R)$ with $R \to \infty$, $dz = i\,d\lambda$

$$\Rightarrow \int_{C_2} dz\, e^{i\nu_m z} G^M_{ij}(z) = -\frac{1}{Z} \int_0^R d\lambda\, i\, \mathrm{Tr}\left(\cancel{e^{-\beta H}}\, \cancel{e^{(\beta+i\lambda)H}}\, c_i\, e^{-(\beta+i\lambda)H} c_j^+\right) e^{i\nu_m(\beta+i\lambda)}$$

$$= -i \int_0^\beta d\lambda\, \frac{1}{Z} \mathrm{Tr}\Big(e^{-\beta H} c_j^+ \underbrace{e^{i\lambda H} c_i e^{-i\lambda H}}_{c_i(\lambda)}\Big) \underbrace{e^{i\nu_m \beta}}_{\pm 1} \cdot e^{-\nu_m \lambda} \quad (41)$$

↳ cyclicity of Tr!

$e^{-\nu_m \lambda}$: For $R \to \infty$, the integral converges only if $\boxed{\nu_m > 0}$! (42)

$$\boxed{\int_{C_2} dz\, e^{i\nu_m z} G^M_{ij}(z) = \mp i \int_0^\infty d\lambda\, e^{-\nu_m \lambda} \langle c_j^+ c_i(\lambda) \rangle \quad (43)}$$

• C_3 : $z = \tau + iR$, with $R \to \infty$, $\tau \in [\beta, 0]$, $dz = d\tau$

$$\Rightarrow \int_{C_3} dz\, e^{i\nu_m z} G^M_{ij}(z) = -\frac{1}{Z} \int_\beta^0 d\tau\, \mathrm{Tr}\left(e^{-\beta H} e^{(\tau+iR)H} c_i\, e^{-(\tau+iR)H} c_j^+\right) e^{i\nu_m \tau}\, e^{-\nu_m R} \quad (44)$$

$e^{-\nu_m R} = 0$ for $\nu_m > 0$ and $R \to \infty$! $\boxed{\int_{C_3} dz\, e^{i\nu_m z} G^M_{ij}(z) \underset{R\to\infty}{=} 0 \ , \nu_m > 0 \quad (45)}$

• C_4: $z = iA$, $A \in (R, 0]$ with $R \to \infty$, $dz = i\,dA$

$$\Rightarrow \int_{C_4} dz\; e^{i\nu_m z}\, G^M_{ij}(z) = -\frac{1}{Z}\, i \int_R^0 dA\, \mathrm{Tr}\Big(e^{-\beta H}\, \underbrace{e^{iAH} c_i e^{-iAH}}_{c_i(A)} c_j^+\Big)\, e^{-\nu_m A} \quad (46)$$

$$\Rightarrow \boxed{\int_{C_4} dz\; e^{i\nu_m z}\, G^M_{ij}(z) \underset{R\to\infty}{=} +i \int_0^\infty dA\, e^{-\nu_m A} \langle c_i(A)\, c_j^+ \rangle} \quad (47)$$

From Eqs. (39) and (40) we find the following expression for $\tilde{G}^M_{ij}$:

$$\underbrace{\int_{C_1} dz\, e^{i\nu_m z} G^M_{ij}(z)}_{\downarrow\, \text{Eq.}(40)} = -\underbrace{\int_{C_2} dz\, e^{i\nu_m z} G^M_{ij}(z)}_{\downarrow\, \text{Eq.}(43)} - \underbrace{\int_{C_3} dz\, e^{i\nu_m z} G^M_{ij}(z)}_{0\,!\ [\text{Eq.}(45)]} - \underbrace{\int_{C_4} dz\, e^{i\nu_m z} G^M_{ij}(z)}_{\downarrow\, \text{Eq.}(47)} \quad (48)$$

$$\tilde{G}^M_{ij}(i\nu_m) = \pm i \int_0^\infty dA\, e^{-\nu_m A} \langle c_j^+ c_i(A) \rangle - 0 - i \int_0^\infty dA\, e^{-\nu_m A} \langle c_i(A) c_j^+ \rangle \quad (49)$$

⇒ We have expressed the Matsubara Green's function in imaginary frequencies by an integral over real times t!

$$\tilde{G}^M_{ij}(i\nu_m) = -i\int_0^{\infty} dt\, e^{-\nu_m t}\left[\langle c_i(t)c_j^+ \mp \langle c_j^+ c_i(t)\rangle\right], \quad \nu_m > 0 \qquad (50)$$

With the definition of the retarded Green's function:

$$\boxed{G^R_{ij}(t) = -i\langle c_i(t)c_j^+ \underset{\text{Fermions}}{\overset{\text{Bosons}}{\mp}} c_j^+ c_i(t)\rangle\,\Theta(t) = -i\left\{\begin{matrix}\langle [c_i(t)c_j^+]\rangle \to \text{commutator} \\ \langle \{c_i(t)c_j^+\}\rangle \to \text{anticommutator}\end{matrix}\right\}\cdot\Theta(t) \qquad (51)}$$

we find:

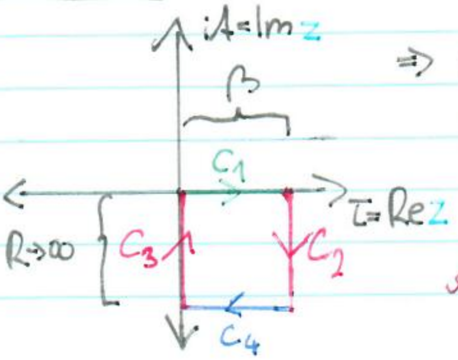
$$\boxed{\tilde{G}^M_{ij}(i\nu_m) = \int_{-\infty}^{+\infty} dt\, e^{-\nu_m t}\, G^R_{ij}(t), \quad \nu_m > 0 \qquad (52)}$$

↳ because we have $\Theta(t)$ in the definition of $G^R_{ij}(t)$!

Note: The time-ordered Matsubara Green's function $G^M_{ij}(\tau)$ is related - via its Fourier transform $\tilde{G}^M_{ij}(i\nu_m)$ - to the retarded Green's function $G^R_{ij}(t)$ on the real time axis, NOT to the time-ordered (causal) Green's function $G^c_{ij}(t)$!

$$\left\{\begin{array}{l} G^c_{ij}(t) = \pm i \langle c_i(t)\, c_j^+ \rangle \Theta(t) + i \langle c_j^+\, c_i(t) \rangle\, \Theta(-t) \\ G^R_{ij}(t) = -i \langle c_i(t)\, c_j^+ \rangle \Theta(t) \pm i \langle c_j^+\, c_i(t) \rangle\, \Theta(t) \end{array}\right] \qquad (53)$$

Question: What about $\boxed{\nu_m < 0\ ?}$



⇒ Consider closed path in the negative imaginary plane:

$$\boxed{\tilde{G}^M_{ij}(i\nu_m) = \int_{-\infty}^{+\infty} dt\, e^{\nu_m t}\, G^A_{ij}(t)} \qquad (54)$$

Advanced Green's function:

$$\boxed{G^A_{ij}(t) = i \langle c_i(t) c_j^+ \mp c_j^+ c_i(t) \rangle \Theta(-t)} \qquad (55)$$

Fourier transform of $G^R_{ij}(t)$ and $G^A_{ij}(t)$:

$$\tilde{G}^R_{ij}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, G^R_{ij}(t) = \int_{0}^{+\infty} dt\, e^{i\omega t}\, G^R_{ij}(t) \qquad (56)$$

$$\tilde{G}^A_{ij}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, G^A_{ij}(t) = \int_{-\infty}^{0} dt\, e^{i\omega t}\, G^A_{ij}(t) \qquad (57)$$

We define a complex frequency variable $z = \omega + i\nu$:

For $\tilde{G}^R_{ij}(\omega)$: $\omega \to z = \omega + i\nu \Rightarrow \tilde{G}^R_{ij}(z) = \int_{0}^{\infty} dt\, e^{i\omega t}\, \boxed{e^{-\nu t}}\, G^R_{ij}(t) \qquad (58)$

$\Rightarrow \tilde{G}^R_{ij}(z)$ is well defined for $\nu = \operatorname{Im} z > 0$ due to the damping factor $e^{-\nu t}$ for $t \in [0, \infty]$!

$\Rightarrow$ $\tilde{G}^R_{ij}(z)$ is an analytic function in the upper half-plane of the complex frequency variable z!

For $\tilde{G}^A_{ij}(\omega)$: $\boxed{\text{$\tilde{G}^A_{ij}(z)$ is an **analytic** function in the lower half-plane of the complex frequency variable z, i.e., for $\mathrm{Im}\, z = v < 0$!}}$

Relation to the Matsubara Green's function $\tilde{G}^M(i\nu_m)$:

$$\tilde{G}^M_{ij}(i\nu_m) = \begin{cases} \int_{-\infty}^{+\infty} dt\; e^{-\nu_m t}\, G^R_{ij}(t) = \tilde{G}^R_{ij}(z = i\nu_m), & \text{for } \nu_m > 0 \quad (59) \\ \int_{-\infty}^{+\infty} dt\; e^{+\nu_m t}\, G^A_{ij}(t) = \tilde{G}^A_{ij}(z = i\nu_m), & \text{for } \nu_m < 0 \quad (60) \end{cases}$$

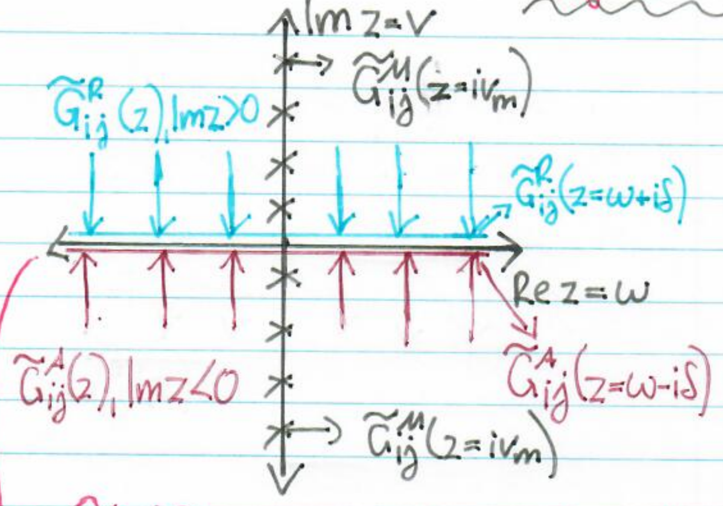
Analytic continuation

Usually, $\tilde{G}^M_{ij}(i\nu_m)$ is „easier" to calculate than $\tilde{G}^R_{ij}(\omega)$ and $\tilde{G}^A_{ij}(\omega)$: Since the Matsubara frequencies have an accumulation point $+\infty$ $(-\infty)$ for $m \to \infty$, we can use **analytical** continuation to calculate $\tilde{G}^R_{ij}(\omega)$ and $\tilde{G}^A_{ij}(\omega)$ from $\tilde{G}^M_{ij}(i\nu_m)$:

$$\boxed{\begin{aligned} \tilde{G}^R_{ij}(\omega) &= \lim_{\delta \to 0+} G^M_{ij}(i\nu \to \omega + i\delta) \quad (61) \\ \tilde{G}^A_{ij}(\omega) &= \lim_{\delta \to 0+} G^M_{ij}(i\nu \to \omega - i\delta) \quad (62) \end{aligned}}$$

Note: In practical numerical calculations, we can calculate $G^M_{ij}(i\nu_m)$ only for a finite number of ν_m ($|m|<N$).
⇒ In this situation, the analytic continuation is not well-defined!

$\tilde{G}_{ij}(z)$ in the entire complex plane



$\tilde{G}^R_{ij}(z) = \int_{-\infty}^{+\infty} dt\, G^R_{ij}(t)\, e^{izt}$ $\qquad$ $\tilde{G}^A_{ij}(z) = \int_{-\infty}^{+\infty} dt\, G^A_{ij}(t)\, e^{izt}$

on real axis: $z = \omega + i\delta$

Im z>0 $\qquad$ Im z<0

$\tilde{G}_{ij}(z)$

$\downarrow z = i\nu_m$

$$\tilde{G}^M_{ij}(i\nu_m) = \int_0^\beta d\tau\, e^{i\nu_m\tau}\, G^M_{ij}(\tau)$$

⇒ applicable for $\nu_m > 0$ and $\nu_m < 0$!

→ $\tilde{G}_{ij}(z)$ has a discontinuity at the real frequency axis: $\tilde{G}^R_{ij}(\omega) \neq \tilde{G}^A_{ij}(\omega)$ ($\Leftrightarrow \tilde{G}_{ij}(z=\omega+i\delta) \neq \tilde{G}_{ij}(z=\omega-i\delta)$ for $\delta \to 0$)

→ $G^R_{ij}(t)$ gives access to $\tilde{G}_{ij}(z)$ for $\mathrm{Im}\,z > 0$ (and to $\tilde{G}^R_{ij}(\omega) = G(z=\omega+i\delta)$),
$G^A_{ij}(t)$ gives access to $\tilde{G}_{ij}(z)$ for $\mathrm{Im}\,z < 0$ (and to $\tilde{G}^A_{ij}(\omega) = G(z=\omega-i\delta)$),
$G^M_{ij}(\tau)$ gives access to $\tilde{G}_{ij}(z)$ for $\mathrm{Im}\,z < 0$ and $\mathrm{Im}\,z < 0$, but only at the discrete Matsubara frequencies ν_m.

→ $\tilde{G}^M_{ij}(i\nu_m)$ can be obtained from $\tilde{G}^R_{ij}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, G^R_{ij}(t)$ by just replacing $\omega \to i\nu_m$ for $\nu_m > 0$ and from $G^A_{ij}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, G^A_{ij}(t)$ by just replacing $\omega \to i\nu_m$ for $\nu_m < 0$!

→ On the contrary, $\tilde{G}^R_{ij}(\omega)$ and $\tilde{G}^A_{ij}(\omega)$ can NOT be obtained from $G^M_{ij}(i\nu_m) = \int d\tau\, e^{i\nu_m \tau}\, G^M_{ij}(\tau)$ by just replacing $i\nu_m \to \omega \pm i\delta$ inside the integral since this formula is valid only for discrete Fourier coefficients
⇒ the analytic continuation must be performed after the τ-integration!

→ For bosonic particles, we have a Matsubara frequency on the real axis, i.e., $\nu_0 = 0$ ($\hat{=}\ z=0$) ⇒ This plays a special role in the linear response theory (see later)!

Properties of $\tilde{G}_{ij}(z)$

→ **Asymptotic behavior for $|z| \to \infty$:**

For $\boxed{\mathrm{Im}\, z > 0}$, $\tilde{G}_{ij}(z) = \int_{-\infty}^{+\infty} dt\, e^{izt}\, G^R_{ij}(t) = -i \int_0^{\infty} dt\, e^{izt} \langle c_i(t) c_j^+ \overset{\text{Bosons}}{\underset{\text{Fermions}}{\mp}} c_j^+ c_i(t) \rangle$

We now use the identity $e^{izt} = \frac{1}{iz} \frac{d}{dt}\left(e^{izt}\right)$ to rewrite the t-integral:

$$\tilde{G}_{ij}(z) = -\cancel{i} \frac{1}{\cancel{i}z} \int_0^{\infty} dt \left(\frac{d}{dt} e^{izt}\right) \langle c_i(t) c_j^+ \mp c_j^+ c_i(t) \rangle$$

$$= -\frac{1}{z} \Big[\left(e^{izt} \langle c_i(t) c_j^+ \mp c_j^+ c_i(t) \rangle\right)\Big|_0^{\infty} - \int_0^{\infty} dt\, e^{izt} \frac{d}{dt} \langle c_i(t) c_j^+ \mp c_j^+ c_i(t) \rangle \Big] \quad (63)$$

↳ partial integration

• $e^{izt} \langle c_i(t) c_j^+ \mp c_j^+ c_i(t) \rangle \Big|_0^{\infty} = e^{i\,\mathrm{Re}\,z \cdot \infty} \underbrace{e^{-\mathrm{Im}\,z \cdot \infty}}_{0,\ \text{because } \mathrm{Im}\,z > 0} \langle c_i(\infty) c_j^+ \mp c_j^+ c_i(\infty) \rangle$

$$- \langle c_i(0) c_j^+ \mp c_j^+ c_i(0) \rangle$$

$$= -\langle c_i c_j^+ \mp c_j^+ c_i \rangle = \begin{cases} \langle [c_i, c_j^+] \rangle & \text{Bosons} \\ \langle \{c_i, c_j^+\} \rangle & \text{Fermions} \end{cases} = -\delta_{ij} \quad (64)$$

• $\frac{d}{d\lambda}\langle c_i(\lambda)c_j^+ \mp c_j^+ c_i(\lambda)\rangle = \langle \frac{dc_i}{d\lambda}(\lambda)c_j^+ \mp c_j^+ \frac{dc_i}{d\lambda}(\lambda)\rangle \underset{\uparrow}{=}$
Heisenberg Eq. of motion

$$= i\langle [H,c_i(\lambda)]c_j^+ \mp c_j^+ [H,c_i(\lambda)]\rangle \quad (65)$$

$$\Rightarrow \widetilde{G}_{ij}(z) = \frac{1}{z}\cdot\delta_{ij} + \underbrace{i\frac{1}{z}\int_0^\infty d\lambda\, e^{iz\lambda}\langle [H,c_i(\lambda)]c_j^+ \mp c_j^+[H,c_i(\lambda)]\rangle}_{I} \quad (66)$$

⇒ Now, the above procedure can be repeated for the integral in the second term, i.e., in I we again use $e^{iz\lambda} = \frac{1}{iz}\left(\frac{d}{d\lambda}e^{iz\lambda}\right)$ and apply partial integration, which leads to:

$$\Rightarrow \widetilde{G}_{ij}(z) = \frac{1}{z}\cdot\delta_{ij} - \frac{1}{z^2}\langle [H,c_i]c_j^+ \mp c_j^+[H,c_i]\rangle - i\frac{1}{z^2}\int_0^\infty d\lambda\, e^{iz\lambda}\frac{d}{d\lambda}\langle [H,c_i(\lambda)]c_j^+ \mp c_j^+[H,c_i(\lambda)]\rangle \quad (67)$$

Heisenberg Eq. of motion: $\frac{d}{d\lambda}\langle [H,c_i(\lambda)]c_j^+ \mp c_j^+[H,c_i(\lambda)]\rangle$

$$= \langle [H,[H,c_i(\lambda)]]c_j^+ \mp c_j^+[H,[H,c_i(\lambda)]] \quad (68)$$

$$\Rightarrow \widetilde{G}_{ij}(z) = \frac{1}{z}\delta_{ij} - \frac{1}{z^2}\langle [H,c_i]c_j^+ \mp c_j^+[H,c_i]\rangle - i\frac{1}{z^2}\int_0^\infty d\lambda\, e^{iz\lambda}\langle [H,[H,c_i(\lambda)]]c_j^+ \mp c_j^+[H,[H,c_i(\lambda)]]\rangle \quad (69)$$

We, hence, define the operator $\boxed{L_H = [H, \bullet] \to L_H^n c_i = \overbrace{[H,[H,\dots,[H,c_i]\dots]]}^{n \text{ times}}}$ (70)

$$\boxed{\tilde{G}_{ij}(z) = \sum_{n=1}^{\infty} \frac{(-1)^n}{z^n} \langle (L_H^{n-1} c_i) c_j^+ \mp c_j^+ (L_H^{n-1} c_i) \rangle = \frac{1}{z}\delta_{ij} + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{z^{n+1}} \cdot \left\langle \begin{matrix} [(L_H^n c_i), c_j^+] \\ \{(L_H^n c_i), c_j^+\} \end{matrix} \right\rangle} \quad (71)$$

for $\mathrm{Im} z > 0$.

For $\mathrm{Im} z < 0$, the same procedure can be performed using the representation of $\tilde{G}_{ij}(z)$ containing $G_{ij}^A(t)$ ⇒ This leads to the same result as Eq. (71). This is also confirmed by an analogous calculation using $G_{ij}^M(\tau)$!

⇒ Eq. (71) represents the asymptotic behavior of $\tilde{G}_{ij}(z)$ in the entire complex plane (but NOT a converging series for $\tilde{G}_{ij}(z)$!).

⇒ For $i \neq j$, the leading asymptotic contribution is $\frac{1}{z}$!

→ Relation between $\tilde{G}^R_{ij}(\omega)$ and $G^A_{ij}(\omega)$

We consider the complex conjugate of $G^R_{ij}(\omega)$:

$$\left(\tilde{G}^R_{ij}(\omega)\right)^* = \left[-i\int_0^\infty dt\, e^{i\omega t}\langle c_i(t)c_j^\dagger \mp c_j^\dagger c_i(t)\rangle\right]^*$$

$$= +i\int_0^\infty dt\, e^{-i\omega t}\langle c_j c_i^\dagger(t) \mp c_i^\dagger(t) c_j\rangle$$

$$|t=-t'| = i\int_{-\infty}^0 dt'\, e^{i\omega t'}\frac{1}{Z}\left[\mathrm{Tr}\left(e^{-\beta H}c_j e^{-it'H}c_i^\dagger e^{it'H}\right)\mp \mathrm{Tr}\left(e^{-\beta H}e^{-it'H}c_i^\dagger e^{it'H}c_j\right)\right]$$

$$|\text{cyclicity of Tr}| \overset{t'=t}{=} i\int_{-\infty}^0 dt\, e^{i\omega t}\frac{1}{Z}\left[\mathrm{Tr}\left(e^{-\beta H}e^{itH}c_j e^{-itH}c_i^\dagger\right)\mp \mathrm{Tr}\left(e^{-\beta H}c_i^\dagger e^{itH}c_j e^{-itH}\right)\right]$$

$$= i\int_{-\infty}^0 dt\, e^{i\omega t}\langle c_j(t)c_i^\dagger \mp c_i^\dagger c_j(t)\rangle = \tilde{G}^A_{ji}(\omega) \quad (72)$$

$$\Rightarrow \boxed{\left(\tilde{G}^R_{ij}(\omega)\right)^* = \tilde{G}^A_{ji}(\omega),\quad \mathrm{Re}\,\tilde{G}^R_{ij}(\omega) = \mathrm{Re}\,\tilde{G}^A_{ji}(\omega),\quad \mathrm{Im}\,\tilde{G}^R_{ij}(\omega) = -\mathrm{Im}\,G^A_{ji}(\omega)} \quad (73)$$

-) Dispersion (or Kramers-Kronig) relations:

Complex differentiability ($\hat{=}$ analyticity) implies strong constraints on a complex functions (e.g.: Cauchy-Riemann differential equations)!

$\Rightarrow$ This leads to a relation between $\mathrm{Re}\,\tilde{G}^R_{ij}(\omega)$ and $\mathrm{Im}\,\tilde{G}^R_{ij}(\omega)$ for real frequencies ω:

We consider $G^R_{ij}(t) \equiv G^R_{ij}(t)\cdot\Theta(t)$ (74)

$\Rightarrow$ We Fourier transform both sides of this equation and apply for the right-hand side the convolution theorem [Eq. (27)] using the Fourier transform of $\Theta(t)$ [Eq. (28)]:

$$\tilde{G}^R_{ij}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega'\, \tilde{G}^R_{ij}(\omega')\cdot \underbrace{\left(\pi\,\delta(\omega-\omega') + iP\frac{1}{\omega-\omega'}\right)}_{\text{Fourier transform of } \Theta(t)} \quad (75)$$

$$\Rightarrow \tilde{G}^R_{ij}(\omega) = \frac{1}{2}\tilde{G}^R_{ij}(\omega) + \frac{i}{2\pi} P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'} \tilde{G}^R_{ij}(\omega') \quad (76)$$

$$\Rightarrow \tilde{G}^R_{ij}(\omega) = \frac{i}{\pi} P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'} \tilde{G}^R_{ij}(\omega') \quad (77)$$

We can now split Eq. (77) into real and imaginary part:

$$\mathrm{Re}\,\tilde{G}^R_{ij}(\omega) + i\,\mathrm{Im}\,\tilde{G}^R_{ij}(\omega) = i\,\frac{1}{\pi}P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'}\mathrm{Re}\,G^R_{ij}(\omega') - \frac{1}{\pi}P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'}\mathrm{Im}\,G^R_{ij}(\omega') \quad (78)$$

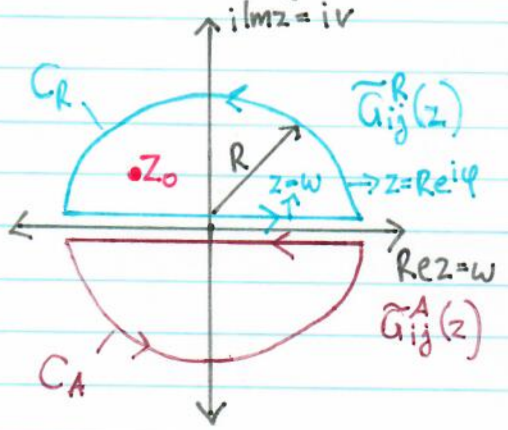
$\Rightarrow$ The equivalence of the real and the imaginary part on the two sides of this equation yields the KRAMERS-KRONIG relations:

$$\boxed{\mathrm{Re}\,\tilde{G}^R_{ij}(\omega) = -\frac{1}{\pi}P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'}\mathrm{Im}\,\tilde{G}^R_{ij}(\omega') \qquad \mathrm{Im}\,\tilde{G}^R_{ij}(\omega) = \frac{1}{\pi}P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'}\mathrm{Re}\,\tilde{G}^R_{ij}(\omega') \quad (79)}$$

Similar relations hold for $G^A_{ij}(\omega)$ where we use the Fourier transform of $\Theta(-t)$ which is given by $\pi\delta(\omega) - iP\frac{1}{\omega}$:

$$\mathrm{Re}\,\tilde{G}^A_{ij}(\omega) = \frac{1}{\pi}P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'}\mathrm{Im}\,G^A_{ij}(\omega') \qquad \mathrm{Im}\,\tilde{G}^A_{ij}(\omega) = -\frac{1}{\pi}P\int_{-\infty}^{+\infty} d\omega' \frac{1}{\omega-\omega'}\mathrm{Re}\,\tilde{G}^A_{ij}(\omega') \quad (80)$$

→ Spectral representation:



Residue theorem:

- $$\oint_{C_R} dz \, \frac{1}{z-z_0} \tilde{G}^R_{ij}(z) = 2\pi i \, \mathrm{Res} \, \frac{\tilde{G}^R_{ij}(z)}{z-z_0} \quad (81)$$

- $$\oint_{C_A} dz \, \frac{1}{z-z_0} \tilde{G}^A_{ij}(z) = 2\pi i \, \mathrm{Res} \, \frac{\tilde{G}^A_{ij}(z)}{z-z_0} \quad (82)$$

Explicit evaluation of the integrals for $R \to \infty$:

- $$\oint_{C_R,\, R\to\infty} dz \, \frac{1}{z-z_0} \tilde{G}^R_{ij}(z) = \lim_{R\to\infty} \int_{-R}^{+R} dw \, \frac{1}{w-z_0} \tilde{G}^R_{ij}(w) + \underbrace{\lim_{R\to\infty} i \int_0^{\pi} d\varphi \, \underbrace{\frac{Re^{i\varphi}}{Re^{i\varphi}-z_0}}_{\to 1 \text{ for } R\to\infty} \overbrace{\tilde{G}^R_{ij}(R \cdot e^{i\varphi})}^{\to 0 \text{ for } R\to\infty}}_{0}$$
$$= \mathrm{Res} \, \frac{\tilde{G}^R_{ij}(z)}{z-z_0} \cdot 2\pi i \quad (83)$$

$\tilde{G}^R_{ij}(z)$ is analytic and, hence, has no poles in the upper complex plane
⇒ contributions to Res can originate only from $\frac{1}{z-z_0}$, if $\mathrm{Im}\, z_0 > 0$!

$$\Rightarrow \operatorname{Res} \frac{\tilde{G}^R_{ij}(z)}{z - z_0} = \tilde{G}^R_{ij}(z_0) \cdot \Theta(\operatorname{Im} z_0) = \tilde{G}_{ij}(z) \cdot \Theta(\operatorname{Im} z_0)$$

$$\Rightarrow \int_{-\infty}^{+\infty} d\omega \, \frac{1}{\omega - z_0} \tilde{G}^R_{ij}(\omega) = 2\pi i \, \tilde{G}_{ij}(z_0) \, \Theta(\operatorname{Im} z_0) \quad (85)$$

⊙ $\oint_{C_A} dz \, \frac{1}{z - z_0} \tilde{G}^A_{ij}(z)$: ⇒ Analogous calculation as for C_R!

$$\int_{-\infty}^{+\infty} d\omega \, \frac{1}{\omega - z_0} \tilde{G}^A_{ij}(z) = -2\pi i \, \tilde{G}_{ij}(z_0) \, \Theta(-\operatorname{Im} z_0) \quad (86)$$

↳ C_A has an integral $\int_{+\infty}^{-\infty} = -\int_{-\infty}^{+\infty}$

Now, we subtract Eq. (86) from Eq. (85) and consider that $\Theta(x) + \Theta(-x) = 1$:

$$\Rightarrow \boxed{\frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega \, \frac{1}{z_0 - \omega} \left[\tilde{G}^A_{ij}(\omega) - \tilde{G}^R_{ij}(\omega) \right] = \tilde{G}_{ij}(z_0) \quad (87)}$$

⇒ Spectral representation of $\tilde{G}_{ij}(\omega)$ in the entire complex plane!

We define : $A_{ij}(\omega) = \frac{1}{2\pi i}\left[\tilde{G}^A_{ij}(\omega) - \tilde{G}^R_{ij}(\omega)\right]$ (88) ... SPECTRAL FUNCTION

$\Rightarrow$ With this definition we can write Eq. (87) as: $\int_{-\infty}^{+\infty} d\omega \, \frac{A_{ij}(\omega)}{z_0 - \omega} = \tilde{G}_{ij}(z_0)$ (89)

Simplifications for $i=j$: From Eqs. (73) we have: $\mathrm{Re}\,\tilde{G}^R_{ii}(\omega) = \mathrm{Re}\,\tilde{G}^A_{ii}(\omega)$

$\mathrm{Im}\,\tilde{G}^R_{ii}(\omega) = -\mathrm{Im}\,\tilde{G}^A_{ii}(\omega)$

$$\Rightarrow \boxed{A_{ii}(\omega) = \frac{1}{2\pi i}(-2i)\,\mathrm{Im}\,\tilde{G}^R_{ii}(\omega) = -\frac{1}{\pi}\mathrm{Im}\,\tilde{G}^R_{ii}(\omega) \quad (90)}$$

$$\Rightarrow \tilde{G}_{ii}(z) = \int_{-\infty}^{+\infty} d\omega \, \frac{1}{z-\omega}\left(-\frac{1}{\pi}\mathrm{Im}\,\tilde{G}^R_{ii}(\omega)\right) \quad (91)$$

(Here, we have set $z = z_0$)

From Eq. (71), we have for the asymptotics: $\tilde{G}_{ii}(z) \underset{|z|\to\infty}{=} \frac{1}{z} + O\left(\frac{1}{z^2}\right)$

$$\Rightarrow \tilde{G}_{ii}(z) = \int_{-\infty}^{+\infty} d\omega \, \frac{1}{z}\frac{1}{1-\frac{\omega}{z}} A_{ii}(\omega) = \sum_{n=0}^{\infty} \frac{1}{z^{n+1}} \underbrace{\int_{-\infty}^{+\infty} d\omega \, \omega^n A_{ii}(\omega)}_{M_n} \quad (92)$$

In particular: $M_0 = \int_{-\infty}^{+\infty} d\omega \, A_{ii}(\omega) = 1$, For fermions we will show $A_{ii}(\omega) \geq 0$

$\Rightarrow A_{ii}(\omega)$ is a probability density function! (M_n... Moments of this probability)

-) Lehmann representation:

How can we evaluate the matrix elements $\langle c_i(t) c_j^+ \rangle$ and $\langle c_j^+ c_i(t) \rangle$ explicitly?

⊙ $\langle c_i(t) c_j^+ \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} e^{itH} c_i e^{-itH} c_j^+ \right) = \frac{1}{Z} \sum_N \langle N | e^{-\beta H} e^{itH} c_i e^{-itH} c_j^+ | N \rangle$, (93)

where the states N form a full eigenbasis of H, $H|N\rangle = E_N |N\rangle$. (94)

$\Rightarrow \langle c_i(t) c_j^+ \rangle = \frac{1}{Z} \sum_N e^{-\beta E_N} e^{itE_N} \langle N | c_i e^{-itH} c_j^+ | N \rangle$ (95)

insert here!

Completness of the basis $|N\rangle$: $\sum_N |N\rangle\langle N| = \mathbb{1}$ ... unity operator

$\Rightarrow \langle c_i(t) c_j^+ \rangle = \frac{1}{Z} \sum_{N,M} e^{-\beta E_N} e^{itE_N} \langle N | c_i e^{-itH} | M \rangle \langle M | c_j^+ | N \rangle$ (96)

$\Rightarrow \langle c_i(t) c_j^+ \rangle = \frac{1}{Z} \sum_{N,M} e^{-\beta E_N} e^{it(E_N - E_M)} \langle N | c_i | M \rangle \langle M | c_j^+ | N \rangle$ (97)

⊙ $\langle c_j^+ c_i(t) \rangle = \frac{1}{Z} \sum_{N,M} e^{-\beta E_M} e^{it(E_N - E_M)} \langle N | c_i | M \rangle \langle M | c_j^+ | N \rangle$ (98)

↳ Here, we have exchanged M and N!

(Analogous equations can be derived for the correlation functions in Matsubara times)

From Eqs. (97) and (98) we can obtain the Lehmann representation for $\tilde{G}^M_{ij}(i\nu_m)$, $\tilde{G}^R_{ij}(\omega)$ and $\tilde{G}^A_{ij}(\omega)$:

$$\boxed{\tilde{G}^R_{ij}(\omega) =} -i \int_0^\infty dt\, e^{i\omega t} \left[\langle c_i(t) c_j^\dagger \rangle \mp \langle c_j^\dagger c_i(t) \rangle \right]$$

$$= -i \frac{1}{Z} \sum_{M,N} \langle N|c_i|M\rangle \langle M|c_j^\dagger|N\rangle \int_0^\infty dt\, e^{i(\omega+E_N-E_M)\cdot t} \left(e^{-\beta E_N} \mp e^{-\beta E_M} \right)$$

$$= -i \frac{1}{Z} \sum_{M,N} \langle N|c_i|M\rangle \langle M|c_j^\dagger|N\rangle \left[\pi\delta(\omega+E_N-E_M) + iP\frac{1}{\omega+E_N-E_M} \right] \times \left(e^{-\beta E_N} \mp e^{-\beta E_M} \right)$$

$$\boxed{\begin{aligned} &= \frac{1}{Z} \sum_{M,N} \langle N|c_i|M\rangle \langle M|c_j^\dagger|N\rangle \cdot e^{-\beta E_N} \cdot \left[P\frac{1}{\omega+E_N-E_M} - i\pi\delta(\omega+E_N-E_M) \right] \times \left(1 \mp e^{-\beta(E_M-E_N)}\right) \\ &= \frac{1}{Z} \sum_{M,N} \langle N|c_i|M\rangle \langle M|c_j^\dagger|N\rangle e^{-\beta E_N} \frac{1}{\omega+i\delta+E_N-E_M} \left(1 \mp e^{-\beta(E_M-E_N)}\right) \qquad (99) \end{aligned}}$$

$$\boxed{\widetilde{G}^{A}_{ij}(\omega)} = +i\int_{-\infty}^{0} dt\, e^{i\omega t}\left[\langle c_i(t)c_j^{+}\rangle \mp \langle c_j^{+}c_i(t)\rangle\right] = \ldots$$ calculations as for $\widetilde{G}^{R}_{ij}(\omega)$

$$= \frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^{+}|N\rangle e^{-\beta E_N}\left[P\frac{1}{\omega+E_N-E_M} + i\pi\,\delta(\omega+E_N-E_M)\right] \times\left(1\mp e^{-\beta(E_M-E_N)}\right)$$

$$= \frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^{+}|N\rangle e^{-\beta E_N}\frac{1}{\omega-i\delta+E_N-E_M}\left(1\mp e^{-\beta(E_M-E_N)}\right) \quad (100)$$

$$\boxed{\widetilde{G}^{M}_{ij}(\omega)} = -\int_{0}^{\beta} d\tau\, e^{i\nu_m\tau}\langle c_i(\tau)c_j^{+}\rangle = -\frac{1}{Z}\int_{0}^{\beta} d\tau\, e^{i\nu_m\tau}\,\mathrm{Tr}\left(e^{-\beta H}e^{\tau H}c_i e^{-\tau H}c_j^{+}\right)$$

$$= -\frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^{+}|N\rangle e^{-\beta E_N}\int_{0}^{\beta} d\tau\, e^{\tau(i\nu_m+E_N-E_M)}$$

$$= -\frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^{+}|N\rangle e^{-\beta E_N}\frac{1}{i\nu_m+E_N-E_M}\left(\overbrace{e^{\beta i\nu_m}}^{\pm 1}e^{\beta(E_N-E_M)}-1\right)$$

$$= \frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^{+}|N\rangle e^{-\beta E_N}\frac{1}{i\nu_m+E_N-E_M}\left(1\mp e^{-\beta(E_M-E_N)}\right) \quad (101)$$

Discussion:

→ The Lehmann representations for $\tilde{G}^R_{ij}(\omega)$, $\tilde{G}^A_{ij}(\omega)$ and $\tilde{G}^M_{ij}(i\nu_m)$ in Eqs. (99) - (101) differ only for the terms marked by the orange circles

⇒ This confirms our previous finding, that we can define a general function $\tilde{G}_{ij}(z)$ in the entire complex frequency plane which is analytic for $\mathrm{Im}\, z > 0$ and $\mathrm{Im}\, z < 0$ and coincides with $\tilde{G}^R_{ij}(\omega)$, $\tilde{G}^A_{ij}(\omega)$ and $\tilde{G}^M_{ij}(i\nu_m)$ in the upper and lower half plane and at the Matsubara frequencies $i\nu_m$!

$$\boxed{\tilde{G}_{ij}(z) = \frac{1}{Z}\sum_{M,N} \langle N|c_i|M\rangle\langle M|c_j^\dagger|N\rangle e^{-\beta E_N}\frac{1}{z+E_N-E_M}\left(1\mp e^{-\beta(E_M-E_N)}\right) = \begin{cases} \tilde{G}^R_{ij}(\omega), & z=\omega+i\delta \\ \tilde{G}^M_{ij}, & z=i\nu_m \\ \tilde{G}^A_{ij}(\omega), & z=\omega-i\delta \end{cases}} \quad (102)$$

$\Rightarrow$ Spectral function: From Eq. (90) we obtain

$$\boxed{A_{ii}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\tilde{G}^R_{ij}(\omega) = \frac{1}{Z}\sum_{M,N} |\langle N|c_i|M\rangle|^2 e^{-\beta E_N}\,\delta(\omega + E_N - E_M)\left(1 \mp e^{-\beta(E_M - E_N)}\right) \quad (103)}$$

(Note: $\langle N|c_i|M\rangle\langle M|c_i^\dagger|N\rangle = \langle N|c_i|M\rangle \cdot \langle N|c_i|M\rangle^* = |\langle N|c_i|M\rangle|^2$

Let us consider the case of fermions, i.e., $\left(1 + e^{-\beta(E_M - E_N)}\right)$ in the last term:

$\Rightarrow A_{ii}(\omega) > 0$, together with Eq. (92): $\int_{-\infty}^{+\infty} d\omega\, A_{ii}(\omega) = 1$

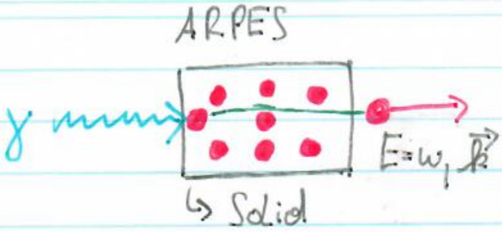
$\Rightarrow A_{ii}(\omega)$ .... probability distribution function

Typical case: $i \triangleq (\vec{k}, \sigma)$ $\vec{k}$... lattice momentum

$\Rightarrow \boxed{A_{ii}(\omega) = A(\omega, \vec{k}) = A(\omega, \vec{k}) \quad (104)}$ $\Rightarrow$ Can be measured by ARPES:

SU(2) symmetry

Angular Resolved PhotoEmission Spectroscopy



1) We excite an electron with a photon (lightpulse) γ.

2) The electron eventually leaves the solid with an energy $E=\omega$ and a momentum $\vec{k}$

$\Rightarrow$ This process is theoretically described by $A(\omega, \vec{k})$!

Eq. (103): ⊙ $|\langle N|c_{\vec{k}}|M\rangle|^2$: A particle with momentum $\vec{k}$ is is removed from the M-particle state $|M\rangle$
$\Rightarrow |M\rangle \rightarrow (M-1) = N$ particle state with probability $|\langle N|c_{\vec{k}}|M\rangle|^2$.

⊙ $\delta(\omega + E_N - E_M)$: The energy of the new state $E_N = E_M - \omega$ is given by the energy E_M of the initial state $-$ energy ω of removed particle

$\Rightarrow A(\omega, \vec{k})$ ... probability for extracting an electron with momentum $\vec{k}$ and energy ω!
For non-interacting case: $A(\omega, \vec{k}) = \delta(\omega - \varepsilon_{\vec{k}})$, $\varepsilon_{\vec{k}}$ ... dispersion relation (see exercise)!

What about $\tilde{G}^c_{ij}(\omega)$?

We have seen : Relevant physical information is included in $\tilde{G}_{ij}(z)$, and in particular in $A_{ii}(\omega) = -\frac{1}{\pi}\mathrm{Im}\,\tilde{G}^R_{ii}(\omega)$!

How is $\tilde{G}^c_{ij}(\omega)$ related to $\tilde{G}_{ij}(z)$ (and $\tilde{G}^R_{ij}(\omega)$, $\tilde{G}^A_{ij}(\omega)$ and $\tilde{G}^M_{ij}(i\nu_m)$) ?

$$\boxed{\tilde{G}^c_{ij}(\omega)} = -i\int_0^\infty dt\, e^{i\omega t}\langle c_i(t)c_j^+\rangle \mp i\int_{-\infty}^0 dt\, e^{i\omega t}\langle c_j^+ c_i(t)\rangle$$

$$= \frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^+|N\rangle\left[e^{-\beta E_N}\frac{1}{\omega+i\delta+E_N-E_M} \mp e^{-\beta E_M}\frac{1}{\omega-i\delta+E_N-E_M}\right]$$

$$= \frac{1}{Z}\sum_{M,N}\langle N|c_i|M\rangle\langle M|c_j^+|N\rangle e^{-\beta E_N}\left[P\frac{1}{\omega+E_N-E_M}\left(1\mp e^{-\beta(E_M-E_N)}\right)\right.$$

$$\left. -i\pi\,\delta(\omega+E_N-E_M)\left(1\pm e^{-\beta(E_M-E_N)}\right)\right] \qquad (105)$$

$\Rightarrow$ $\tilde{G}^c_{ij}(\omega)$ is NOT analytic (neither in the upper nor in the lower halfplane) since it contains both $\frac{1}{\omega+i\delta+E_N-E_M}$ AND $\frac{1}{\omega-i\delta+E_N-E_M}$!

For the diagonal components $i=j$, we find:
If we consider $\mathrm{Re}\,\tilde{G}^c_{ii}(\omega)$ and $\mathrm{Im}\,\tilde{G}^c_{ii}(\omega)$ separately, we find:

- $$\boxed{\mathrm{Re}\,\tilde{G}^c_{ii} = \mathrm{Re}\,\tilde{G}^R_{ii}(\omega) = \mathrm{Re}\,\tilde{G}^A_{ii}(\omega) = \frac{1}{Z}\sum_{N,M} \langle N|c_i|M\rangle\langle M|c_i^+|N\rangle e^{-\beta E_N}\, P\frac{1}{\omega+E_N-E_M}\left(1\mp e^{-\beta(E_M-E_N)}\right)}$$
  where $\langle N|c_i|M\rangle\langle M|c_i^+|N\rangle = |\langle N|c_i|M\rangle|^2 \in \mathbb{R}$

- For $\mathrm{Im}\,\tilde{G}^c_{ii}(\omega)$, we have the problem that in the last term $(1\pm e^{-\beta(E_M-E_N)})$ the signs are exchanged w. r. t. $\mathrm{Im}\,\tilde{G}^R_{ii}(\omega)$ and $\mathrm{Im}\,\tilde{G}^A_{ii}(\omega)$!

$$\Rightarrow \quad 1\pm e^{-x} = \left(1\mp e^{-x}\right)\cdot \begin{cases} \coth\left(\frac{x}{2}\right), & \text{BOSONS} \\ \tanh\left(\frac{x}{2}\right), & \text{FERMIONS} \end{cases} \quad x=\beta(E_M-E_N)=\beta\cdot\omega \text{ due to } \delta(\omega+E_N-E_M)! \qquad (107)$$

$$\boxed{\begin{aligned}\mathrm{Im}\,\tilde{G}^c_{ii}(\omega) &= \mathrm{Im}\,\tilde{G}^R_{ii}(\omega)\cdot\begin{Bmatrix}\coth\left(\frac{\beta\omega}{2}\right)\\ \tanh\left(\frac{\beta\omega}{2}\right)\end{Bmatrix} = -\mathrm{Im}\,\tilde{G}^A_{ii}(\omega)\begin{Bmatrix}\coth\left(\frac{\beta\omega}{2}\right)\\ \tanh\left(\frac{\beta\omega}{2}\right)\end{Bmatrix}\\ &= -\frac{1}{Z}\sum_{N,M}\langle N|c_i|M\rangle\langle M|c_i^+|N\rangle e^{-\beta E_N}\,\pi\,\delta(\omega+E_N-E_M)\left(1\pm e^{-\beta(E_M-E_N)}\right)\end{aligned}} \qquad (108)$$

Limit $T \to 0$ ($\beta \to \infty$):

$$\lim_{\beta \to \infty} \tanh\left(\frac{\beta\omega}{2}\right) \Big| \coth\left(\frac{\beta\omega}{2}\right) = \mathrm{sign}(\omega) \qquad (109)$$

$$\Rightarrow \boxed{\omega < 0:} \; \tilde{G}^{c}_{ii}(\omega) = \tilde{G}^{A}_{ii}(\omega) \qquad \boxed{\omega > 0:} \; \tilde{G}^{c}_{ii}(\omega) = \tilde{G}^{R}_{ii}(\omega) \qquad (110)$$

Note: In the literature, one sometimes finds the conditions $\omega < \mu$ and $\omega > \mu$ instead of $\omega < 0$ and $\omega > 0$. The difference originates from the fact, that we have included the term μN from the grand canonical ensemble in the Hamiltonian!

Question: $\tilde{G}^{c}_{ij}(\omega)$ has in contrast to $\hat{G}_{ij}(z)$ „unfavorable" properties (it is not analytic!) and it does not correspond directly to experimentally measurable quantities (such as $A_{ii}(\omega)$).

Why do we need it at all? $\Rightarrow$ For the answer: see chapter 4 about perturbation theory!