Condensed Matter Theory

Many-Body Physics

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SS 2008

3h/week 2h exercises/week

Exercises: Tobias Langenbruch

Presumed knowledge
- Quantum mechanics I, II
- not thermodynamics and statistics

Contents

5. Magnetism and strong correlations

- Quantum mechanical origin of magnetism (Anderson model etc.)
- Magnetic defects in metals: Kondo effect
- Concept of renormalization group
- Magnetic lattice systems

Types of magnetic coupling

- Hund's rule: FM
- exchange, (superexchange) AFM
- Dipole: FM
- RKKY: FM, AFM

Models: Heisenberg; Hubbard, t-J

6. Metal-insulator transition in strongly correlated systems

- Hubbard model
- Dynamical mean field theory (DMFT).

Important general concepts:

- Continuity: quasiparticles
- Collective phenomena of many particles
- Spontaneous symmetry breaking: discontinuity (phase transitions see next semester) ordering by (weak) interactions
- Renormalization: Strong correlations out of weak interactions

Confinement.

1. Quantum field theory at finite temperature

1.1 Reminder: fundamentals

1.1.1 Second quantization

Let $\mathbb{B}^{(1)} = \{ |k\rangle \mid \forall\, k \text{, complete set of quantum nos.} \}$ be a basis of the single-particle Hilbert space.

Then $\mathbb{B}^{(N)} = \{ |k_1, k_2, \dots, k_N\rangle \mid \forall\, k_1, \dots, k_N \}$ is a basis of the N-particle Hilbert space.

$$|k_1, \dots, k_N\rangle = \mathcal{N} \sum_{P(1,\dots,N)} \overset{\text{bosons}}{\underset{\text{fermions}}{(\pm 1)^P}} |k_{P(1)}\rangle \cdots |k_{P(N)}\rangle$$

is a completely symmetrized / antisymmetrized (bosons / fermions) product state of 1-particle states.

$\mathbb{B} = \bigcup_{N=0}^{\infty} \mathbb{B}^{(N)}$ is a complete basis of the Fock space with variable particle number.

Occupation number representation:

Specifying the number n_k of particles in each single-particle state $|k\rangle$ instead of specifying for each particle in which state it is, one can identify:

$$|n_1, n_2, \dots\rangle \equiv |k_1, \dots, k_N\rangle$$

($n_1, n_2, \dots$: quantum numbers; $k_1, \dots, k_N$: particle index)

and $\mathbb{B} = \{ |n_1, n_2, \dots\rangle \mid \forall\, n_i,\ i = 1, \dots, \infty \}$,

with $n_i = 0, 1, 2, \dots$ bosons

$n_i = 0, 1$ fermions.

Each state of the interacting many-body system can be expanded in the basis $\mathbb{B}$.

Creation and destruction operators acting on the Fock space are defined as

Bosons: $n_k = 0, 1, 2, \dots$

$$a_k |\dots, n_k, \dots\rangle = \sqrt{n_k}\, |\dots, n_k - 1, \dots\rangle$$

$$a_k^+ |\dots, n_k, \dots\rangle = \sqrt{n_k + 1}\, |\dots, n_k + 1, \dots\rangle$$

$$[a_k, a_{k'}^+] = \delta_{kk'}$$

$$[a_k, a_{k'}] = [a_k^+, a_{k'}^+] = 0$$

Fermions: $n_k = 0, 1$

$$c_k |\dots, n_k, \dots\rangle = (1 - n_k) |\dots, n_k + 1, \dots\rangle$$

$$c_k^+ |\dots, n_k, \dots\rangle = (1 - n_k) |\dots, n_k + 1, \dots\rangle$$

1.1.2 Heisenberg and interaction pictures

Schrödinger:

state: $i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$

operator: $\hat{A}$ (time independent)

$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$

expectation value: $\langle A\rangle = \langle\psi(t)|\hat{A}|\psi(t)\rangle$

$= \langle\psi(0)|e^{+iHt}\hat{A}e^{-iHt}|\psi(0)\rangle$

Heisenberg:

state: $|\psi\rangle_H = |\psi(0)\rangle$ (time independent)

operator: $\hat{A}_H(t) = e^{iHt}\hat{A}e^{-iHt}$

$i\frac{d}{dt}\hat{A}_H(t) = \left[\hat{A}_H(t), H\right]$

(Heisenberg - Bew. - Gleichung)

Dirac (interaction picture): $H = H_0 + \hat{V}(t)$

state: $|\psi(t)\rangle_I = e^{+iH_0t}|\psi(t)\rangle$

(time evolution "only" wrt. $\hat{V}(t)$)

$\Rightarrow$ operator: $\hat{A}_I(t) = e^{+iH_0t}\hat{A}e^{-iH_0t}$

(time evolution only wrt. H_0)

$i\frac{d}{dt}\hat{A}_I(t) = \left[\hat{A}_I(t), H_0\right]$

$i\frac{d}{dt}|\psi(t)\rangle_I = \hat{V}_I(t)|\psi(t)\rangle_I$

$\hat{V}_I(t) = e^{iH_0t}\hat{V}e^{-iH_0t}$

1.1.3 Statistical physics

We will consider many-particle systems which are coupled to a heat bath (reservoir) with energy and particle exchange, i.e.
energy E and
particle number N of the system
are fixed on average only (grand canonical ensemble)

The eigenstates and eigenenergies of the N-particle system are denoted by

$|\Psi_n^N\rangle$

E_n^N , $n =$ (set of quantum numbers uniquely describing the state)

$n = 0$: ground state

Important quantities:

- Chemical potential μ:
  Change of the ground state energy when the particle number is increased by 1:

$$\mu = E_0^{N+1} - E_0^N \underset{N \gg 1}{=} E_0^N - E_0^{N-1} \underset{N \gg 1}{=} \frac{dE_0^N}{dN} .$$

- Probability that the N-particle system is in the state $|\psi_n^N\rangle$:

$$P(N,n) = \frac{1}{Z_G} e^{-\beta(E_n^N - \mu N)}$$

"Boltzmann distribution"

$\beta = \frac{1}{k_B T}$, T = temperature

[convention: in the following $\hbar = 1$, $c = 1$, $k_B = 1$]

normalization factor:

$$Z_G(T) = \sum_{N,n} e^{-\beta(E_n^N - \mu N)}$$

"grand canonical partition sum, partition function"

Note: $P(N,n)$ depends, for fixed temperature T, only on the total particle number N and the total energy E_n^N of the system!

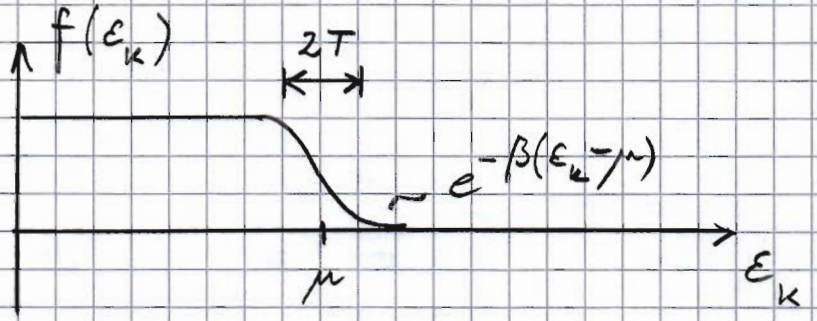
- Average occupation number n_k of a given single-particle state within the N-particle $|k\rangle$ system:

Fermions: $$n_k = \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1} =: f(\varepsilon_k - \mu)$$

Bosons: $$n_k = \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} =: b(\varepsilon_k - \mu)$$

depends only on single particle energy (for fixed T, μ).

Fermions



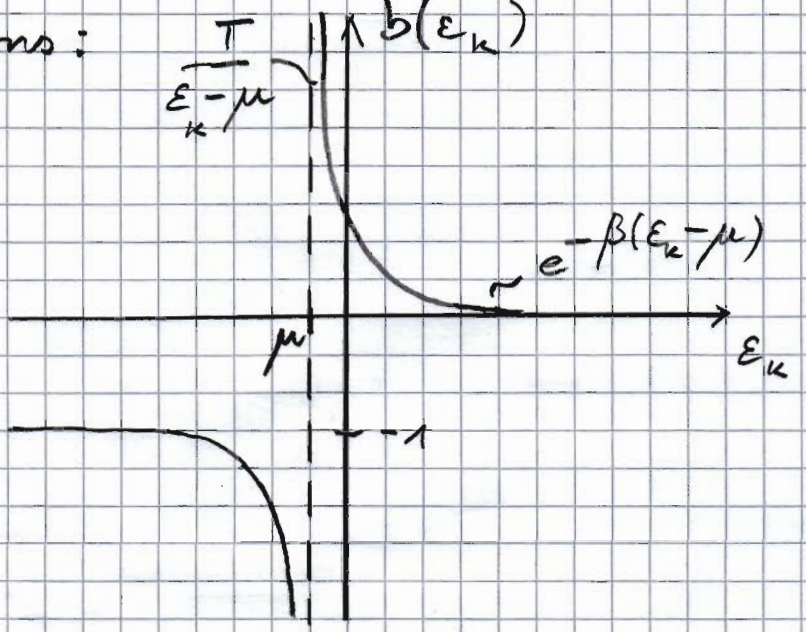
$\mu \geq 0$

at $T = 0$

$\mu(T=0) \equiv \varepsilon_F$

Fermi energy

Bosons:



$\mu < 0$

in general

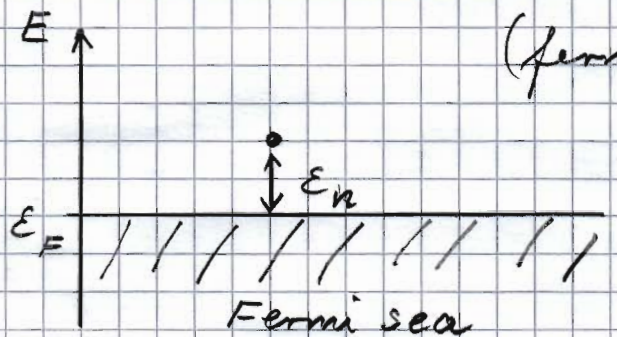
$(\varepsilon_k \geq 0)$

1.2 Green's functions at finite temperature

The excitation energy of a many-body system due to adding one additional particle is usually measured wrt. the chemical potential:

$$E_n^{N+1} - E_0^N = \underbrace{E_n^{N+1} - E_0^{N+1}}_{\varepsilon_n} + \underbrace{E_0^{N+1} - E_0^N}_{\mu} = \varepsilon_n + \mu$$

$T = 0$ (fermions)



Therefore, we define the Schrödinger equation of the many-particle system with the Hamilton operator $\hat{H} - \mu \hat{N}$ where $\hat{N} = \sum_k c_k^+ c_k$ is the total particle number operator.

$$i \frac{d}{dt} |\Psi(t)\rangle = (\hat{H} - \mu \hat{N}) |\Psi(t)\rangle$$

For a change of particle number by 1, the term $-\mu \hat{N}$ just subtracts the energy μ needed to add 1 particle in the ground state, i.e. $\hat{H} - \mu \hat{N}$ measures the excitation energy ε_n.

In the Heisenberg picture the creation/destruction operators have the form

$$c_k(t) = e^{i(H-\mu N)t}\, c_k\, e^{-i(H-\mu N)t}$$

$$c_k^+(t) = e^{i(H-\mu N)t}\, c_k^+\, e^{-i(H-\mu N)t}$$

Denoting now k specifically as the momentum (wave vector), the field operators are defined by the Fourier transform

$$\Psi(\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\vec{r}}\, c_k \quad \text{destruction} \Big\} \text{operator for a particle at position } \vec{r}.$$

$$\Psi^+(\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, e^{-i\vec{k}\vec{r}}\, c_k^+ \quad \text{creation} \Big\} \text{operator for a particle at position } \vec{r}.$$

(Note: these operators may also carry a spin index, which is suppressed here for clarity.)

1.2.1 Definition of the $T>0$ Green's functions

The retarded / advanced thermal Green's function is the thermal average of the q.m. expectation value for creating a particle at $x=(t',\vec{r}')$ and removing it at $x=(t,\vec{r})$, i.e.

$$G^R(x,x') = -i\theta(t-t')\, \frac{tr\{e^{-\beta(H-\mu N)}\,[\Psi(x),\Psi^+(x')]_{\mp}\}}{tr\{e^{-\beta(H-\mu N)}\}}$$

($\mp$: $-$ for Bosons, $+$ for Fermions)

$$G^A(x,x') = +i\theta(t'-t)\, \frac{tr\{e^{-\beta(H-\mu N)}\,[\Psi(x),\Psi^+(x')]_{\mp}\}}{tr\{e^{-\beta(H-\mu N)}\}}$$

(causal Green's functions)

where the trace is over all q.m. states of the N-particle system, and summed over $N = 0, 1, \ldots \infty$, and all expressions are taken in the Heisenberg picture.

Explicitly:

$$G^R(x,x') = -i\theta(t-t') \frac{\sum_{N,n} \langle \psi_n^N | e^{-\beta(H-\mu N)} [\psi(x), \psi^+(x')]_\mp | \psi_n^N \rangle}{\sum_{N,n} \langle \psi_n^N | e^{-\beta(H-\mu N)} | \psi_n^N \rangle}$$

$$tr\{e^{-\beta(H-\mu N)}\} = Z_G. \quad \text{grand canonical partition function}$$

From time-dependent perturbation theory we know that time-ordered products of the perturbation appear.
In a many-particle system the time dependence of the particle operators necessarily introduces time-dependent interactions for a single particle.
In order to develop the perturbation theory for many-particle systems in a later chapter, we therefore introduce also the

<u>time-ordered Green's function</u>

$$G(x,x') = -i \frac{tr\{e^{-\beta(H-\mu N)} \hat{T}(\psi(x)\psi(x'))\}}{tr\{e^{-\beta(H-\mu N)}\}}$$

with $\hat{T}$ the time ordering operator for bosons or fermions.

	physical time evolution	perturbation theory
$G^{R/A}$	✓	no
G	no	✓

→ One first calculates G, e.g., using P.T., and then obtains $G^{R/A}$ from G in a second step. While in time-space there is no simple relation between G and $G^{R/A}$, this relation is very simple in frequency space through the analytical properties in the complex ω plane.

The analytical properties of G, $G^{R/A}$ will also tell how to obtain physical properties like excitation energy, decay rates, spectral density from the Green's function.

Therefore we investigate the analytical properties of the Green's functions.

The invariance of the tr under cyclic permutations will introduce significant simplifications which are not present in the $T=0$ formalism, where only the ground state expectation value is taken.

1.2.2 Analytical properties

$$G(x,x') = -\frac{i}{Z_G}\,\mathrm{tr}\Big\{ e^{-\beta(H-\mu N)}\, \mathcal{T}\Big[e^{+i(H-\mu N)t}\,\psi(\vec r)\, e^{-i(H-\mu N)(t-t')}\,\psi^+(\vec r')\, e^{-i(H-\mu N)t'}\Big]\Big\}$$

cyclic invariance under tr

$$= \begin{cases} -\frac{i}{Z_G}\,\mathrm{tr}\Big\{ e^{-\beta(H-\mu N)}\, e^{i(H-\mu N)(t-t')}\,\psi(\vec r)\, e^{-i(H-\mu N)(t-t')}\,\psi^+(\vec r')\Big\} \\ \qquad (N+1)\text{-particle basis: } \sum_m |\psi_m^{N+1}\rangle\langle\psi_m^{N+1}| \\ \qquad =: G^>(x,x') \quad , \quad t > t' \\ \pm\frac{i}{Z_G}\,\mathrm{tr}\Big\{ e^{-\beta(H-\mu N)}\,\psi^+(\vec r')\, e^{+i(H-\mu N)(t-t')}\,\psi(\vec r)\, e^{-i(H-\mu N)(t-t')}\Big\} \\ \qquad =: G^<(x,x') \quad , \quad t < t' \end{cases}$$

(F: $-$, B: $+$)

The functions $G^>$ and $G^<$ are defined for all times t, t' and coincide with G for $t > t'$ and $t < t'$, respectively.

Since $G(x,x')$ depends only on the difference $t-t'$, we set $t' = 0$, i.e. $t - t' = t$ from now on.

Formal analogy: $\boxed{\beta = \frac{1}{T} \quad \leftrightarrow \quad it}$

This motivates the

Analytic continuation to complex times

We must ensure the absolute convergence of the exponentials under the trace. This sets the range of definition for $G^>$, $G^<$ in the complex time plane:

E_n^N, E_m^{N+1} eigenvalues of H. $\tau := \mathrm{Im}\, t$.

We can set $E_0^N = 0$ (without loss of generality)

$\underline{G^>}$: must require

$$-\beta E_n^N - \underbrace{(E_n^N - E_m^{N+1} + \mu)\tau}_{= E_n^N - E_m^{N+1} + E_0^{N+1} - E_0^N \leq E_n^N \;\forall m} < 0 \quad \forall n, m$$

→ for $\tau \leq 0$:

$$-\beta E_n^N - (E_n^N - E_m^{N+1} + \mu)\tau \leq -E_n^N(\beta + \tau) < 0 \quad \forall n > 1 \text{ for } \tau > -\beta$$

→ $G^>$ converges for $-\beta \leq \tau \leq 0$

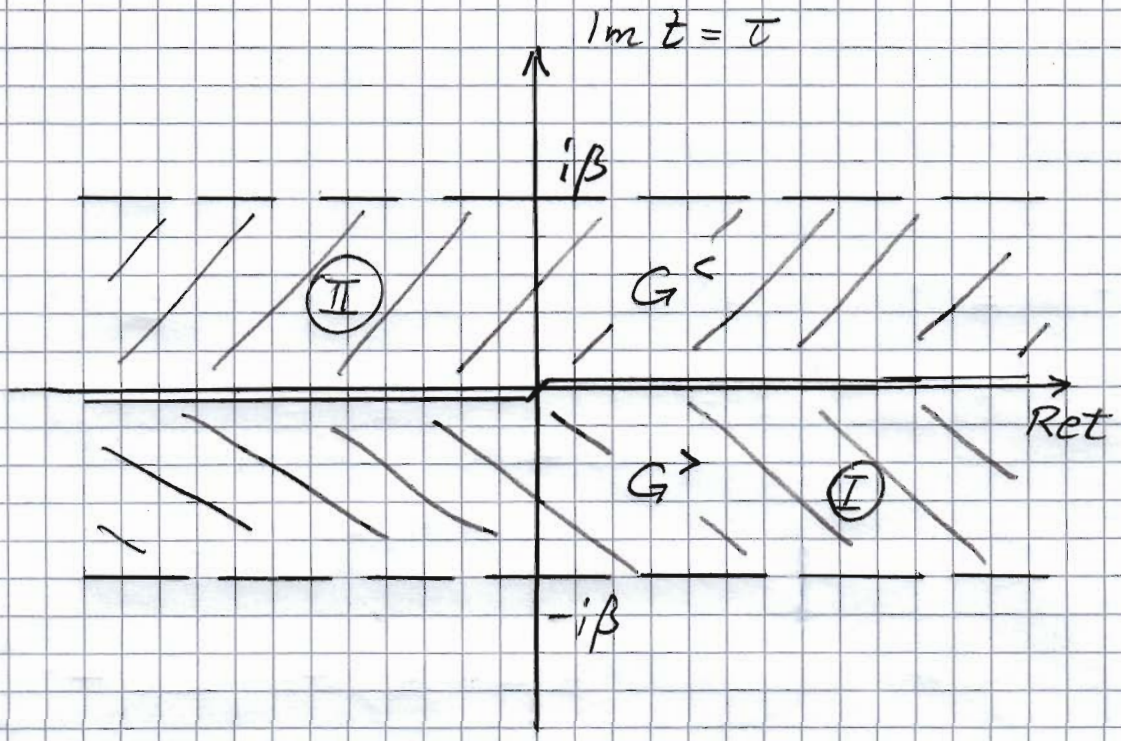
$\underline{G^<}$: must require

$$-\beta E_n^N + \underbrace{(E_n^N - E_m^{N-1} - \mu)\tau}_{E_n^N - E_m^{N-1} - E_0^N + E_0^{N-1} \leq E_n^N \;\forall m}$$

→ for $\tau \geq 0$:

$$-\beta E_n^N + (E_n^N - E_m^{N-1} + \mu)\tau \leq -E_n^N(\beta - \tau) < 0 \quad \forall n > 1 \text{ for } \tau < \beta$$

→ $G^<$ converges for $0 \le \tau \le \beta$



<u>Periodicity along the imaginary axis</u>

for $0 < \mathrm{Im}\, t < i\beta$

$$G^>(t - i\beta) = -\frac{i}{Z_G} \mathrm{tr}\left\{ e^{-\beta(H-\mu N)} e^{i(H-\mu N)(t-i\beta)} \psi(\vec{r}) e^{-i(H-\mu N)(t-i\beta)} \psi^+(\vec{r}') \right\}$$

(cyclic)

$$= -\frac{i}{Z_G} \mathrm{tr}\left\{ e^{-i(H-\mu N)(-i\beta)} \psi^+(\vec{r}') e^{i(H-\mu N)t} \psi(\vec{r}) e^{-i(H-\mu N)t} \right\}$$

$$= \mp G^<(t)$$

$$\boxed{G^>(t - i\beta) = \overset{F}{\underset{B}{\mp}} G^<(t)} \qquad 0 < \mathrm{Im}\, t < i\beta$$

$$\boxed{G(t - i\beta) = \mp G(t)}$$

(using general def. of G in terms of $G^>$, $G^<$.)

Using these relations, G is continued periodically (bosons) / antiperiodically (fermions) along the imaginary axis to the complete time plane.

Fourier transformation and spectral representation

Distinguish $G^>$, $G^<$, G (different supports)

for $t>0$: $G = G^>$ for $t<0$: $G = G^<$ (*)

$$G^>(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} G^>(\omega) e^{-i\omega t} \qquad G^<(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} G^<(\omega) e^{-i\omega t}$$

The F.T. is evaluated using contour integration in the complex time plane:

$$G^>(\omega) = \int_{C_0} dt\, e^{i\omega t} G^>(t) = \int_{C_1} dt' e^{i\omega(t'-i\beta)} \underbrace{G^>(t'-i\beta)}_{\mp G^<(t')}$$

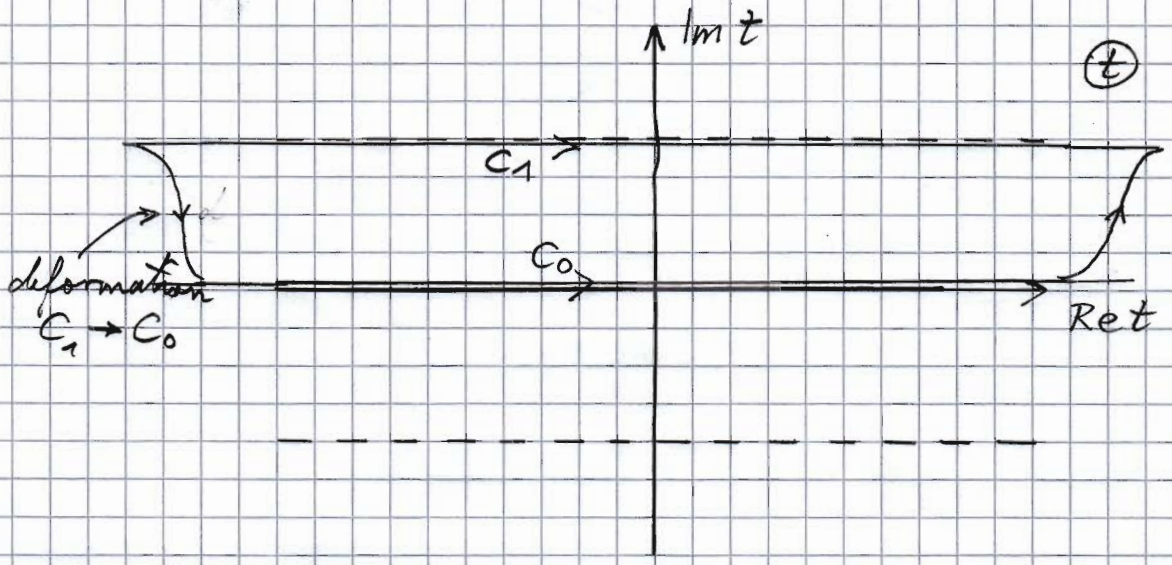
$t' = t + i\beta$

$$= \mp e^{\beta\omega} \int_{C_1} dt' e^{i\omega t'} G^<(t') =$$

$$= \mp e^{\beta\omega} \int_{C_0} dt' e^{i\omega t'} G^<(t') = \mp e^{\beta\omega} G^<(\omega)$$

analyticity in (B): $C_1 \to C_0$

$$\boxed{G^>(\omega) = \underset{B}{\overset{F}{\mp}} e^{\beta\omega} G^<(\omega)} \qquad \omega \in \mathbb{R} \quad (**)$$



FT of $G(t)$:

$$G(t) = \int \frac{d\omega}{2\pi} G(\omega) e^{-i\omega t}$$

$$G(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t} G(t) = \int_{-\infty}^{0} dt\, e^{i\omega t} G^{<}(t) + \int_{0}^{\infty} dt\, e^{i\omega t} G^{>}(t)$$

$$\overset{(*)}{=} \int_{-\infty}^{0} dt \int \frac{d\omega'}{2\pi} e^{i(\omega-\omega'-i\eta)t} G^{<}(\omega')$$

$$\eta \to 0^{+} \qquad + \int_{0}^{\infty} dt \int \frac{d\omega'}{2\pi} e^{i(\omega-\omega'-i\eta)t} G^{>}(\omega')$$

$$\boxed{G(\omega) = i \int \frac{d\omega'}{2\pi} \left[\frac{G^{>}(\omega')}{\omega - \omega' + i\eta} - \frac{G^{<}(\omega')}{\omega - \omega' - i\eta} \right]} \qquad (***)$$

Our goal is to extract the retarded / advanced Green's functions $G^{R/A}(\omega)$ from the time-ordered one $G(\omega)$.

To that end we define the so-called

<u>Spectral function</u> ($\vec{r}, \vec{r}'$ or $\vec{k}, \vec{k}'$ variables suppressed for clarity.)

$$A(\omega) := \frac{i}{2\pi}\left[G^{>}(\omega) - G^{<}(\omega)\right] .$$

We use $A(\omega)$ to express the time-ordered G-functions:

Using (**):

$$A(\omega) = \begin{cases} \mp \frac{i}{2\pi}\left(e^{\beta\omega} \pm 1\right) G^{<}(\omega) & \text{or} \\ \frac{i}{2\pi}\left(1 \pm e^{-\beta\omega}\right) G^{>}(\omega) \end{cases}$$

$$G^{<}(\omega) = \mp 2\pi i \underbrace{\frac{1}{e^{\beta\omega} \pm 1}}_{f,\,b} A(\omega) = \begin{cases} 2\pi i\, f(\omega)\, A(\omega), & F \\ -2\pi i\, b(\omega)\, A(\omega), & B \end{cases}$$

$$G^{>}(\omega) = -2\pi i \frac{1}{1 \pm e^{-\beta\omega}} A(\omega) = \begin{cases} -2\pi i\,(1-f(\omega))\, A(\omega), & F \\ -2\pi i\,(1+b(\omega))\, A(\omega), & B \end{cases}$$

$$\frac{1}{1+e^{-\beta\omega}} = \frac{e^{\beta\omega}+1-1}{e^{\beta\omega}+1} = 1 - f(\omega) = f(-\omega)$$

$$\frac{1}{1-e^{-\beta\omega}} = \frac{e^{\beta\omega}-1+1}{e^{\beta\omega}-1} = 1 + b(\omega) = -b(-\omega)$$

in integral representation for $G(\omega)$ (***):

$$G(\omega) = \int d\omega' \, A(\omega') \left[\frac{1 - f(\omega')}{\omega - \omega' + i\eta} + \frac{f(\omega')}{\omega - \omega' - i\eta} \right] \qquad F$$

($A(\omega')$: spectral information; $1 - f(\omega')$: statistical)

$$G(\omega) = \int d\omega' \, A(\omega') \left[\frac{1 + b(\omega')}{\omega - \omega' + i\eta} - \frac{b(\omega')}{\omega - \omega' - i\eta} \right] \qquad B$$

Lehmann or spectral representation

Spectral representation for the Retarded / advanced Green's function

$$G^R(t) = -i \frac{1}{Z_G} \Theta(t) \, \mathrm{tr}\left\{ e^{-\beta(H - \mu N)} \left[\psi(t), \psi^+(0) \right]_{\pm} \right\} \quad (F \text{ or } B)$$

$$= \Theta(t) \left[G^>(t) - G^<(t) \right]$$

(def. of $G^>, G^<$)

(for both, F and B)

FT:

$$G^R(\omega) = \int dt \, e^{i\omega t} \, G^R(t) = \int_0^\infty dt \, e^{i(\omega + i\eta)t} \left[G^>(t) - G^<(t) \right]$$

($\eta \to 0+$: convergence factor)

$$G^{>,<}(t) = \int \frac{d\omega'}{2\pi} \, e^{-i\omega' t} \, G^{>,<}(\omega')$$

$$= i \int \frac{d\omega'}{2\pi} \, \frac{G^>(\omega') - G^<(\omega')}{\omega - \omega' + i\eta}$$

$$G^R(\omega) = \int d\omega' \frac{A(\omega')}{\omega - \omega' + i\eta}$$

analogous:

$$G^A(\omega) = \int d\omega' \frac{A(\omega')}{\omega - \omega' - i\eta} = G^R(\omega)^*$$

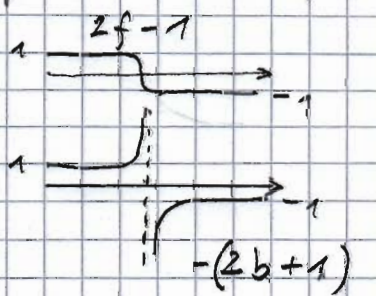
The spectral function $A(\omega)$ provides the link for calculating the physical Green's functions $G^{R/A}$:

1. Calculate the time-ordered $G(\omega)$
   - convenient periodic properties in imaginary time (see Matsubara technique, analytic continuation)
   - accessible by perturbation theory (see Wick's theorem)

2. Obtain the spectral function $A(\omega)$ from $\mathrm{Im}\, G(\omega)$:

F: $\mathrm{Im}\, G(\omega) = \pi A(\omega)\,(2f(\omega) - 1)$

B: $\mathrm{Im}\, G(\omega) = -\pi A(\omega)\,(2b(\omega) + 1)$



3. Compute $G^{R/A}(\omega)$ from $A(\omega)$.

The physical meaning of A(ω)

From the definition of A(ω) we have in time space:

$$A(\vec{r},\vec{r}',t) = \frac{1}{2\pi}\frac{1}{Z_G} tr\Big\{ e^{-\beta(H-\mu N)} e^{i(H-\mu N)t} \psi(\vec{r}) e^{-i(H-\mu N)t} \psi^+(\vec{r}')$$

$$\sum_{N,n} |\psi_n^N\rangle\langle\psi_n^N| \qquad \sum_m |\psi_m^{N+1}\rangle\langle\psi_m^{N+1}|$$

$$\pm\, e^{-\beta(H-\mu N)} \psi^+(\vec{r}') e^{i(H-\mu N)t} \psi(\vec{r}) e^{-i(H-\mu N)t} \Big\}$$

$$\sum_m |\psi_m^{N-1}\rangle\langle\psi_m^{N-1}| \qquad |\psi_n^N\rangle$$

$$= \frac{1}{2\pi}\frac{1}{Z_G}\sum_{N,n,m} e^{-\beta(E_n^N-\mu N)} \Big\{ e^{-i(E_m^{N+1}-E_n^N-\mu)t} \langle\psi_n^N|\hat\psi(\vec{r})|\psi_m^{N+1}\rangle\langle\psi_m^{N+1}|\hat\psi^+(\vec{r}')|\psi_n^N\rangle$$

$$\pm\, e^{-i(E_n^N-E_m^{N-1}-\mu)t} \langle\psi_n^N|\hat\psi^+(\vec{r}')|\psi_m^{N-1}\rangle\langle\psi_m^{N-1}|\hat\psi(\vec{r})|\psi_n^N\rangle \Big\}$$

FT in space; transl. inv.: only dependent on $\vec{r}-\vec{r}'$.

$$\int d^3r \int d^3r'\, e^{-i\vec{p}\vec{r}} e^{+i\vec{p}'\vec{r}'} \ldots =$$

$$= \int d^3r \int d^3r'\, e^{-i\vec{p}(\vec{r}-\vec{r}')} e^{i(\vec{p}-\vec{p}')\vec{r}'} \ldots$$

$$\vec{r}-\vec{r}' = \tilde{\vec{r}} \qquad \to \delta_{pp'}$$

$$= \int d^3\tilde{r}\, e^{-i\vec{p}\tilde{\vec{r}}}\, \delta_{pp'}$$

$$\psi(r)\psi^+(\vec{r}') \to \sum_p c_p\, c_p^+$$

a) Fermions:

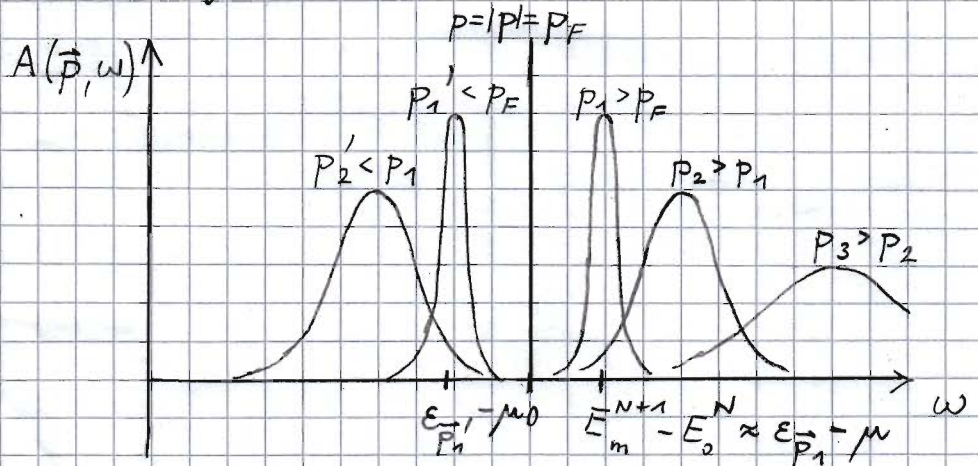
At $T=0$ injection of a particle is only possible above ε_F (1. term in $A(\vec{p},\omega)$)

removal " " " " " " below ε_F (2. term in $A(\vec{p},\omega)$).

The level spacing in a system of volume V is typically $E_{n+1}^{N+1} - E_n^N \sim \frac{1}{V}$, i.e. for a macroscopic system, $V \to \infty$, $A(\vec{p},\omega)$ can be considered as a continuous function of ω.

(i) Typical shape of $A(\vec{p},\omega)$ for $T=0$:

$T=0$: Only $|\Psi_0^N\rangle$ contributes to the thermal average,



(measurements: photoemission)

(ii) In general, the many-body eigenstate $|\Psi_m^{N+1}\rangle$ is not an eigenstate of the single-particle momentum $\vec{p}$: By many-body interactions, a single-particle momentum state can decay.

Therefore, several of the matrix elements in $A(\vec{p},\omega)$ contribute for a given $\vec{p}$.

FT wrt. time: $\int dt\, e^{i\omega t} \ldots$:

$$A(\vec{p},\omega) = \sum_{N,nm} \frac{e^{-\beta(H-\mu N)}}{Z_G} \Big\{ \delta\big(\omega - (\underbrace{E_m^{N+1} - E_n^N}_{\text{energy difference of final and initial state}} - \mu)\big) \left| \langle \Psi_m^{N+1} | C_{\vec{p}}^{+} | \Psi_n^N \rangle \right|^2$$

$$\pm\, \delta\big(\omega + (E_m^{N-1} - E_n^N + \mu)\big) \left| \langle \Psi_m^{N-1} | C_{\vec{p}} | \Psi_n^N \rangle \right|^2$$

energy difference counted negative

Properties of the spectral function:

1. $A(\vec{p},\omega)$ is real. $\quad A(\vec{p},\omega) \in \mathbb{R}$

2. Fermions: $\quad A(\vec{p},\omega) \geq 0 \quad \forall\, \omega \in \mathbb{R}$

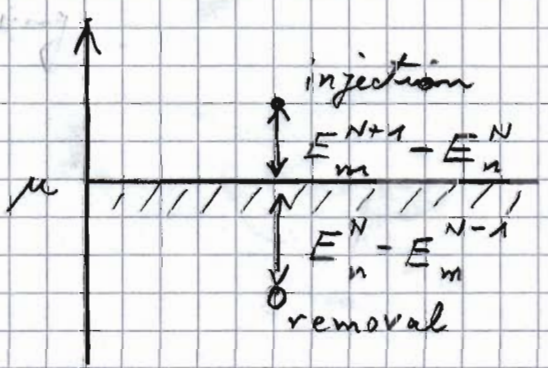
   Bosons: $\quad A(\vec{p},\omega) \begin{cases} \geq 0 & \forall\, \omega \geq 0 \\ \leq 0 & \forall\, \omega < 0 \end{cases}$

   $$\omega\, A(\vec{p},\omega) \geq 0 \quad \forall\, \omega \in \mathbb{R}$$

   (ω measured relative to μ.)

3. Interpretation and further properties

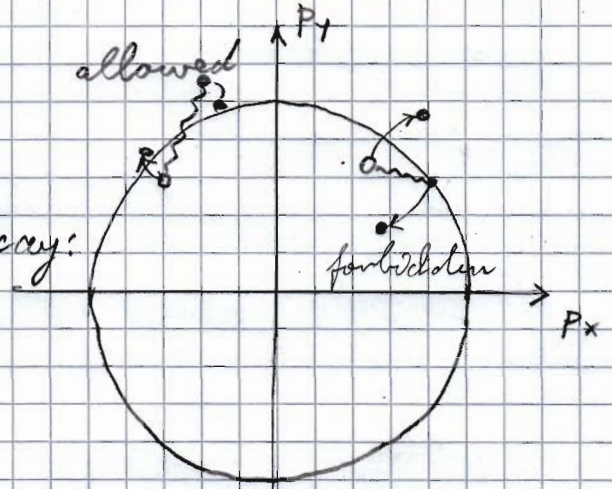
   $A(\vec{p},\omega)$ is the (thermodynamic and quantum mechanical) probability for injecting or removing a particle with momentum $\vec{p}$ at energy ω (w.r.t. μ).



fermions

→ In general, for fixed $\vec{p}$ $A(\vec{p},\omega)$ is not a single δ-function, but a broadened peak.
The phase space for decay ⊛ ($\hat{=}$ number of states available to decay into) is the larger the further away $|\vec{p}|$ is from p_F. For $|\vec{p}| = p_F$ no decay is possible because of phase space restrictions.
Therefore, the peak width of $A(\vec{p},\omega)$ increases with $||\vec{p}| - p_F|$.

⊛ phase space restriction on decay: Pauli principle → Landau Fermi liquid theory



At $T>0$ the peaks are additionally broadened.

(ii) $A(\vec{p},\omega) \neq 0$ only if there exists ω such that $\omega \approx \varepsilon_{\vec{p}}$ single-particle energy, i.e. inside the energy bands.

(iii) Normalization:

$$\int_{-\infty}^{+\infty} d\omega\, A(\vec{p},\omega) = 1$$

[Proof: represent $\int d\omega\, A(\vec{p},\omega)$ as equal-time expectation value of $c_p\, c_p^+ \pm c_p^+\, c_p$ and use (anti-) commutation rules.]

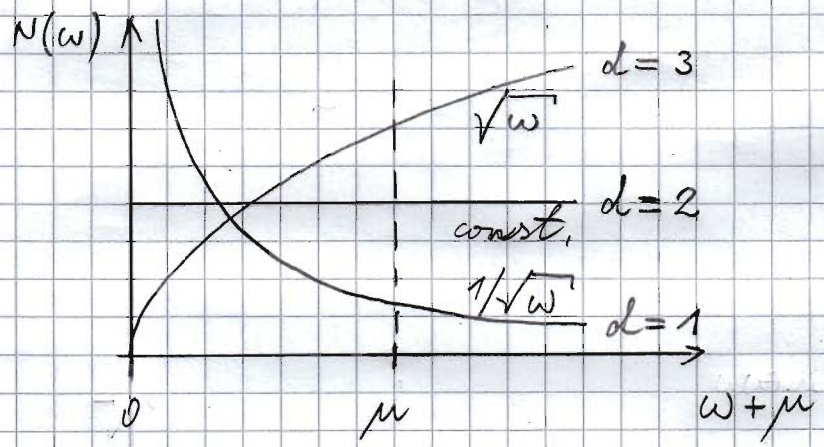
(iv) The density of states $N(\omega)$

$$N(\omega) = \sum_{\vec{p}} A(\vec{p}, \omega)$$

From the definition of $A(\vec{p}, \omega)$ as a probability density it follows that

$N(\omega)\,d\omega$ the number of single-particle states that exist in the infinitesimal energy interval $d\omega$ in a system of volume V.

→ $N(\omega)$ is the single-particle density of states (DOS)



DOS of a free electron gas

(→ exercise)

free electron gas: $\varepsilon_p = \frac{p^2}{2m}$: $\boxed{N(\omega) \sim \omega^{(d-2)/2}}$

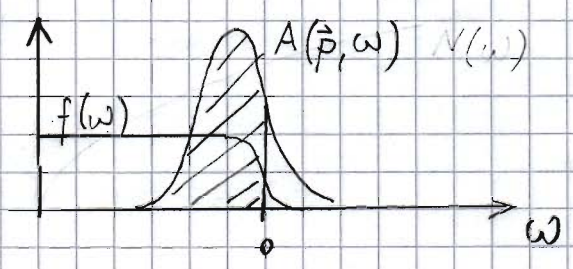
(v) The particle number

$$n_{\vec{p}} = \int d\omega\, f(\omega)\, A(\vec{p}, \omega) \geq 0$$

(see formal calculation using Matsubara below.)

$f(\omega)$: probability that the state at $\vec{p}, \omega$ is occupied

$A(\vec{p}, \omega)$: probability that there exists a state at $\vec{p}, \omega$



- <u>Bosons</u>

Most properties of $A(\vec{p},\omega)$ and $N(\omega)$ hold for bosons like for fermions, with 2 exceptions:

(i) The concept of well-defined quasiparticles near ε_F (i.e. no decay) does not hold in the same way because there is no Pauli principle. At low T a new phenomenon appears: BEC.

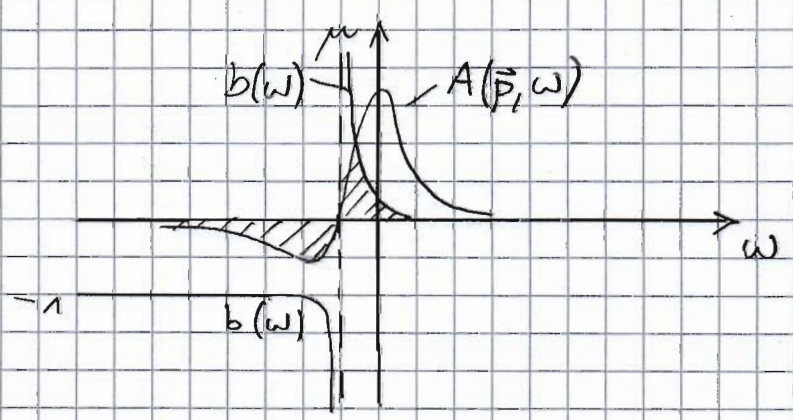
(ii) The probability density is not positive definite!

$$\omega A(\vec{p},\omega) \geq 0$$

This is physically meaningful, because the particle number is

$$n_{\vec{p}} = \int d\omega \; b(\omega) A(\vec{p},\omega)$$

i.e. the product $b(\omega)A(\vec{p},\omega)$ is positive semidefinite and $n_{\vec{p}}$ has only positive contributions.



Analytical continuation to complex ω and Kramers-Kronig relations

Using the spectral representation of the t-ordered Green's function

(similar for bosons)

$$G(\omega) = \int d\omega' A(\omega') \left[\frac{1-f(\omega')}{\omega - \omega' + i\eta} + \frac{f(\omega')}{\omega - \omega' - i\eta} \right],$$

where $A(\omega') \in \mathbb{R}$,

$G(\omega)$ can be analytically continued by setting

$\omega \to z \in \mathbb{C}$.

Then the infinitesimal imaginary parts η are irrelevant, and we have

$$\boxed{G(z) = \int d\omega' \frac{A(\omega')}{z - \omega'}}$$

By construction, $G(z)$

- is analytical in the upper and in the lower half complex plane.
- has a branch cut at the real axis ($\mathrm{Im}\, z = 0$)

$$G(\omega + i\eta) - G(\omega - i\eta) = \int d\omega' A(\omega') \left[\frac{1}{\omega - \omega' + i\eta} - \frac{1}{\omega - \omega' - i\eta} \right]$$

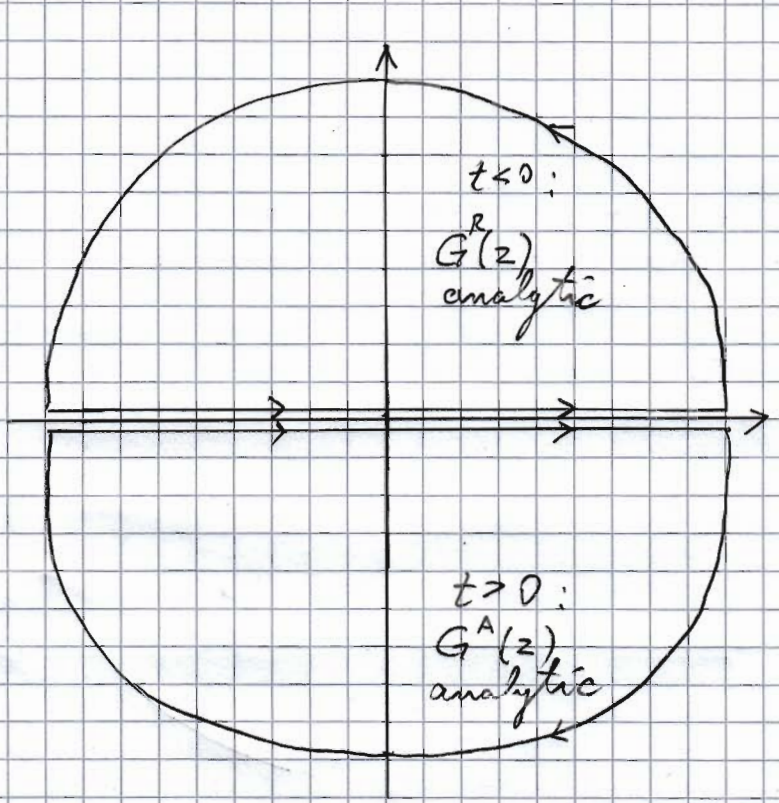
$$= \int d\omega' A(\omega') \left(-2\pi \delta(\omega - \omega') \right)$$

$$= -2\pi i A(\omega).$$

The step at the branch cut is $-2\pi i A(\omega)$.

Causality requires that $G^{R/A}(z)$ is analytic in the upper / lower half plane:

Proof:



$$0 \overset{!}{=} G^R(t<0) = \int \frac{d\omega}{2\pi} e^{-i\omega t} G^R(\omega) = \oint \frac{dz}{2\pi} e^{-izt} G^R(z)$$

converges in upper z-plane for $t<0$

$\Rightarrow$ $G^R(z)$ analytic for $\mathrm{Im}\, z > 0$.

$$0 \overset{!}{=} G^A(t>0) = \int \frac{d\omega}{2\pi} e^{-i\omega t} G^A(\omega) = \oint \frac{dz}{2\pi} e^{-izt} G^A(z)$$

converges in lower z-plane for $t>0$

$\Rightarrow$ $G^A(z)$ analytic for $\mathrm{Im}\, z < 0$

Since the analytic continuation of a function given on the closed rim of the region of analyticity is unique, the retarded / advanced G-functions

$$G^{R/A}(\omega) = \int d\omega' \frac{A(\omega')}{\omega - \omega' \pm i\eta}$$

are analytically continued to the upper / lower half plane by $\omega \to z \in \mathbb{C}$, $\mathrm{Im}\, z \gtrless 0$.
$G^{R/A}(z)$ must have pole in lower/upper half plane, since $G^R(t>0) \neq 0$, $G^A(t<0) \neq 0$.
Hence we have

$$G^R(z) = G(z) \qquad \mathrm{Im}\, z > 0$$

$$G^A(z) = G(z) \qquad \mathrm{Im}\, z < 0$$

and in particular for $z \to \omega \pm i\eta$, $\omega \in \mathbb{R}$

$$\boxed{\begin{aligned} G(\omega + i\eta) &= G^R(\omega) \\ G(\omega - i\eta) &= G^A(\omega) \end{aligned}} \qquad \omega \in \mathbb{R}$$

In this way, $G^{R/A}(\omega)$ can be easily obtained from the (analytically continued) t-ordered function $G(z)$.

Kramers – Kronig relation:

An arbitrary function $G^{R/A}$ analytic in the upper/lower half plane can be uniquely written on the real axis as

$$G^{R/A}(\omega) = \int d\omega' \frac{A(\omega')}{\omega - \omega' \pm i\eta} = \mathcal{P}\int d\omega' \frac{A(\omega')}{\omega - \omega'} \mp i\pi A(\omega)$$

with a real function $A(\omega')$.

Hence we have

$$\boxed{\begin{aligned} \mathrm{Im}\, G^{R/A}(\omega) &= \mp \pi A(\omega) \\ \mathrm{Re}\, G^{R/A}(\omega) &= \mp \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\, G^{R/A}(\omega)}{\omega - \omega'} \end{aligned}}$$

— must Kramers – Kronig

1.2.3 The Matsubara technique

It is more convenient to evaluate Green's functions on the imaginary axis, because

- $G(t)$ is periodic along the imaginary time axis
- there are no statistical factors $f(\omega)$, $b(\omega)$ in $G(z)$ on the imaginary frequency axis,

$$G(z) = \int d\omega' \frac{A(\omega')}{z - \omega'}$$

in contrast to the spectral representation of $G(\omega)$ on the real axis.

The statistical factors would complicate integrals over $G(\omega)$.

→ We evaluate expressions first on the imaginary ω axis. The information about the statistical occupation probabilities, $f(\omega)$ or $b(\omega)$, will enter naturally through the "Matsubara frequency summation" and the subsequent analytical continuation to the real axis.

To exploit the periodicity (anti-) of $G(t)$ along the imaginary time axis, we define the imaginary time as

$$\boxed{t = -i\tau}$$

"Wick rotation" in complex plane by $\varphi = +\frac{\pi}{2}$

$$\left(\tau = e^{i\frac{\pi}{2}} t\right)$$

We further define the "thermal Green's function"

$$\boxed{\tilde{G}(\tau) = -i\, G(-i\tau)} \quad , \qquad \tau \in \mathbb{R}$$

Since $\tilde{G}(\tau)$ is antiperiodic / periodic in τ, it can be represented as a Fourier series ("Matsubara series"):

$$\boxed{\begin{aligned} \tilde{G}(\tau) &= \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau}\, \tilde{G}(\omega_n) \\ \tilde{G}(\omega_n) &= \int_0^\beta d\tau\, e^{+i\omega_n \tau}\, \tilde{G}(\tau) \end{aligned}} \qquad \text{with}$$

The values for ω_n follow from the (anti-) periodicity:

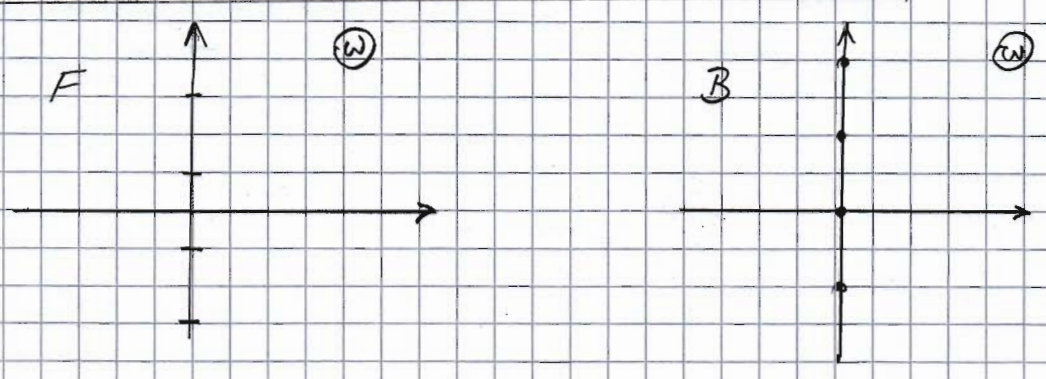
$$\tilde{G}(\tau - \beta) = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n(\tau-\beta)}\, \tilde{G}(\omega_n)$$

$$F \to \; \stackrel{!}{=} \; -\frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau}\, \tilde{G}(\omega_n)$$

$$B \to$$

$$\Leftrightarrow \qquad e^{i\omega_n \beta} = -1 \qquad \text{or}$$

$$\boxed{\begin{aligned} \omega_n &= \frac{\pi}{\beta}(2n+1) && \text{fermions} \\ \omega_n &= \frac{\pi}{\beta} \cdot 2n && \text{bosons} \end{aligned} \qquad n = 0, \pm 1, \pm 2, \ldots}$$



How can the physical functions $G^{R/A}$ be obtained from the thermal one $\tilde{G}$?

$$G(t) \xrightarrow[\text{to imaginary time}]{\text{analyt. cont.}} \tilde{G}(\tau) = -i\,G(-i\tau),\ \tau \in \mathbb{R}$$

$$\downarrow \text{FT} \qquad\qquad \downarrow \text{FT (period. in } \tau)$$

$$G(\omega) = \int dt\, e^{+i\omega t} G(t) \qquad \tilde{G}(\omega_n) = \int_0^\beta d\tau\, e^{+i\omega_n \tau} \tilde{G}(\tau)$$

$$\downarrow \text{analytic cont. to complex frequency} \qquad \downarrow \text{analyt. cont.}\ (*)$$

$$G(z) = \int d\omega' \frac{A(\omega')}{z-\omega'} \quad \overset{?}{\Longleftrightarrow} \quad \tilde{G}(z)$$

However: (for fermions; bosons analogous)

$$\tilde{G}(\omega_n) = -i \int_0^\beta d\tau\, e^{i\omega_n \tau} G^{\rightarrow}(-i\tau)$$

$$= -i \int_0^\beta d\tau\, e^{i\omega_n \tau} \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} e^{-i\omega'(-i\tau)} \left[\frac{2\pi}{i} A(\omega') f(-\omega')\right]$$

$$= -\int d\omega' f(-\omega') A(\omega') \frac{(e^{i\omega_n \beta} e^{-\omega'\beta} - 1)^{-1}}{i\omega_n - \omega'} = \int d\omega' \frac{A(\omega')}{i\omega_n - \omega'}$$

$$\xrightarrow[\text{analyt. continuation}]{(*)} \int d\omega' \frac{A(\omega')}{z-\omega'} = \tilde{G}(z)$$

$\Rightarrow$ $\tilde{G}(z)$ and $G(z)$ are identical!

$G^{R/A}(\omega)$ is obtained from $\tilde{G}(\omega_n) \equiv G(i\omega_n)$ simply by $i\omega_n \to \omega \pm i\eta$.