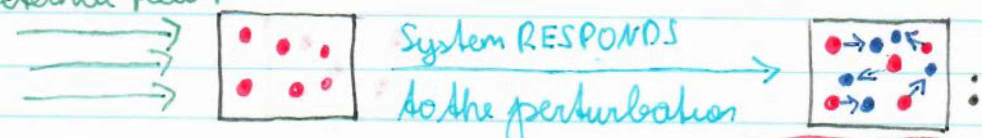
5. Linear response Theory

external field F F... electric field, magnetic field, ...



: Expectation value of an operator O, $\langle O \rangle$, depends on field: $\boxed{\langle O \rangle = \langle O \rangle(F)}$

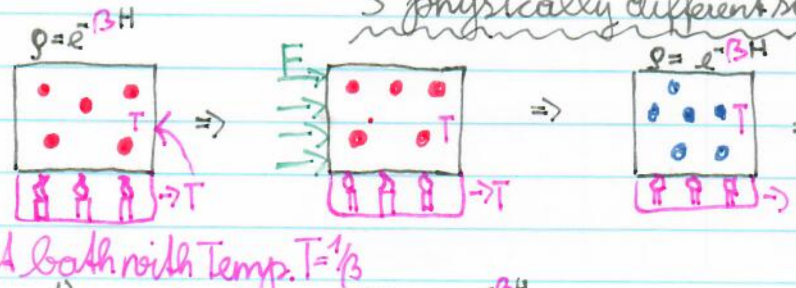
LINEAR response: $\langle O \rangle(F) = \underbrace{\langle O \rangle}_{\text{without field}} + \boxed{\left.\frac{\partial \langle O \rangle(F)}{\partial F}\right|_{F=0} \cdot F} + O(F^2)$ (1)

↳ LINEAR response term!

$$\left.\frac{\partial \langle O \rangle(F)}{\partial F}\right|_{F=0} = \chi \text{... SUSCEPTIBILITY (which is related to a 2-particle GF } G^{(2)}\text{)} \quad (2)$$

3 physically different situations

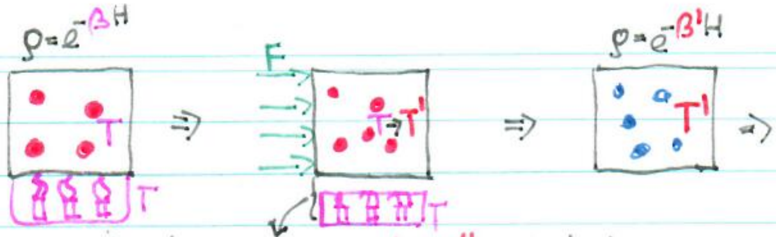
a)



⇒ (grand) canonical ensemble: $\rho = e^{-\beta H}$

⇒ ISOTHERMAL response:
⇒ System remains coupled to the bath when F is applied
→ $\rho = e^{-\beta H}$ after F is applied!
→ β... unchanged!

b)



System is „essentially" isolated when F is applied; Only a „small" coupling to the bath remains!

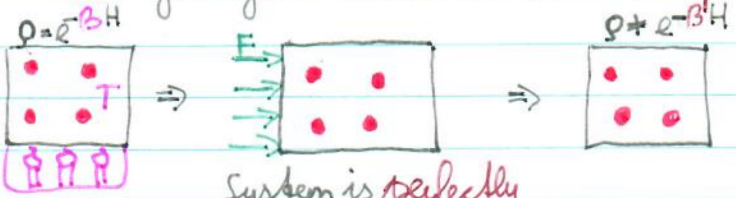
ADIABATIC response:

⇒ System remains in a thermal state (grand canonical ensemble) but with a different temperature:

→ $\rho = e^{-\beta' H}$

→ $\beta \Rightarrow \beta'$ during the process

c)



System is perfectly isolated!

KUBO (ISOLATED) response:

⇒ Initially (grand) canonical ensemble, does NOT remain canonical!

⇒ $\rho \neq e^{-\beta H}$!

In all three situations, we can calculate the respective susceptibility, i.e., the isothermal susceptibility χ^I, the adiabatic susceptibility χ^A or the Kubo susceptibility χ^K.

⇒ In the following we will discuss χ^I and χ^K!

Hamiltonian in the presence of the external field: $H \rightarrow H(F)$

$\Rightarrow$ Since we are interested only in the LINEAR response, we can expand $H(F)$ in terms of F: $H(F) = \underbrace{H(F=0)}_{H} + F \underbrace{H'(F=0)}_{H_1} + O(F^2)$ (3)

$\Rightarrow$ The Hamiltonian takes the form: $H(F) = \overset{\text{Hamiltonian without external field } F}{H} + F \cdot \overset{\text{operator, which couples linearly to the external field } F}{H_1}$

Note: Typically, an external field couples only linearly to an external field anyway! (E.g., Gauge fields in relativistic QFT.)

Examples:

$\rightarrow$ Coupling of $\boxed{\text{spin}}$ to a magnetic field: $H_1 = \overset{\hat{=} F}{B} \cdot \sum_i (n_{i\uparrow} - n_{i\downarrow})$ (4)

$\rightarrow$ Coupling of the $\boxed{\text{current}}$ to an electromagnetic field: $H_1 = -\frac{1}{c} \int d^3r \, \overset{\text{current operator}}{\vec{j}(\vec{r})} \vec{A}(\vec{r})$

$\Rightarrow \vec{j}(\vec{r}) = \underbrace{-\frac{ie\hbar}{2m} \left[\psi_\sigma^+(\vec{r}) \vec{\nabla} \psi_\sigma(\vec{r}) - (\vec{\nabla} \psi_\sigma^+(\vec{r})) \psi_\sigma(\vec{r}) \right]}_{\text{paramagnetic current}} + \underbrace{\frac{e^2}{mc} \psi_\sigma^+(\vec{r}) \psi_\sigma(\vec{r}) \vec{A}(\vec{r})}_{\text{diamagnetic current}}$ (5)

vector potential $\hat{=} F$

ⓐ Isothermal response:

The form of the density matrix does not change, when the field F is applied:

$\Rightarrow \langle O \rangle(F) = \frac{1}{Z(\beta, F)} \mathrm{Tr}\left(e^{-\beta H(F)} O\right)$, with $Z(\beta, F) = \mathrm{Tr}\left(e^{-\beta H(F)}\right)$ (6)

$\Rightarrow$ Calculating the derivative $\frac{d}{dF}\langle O \rangle(F)$ requires $\boxed{\frac{d}{dF} e^{-\beta H(F)}}$!

„Naive" attempt: $\frac{d}{dF} e^{-\beta H(F)} = \underbrace{e^{-\beta H(F)} \frac{dH(F)}{dF}(-\beta)}_{(1)}$ $\boxed{\text{or}}$ $\underbrace{\frac{dH(F)}{dF} e^{-\beta H(F)}(-\beta)}_{(2)}$ (7)

Problem: When $\left[H(F), \frac{dH(F)}{dF}\right] \neq$ (which is generally the case), expressions (1) and (2) are different $\rightarrow$ „naive" attempt does not work.

Possible solution: Consider Taylor series for $e^{-\beta H(F)} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \beta^n \left(H(F)\right)^n$ (8)

$\Rightarrow$ Here, one can take directly the derivative w.r.t. F, but this gets a bit „messy"!

$\rightarrow$ Alternative: Differential Equation!

We define: $\underline{A(\beta, F) = \frac{\partial}{\partial F} e^{-\beta H(F)}}$ $\Rightarrow$ take a derivative w. r. t. β:

- $\frac{\partial}{\partial\beta} A(\beta, F) = \frac{\partial}{\partial\beta}\frac{\partial}{\partial F} e^{-\beta H(F)} = \frac{\partial}{\partial F}\frac{\partial}{\partial\beta} e^{-\beta H(F)} = -\frac{\partial}{\partial F}\left[H(F)\, e^{-\beta H(F)}\right] =$

$$= -H(F)\underbrace{\left[\frac{\partial}{\partial F} e^{-\beta H(F)}\right]}_{A(\beta, F)} - \underbrace{\frac{\partial H(F)}{\partial F}}_{H'(F)} e^{-\beta H(F)} \quad (9)$$

- $A(\beta = 0, F) = \frac{\partial}{\partial F}\mathbb{1} = 0$ (10)

$$\Rightarrow \boxed{\frac{\partial}{\partial\beta} A(\beta, F) = -H(F) A(\beta, F) - H'(F)\, e^{-\beta H(F)}, \quad A(\beta = 0, F) = 0} \quad (11)$$

$\Rightarrow$ Autonomous, inhomogeneous, linear first order differential Eq. for $A(\beta, F)$ with the initial condition $A(\beta = 0, F) = 0$!

Solution of homogeneous equation: $\frac{\partial}{\partial\beta} A_0(\beta, F) = -H(F) A_0(\beta, F) \Rightarrow \underline{A_0(\beta, F) = e^{-\beta H(F)}}$ (12)

Ansatz for inhomogeneous equation: $A(\beta, F) = A_0(\beta, F) \cdot G(\beta, F)$ (variation of parameters) (13)

$$\Rightarrow \frac{\partial}{\partial\beta} A(\beta,F) = -\cancel{H(F)A(\beta,F)} + e^{-\beta H(F)} \frac{\partial G(\beta,F)}{\partial \beta\, \partial F} = -\cancel{H(F)A(\beta,F)} - H'(F)\, e^{-\beta H(F)} \quad (14)$$

$$\Rightarrow \frac{\partial G(\beta,F)}{\partial\beta} = -e^{\beta H(F)} H'(F)\, e^{-\beta H(F)} \Rightarrow G(\beta,F) = \underbrace{G_0}_{G(0,F)} - \int_0^\beta d\tau\, e^{\tau H(F)} H'(F)\, e^{-\tau H(F)} \quad (15)$$

$$\Rightarrow A(\beta,F) = e^{-\beta H(F)} G_0 - e^{-\beta H(F)} \int_0^\beta d\tau\, e^{\tau H(F)} H'(F)\, e^{-\tau H(F)} \quad (16)$$

Initial condition: $A(\beta=0,F) = G_0 \equiv 0$ (17)

$$\Rightarrow A(\beta,F) = \boxed{\frac{\partial}{\partial F} e^{-\beta H(F)} = -e^{-\beta H(F)} \int_0^\beta d\tau\, e^{\tau H(F)} \frac{dH}{dF}(F)\, e^{-\tau H(F)} \quad (18)}$$

This result allows us now to calculate the change of the expectation value $\langle O\rangle$ due to the external field F to linear order:

$$\frac{\partial}{\partial F}\left[\frac{1}{Z(\beta,F)} \mathrm{Tr}\left(e^{-\beta H(F)} O\right)\right] = -\frac{1}{Z(\beta,F)^2} \cdot \frac{\partial Z(\beta,F)}{\partial F} \cdot \mathrm{Tr}\left(e^{-\beta H(F)} O\right) + \frac{1}{Z(\beta,F)} \mathrm{Tr}\left(\left[\frac{\partial}{\partial F} e^{-\beta H(F)}\right] O\right) \quad (19)$$

$$\odot\ \frac{\partial Z(\beta,F)}{\partial F} = \mathrm{Tr}\left(\frac{\partial}{\partial F} e^{-\beta H(F)}\right) = -\int_0^\beta d\tau\, \mathrm{Tr}\left(e^{-\beta H(F)} e^{\tau H(F)} \frac{dH}{dF}(F)\, e^{-\tau H(F)}\right)$$

$$= -\int_0^\beta d\tau\, \mathrm{Tr}\left(e^{-\beta H(F)} \cdot H'(F)\right) = -\beta \langle H'(F)\rangle \cdot Z(\beta,F) \quad (20)$$

$$\Rightarrow -\frac{1}{Z(\beta,F)^2}\cdot\frac{\partial Z}{\partial F}(\beta,F)\,\mathrm{Tr}\left(e^{-\beta H(F)}\cdot O\right) = \beta\cdot\langle O\rangle\cdot\langle H(F)\rangle \quad (21)$$

$$\odot\ \mathrm{Tr}\left(\left[\frac{\partial}{\partial F}e^{-\beta H(F)}\right]O\right) = -\int_0^\beta d\tau\,\mathrm{Tr}\Big(e^{-\beta H(F)}\underbrace{e^{\tau H(F)}H'(F)e^{-\tau H(F)}}_{\text{Matsubara time evolution of operator } H'(F):\ H'(F,\tau) := H'_F(\tau)}O\Big) \quad (22)$$

$$= -\int_0^\beta d\tau\,\mathrm{Tr}\left(e^{-\beta H(F)}H'_F(\tau)\,O\right) = -\int_0^\beta d\tau\,\langle H'_F(\tau)\,O\rangle\,Z(\beta,F) \quad (23)$$

$$\Rightarrow \frac{1}{Z(\beta,F)}\mathrm{Tr}\left(\left[\frac{\partial}{\partial F}e^{-\beta H(F)}\right]O\right) = -\int_0^\beta d\tau\,\langle H'_F(\tau)\,O\rangle \quad (24)$$

$$\Rightarrow \boxed{\frac{\partial}{\partial F}\langle O\rangle(F)\Big|_{F=0} = -\int_0^\beta d\tau\left[\langle H_1(\tau)\,O\rangle - \langle H_1\rangle\langle O\rangle\right] \quad (25)} \qquad \left(H_1(\tau) = H'_{F=0}(\tau)\right)$$

where the expectation values are taken for $F=0$!

Interpretation: The isothermal response is given by the correlation function between H_1 and O, averaged over imaginary times τ!

$\Rightarrow$ Matsubara time evolution appears NATURALLY here!

$\Rightarrow$ Question: What is the connection to Matsubara Green's functions?

(Remark: The uncorrelated contribution $\langle H_1\rangle\langle O\rangle$ can be always set to 0 by redefining $O \to O - \langle O\rangle$!)

Let us define a more general Matsubara Green's function for two bosonic operators A and B:

$\frac{2m\pi}{\hbar\beta}$ ... bosonic Mat. Frequ.

$$G^M_{AB}(\tau) = -\langle A(\tau)\, B\rangle \Theta(\tau) - \langle B A(\tau)\rangle \Theta(-\tau) \qquad \tilde{G}^M_{AB}(i\Omega_m) = \int_0^\beta d\tau\, e^{i\Omega_m \tau}\, G^M_{AB}(\tau) \quad (26)$$

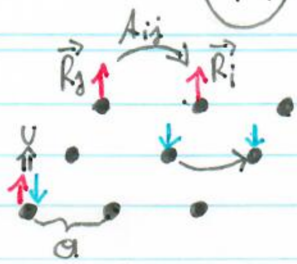
⇒ This allows us to express Eq. (25) in terms of this (generalized) bosonic Matsubara Green's function:

$$\boxed{\chi^I_{H_1 O} = \frac{\partial}{\partial F}\langle O\rangle(F)\Big|_{F=0} = \tilde{G}^M_{H_1 O}(i\Omega_m = 0) \quad (\text{assuming } \langle O\rangle = 0) \quad (27)}$$

⇒ The isothermal linear response of $\langle O\rangle$ to an external field F which is coupled to the system by $H \to H + F\cdot H_1$ is given by the Matsubara Green's function $\tilde{G}^M_{H_1 O}(i\Omega_m)$ at zero frequency $i\Omega_m = 0$!

⇒ This illustrates the „special" role of $i\Omega_m = 0$ for bosonic Green's functions!

Note: The generalized Matsubara Green's function $\tilde{G}^M_{H_1 O}(i\Omega_m)$ has the same analytic properties as the standard $\tilde{G}^M_{ij}(i\Omega_m)$.



Examples and relation to two-particle Green's functions:

We consider the Hubbard model [see chapter 2, Eq. (34)] :

$$H = \sum_{ij,\sigma} A_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (28)$$

$n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ ... particle number (density)

$i \hat{=} \vec{R}_i$ ... lattice site

A_{ij} ... hopping amplitud from lattice site $\vec{R}_j$ to $\vec{R}_i$

U ... local Coulomb (Hubbard) repulsion between electrons at site $\vec{R}_i$

⇒ Let us now consider different fields, which can be applied to this model :

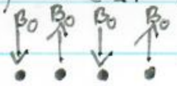
ⓐ Static Magnetic Field: $H_1 = \sum_i B_i \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$, $\frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) = S_{i,z}$ is the spin operator in z-direction at lattice site $\vec{R}_i$

→ Spin operator

Note: The site-dependence of the field B_i determines its spatial structure:

$$B_i = B_0 e^{-i\vec{q}\vec{R}_i} \quad (29) : q_x, q_y, q_z \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right) \quad \begin{pmatrix} R_x \\ R_y \\ R_z \end{pmatrix} = a \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$$

$n_x, n_y, n_z \in \mathbb{Z}$, a ... lattice constant of cubic lattice

e.g.: $\vec{k} = \begin{pmatrix} \pi \\ \pi \\ \pi \end{pmatrix}$: $B_i = B_0 e^{i\pi(n_x+n_y+z_z)} = \pm 1$ ⇒  ⇒ STAGGERED magnetic field or $\vec{q} = \binom{0}{0}$: $B_i = B_0 \Rightarrow \overset{B_0}{\uparrow}\ \overset{B_0}{\uparrow}\ \overset{B_0}{\uparrow}\ \overset{B_0}{\uparrow} \Rightarrow$ UNIFORM magnetic field

What is the effect of the magnetic field on the **magnetization** of the system?

(This is often the case!)

$$\underbrace{m_i = m}_{\text{translational invariance}} = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) = S_{i,z} = O \Rightarrow O \text{ and } H_1 \text{ are equivalent!} \quad (30)$$

Since for $B_0 = 0$ the system is $SU(2)$ spin symmetric, $\langle O \rangle = \langle m_i \rangle = 0$, the linear response of the magnetization m to an magnetic field B_0 becomes:

$$\frac{\partial \langle m \rangle}{\partial B_0}\bigg|_{B_0=0} = \sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \, \langle S_{j,z}(\tau) S_{i,z} \rangle = \frac{1}{4} \sum_j e^{i\vec{q}\vec{R}_j} \int_0^\beta d\tau \, \langle [n_{j\uparrow}(\tau) - n_{j\downarrow}(\tau)][n_{0\uparrow} - n_{0\downarrow}] \rangle$$

i can be set to 0 ($\hat{=}\ \vec{R}_0 = \binom{0}{0}$)

$$= \frac{1}{4} \sum_j e^{i\vec{q}\vec{R}_j} \int_0^\beta d\tau \, \langle n_{j\uparrow}(\tau) n_{0\uparrow} + n_{j\downarrow}(\tau) n_{0\downarrow} - n_{j\uparrow}(\tau) n_{0\downarrow} - n_{j\downarrow}(\tau) n_{0\uparrow} \rangle \quad (31)$$

Because of $SU(2)$ symmetry we have: $\langle n_{j\uparrow}(\tau) n_{0\uparrow} \rangle = \langle n_{j\downarrow}(\tau) n_{0\downarrow} \rangle$ and $\langle n_{j\uparrow}(\tau) n_{0\downarrow} \rangle = \langle n_{j\downarrow}(\tau) n_{0\uparrow} \rangle$ (32)

$$\Rightarrow \boxed{\frac{\partial \langle m \rangle}{\partial B_0}\bigg|_{B_0=0} = \frac{1}{2} \sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \left[\langle n_{j\uparrow}(\tau) n_{0\uparrow} \rangle - \langle n_{j\uparrow}(\tau) n_{0\downarrow} \rangle \right] \quad (33)}$$

Considering that $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$, Eq. (33) can be expressed in terms of two-particle Green's functions:

$$\frac{\partial \langle m \rangle}{\partial B_0}\bigg|_{B_0=0} = \frac{1}{2} \sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \left[\langle c^{+}_{j\uparrow}(\tau) c_{j\uparrow}(\tau) c^{+}_{0\uparrow} c_{0\uparrow} \rangle - \langle c^{+}_{j\uparrow}(\tau) c_{j\uparrow}(\tau) c^{+}_{0\downarrow} c_{0\downarrow} \rangle \right]$$

$$= \frac{1}{2} \sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \left[G^{(2),M}_{jj00,\uparrow\uparrow}(\tau,\tau,0) - G^{(2),M}_{jj00,\uparrow\downarrow}(\tau,\tau,0) \right] \quad (34)$$

This corresponds to the definition of the susceptibility in Eq. (120) in Chapter 3:

$$\tilde{\chi}^{M}_{(i\sigma)(0\sigma')}(i\Omega) =: \int_0^\beta d\tau\, e^{i\Omega\tau}\, G^{(2),M}_{ii00,\sigma\sigma'}(\tau,\tau,0),$$ which is Fourier transformed w.r.t. i in Eq. (34) $[\sum_j e^{-i\vec{q}\vec{R}_j}]$!

Defining the magnetic susceptibility as $\boxed{\tilde{\chi}^{M}_{i0,m}(i\Omega) = \tilde{\chi}^{M}_{(i\uparrow)(0\uparrow)}(i\Omega) - \tilde{\chi}^{M}_{(i\uparrow)(0\downarrow)}(i\Omega) \quad (35)}$

we obtain: $\boxed{\frac{\partial \langle m \rangle}{\partial B_0}\bigg|_{B_0=0} = \frac{1}{2} \tilde{\chi}^{M}_{\vec{q},m}(i\Omega=0) = \frac{1}{2} \sum_j e^{-i\vec{q}\vec{R}_j} \tilde{\chi}^{M}_{j0,m}(i\Omega=0) \quad (36)}$

⇒ This corresponds to the thermodynamic definition of a susceptibility in classical statistical mechanics!

Physical interpretation:

$\tilde{\chi}^{M}_{\vec{q},m}(i\Omega=0)$ is the linear paramagnetic (i.e. spin polarization) response of the system to an applied magnetic field $B_i = B_0\, e^{-i\vec{q}\vec{R}_i}$, whose spatial structure is given by the wave vector $\vec{q}$.

If for a specific value of $\vec{q} = \vec{q}_0$, $\tilde{\chi}^{M}_{\vec{q}_0,m}(i\Omega=0) \to \infty$, this indicates a phase transition to phase with a long-range spin order, whose spatial pattern is given by the vector $\vec{q}_0$:

$\tilde{\chi}^{M}_{\vec{q}_0,m}(i\Omega=0)=\infty \iff \left.\frac{\partial\langle m\rangle}{\partial B_0}\right|_{B_0=0} \cong \frac{\Delta\langle m\rangle}{\Delta B_0} = \infty$: An infinitesimal small small change of the field ΔB_0, leads to a finite change $\Delta\langle m\rangle$ in the magnetization, i.e., a spontaneous magnetization!

Spatial pattern of the spins $\Rightarrow$ described by $e^{-i\vec{q}_0\vec{R}_i}$:

$\vec{q}_0 = \begin{pmatrix}0\\0\\0\end{pmatrix}$ = uniform magnetization

ferromagnetism

$\vec{q}_0 = \begin{pmatrix}\pi\\\pi\\\pi\end{pmatrix}\frac{1}{a}$ = stagged magnetization

CHECKERBOARD $\Rightarrow$ ORDER!

antiferromagnetism

(b) Static Electric Field: $H_1 = \sum_i E_i \overset{\text{Charge of electron}}{\overset{\uparrow}{(-e)}} (n_{i\uparrow} + n_{i\downarrow})$, $(-e)(n_{i\uparrow}+n_{i\downarrow}) = \rho_i$ is the charge density operator at site $\vec{R}_i$

⇒ Here, we are typically interested in the response of the charge density $\langle \rho_i \rangle = \langle \rho \rangle$ to the electric field $E_i = E_0 \, e^{-i\vec{q}\vec{R}_i}$!

⇒ Completely analogous calculation as for the Spin-response in the previous section, with the only difference that we consider $n_{i\uparrow} + n_{i\downarrow}$ instead of $n_{i\uparrow} - n_{i\downarrow}$ (and a factor $(-e)$ instead of $\frac{1}{2}$).

⇒ Note that, in contrast to the spin-operator where $\langle S_{iz} \rangle = 0$, here we have $\langle \rho_i \rangle \neq 0$

⇒ Usually we redifine the operator $\rho_i \to \rho_i - \langle \rho_i \rangle$.

$$\Rightarrow \boxed{\left.\frac{\partial \langle \rho \rangle}{\partial E_0}\right|_{E_0=0} = 2e^2 \, \tilde{\chi}^{M}_{\vec{q},d}(i\Omega = 0) \quad , \quad \tilde{\chi}^{M}_{\vec{q},d}(i\Omega) = \sum_j e^{-i\vec{q}\vec{R}_j} \left[\tilde{\chi}^{M}_{(j\uparrow)(0\uparrow)}(i\Omega) + \tilde{\chi}^{M}_{(j\uparrow)(0\downarrow)} - 2\overset{(\text{or } \langle n_{i\downarrow}\rangle^2)}{\overset{\uparrow}{\langle n_{i\uparrow} \rangle^2}} \right]} \quad (37)$$

Remark: Eqs. (36) and (37) allow for the calculation of the magnetic permeability constant μ and the dielectric constant ε which are used in the phenomenological theory of electro- and magnetostatics in matter:

$\mu = 1 + 4\pi \, \tilde{\chi}^{M}_{\vec{q},m}(i\Omega = 0)$ and $\varepsilon = 1 + 4\pi \, \tilde{\chi}^{M}_{\vec{q},d}(i\Omega = 0)$ [The prefactor 4π depends on the units].

ⓒ Static pairing field - Superconductivity: $H_1 = \sum_i P_i \left(c^+_{i\downarrow} c^+_{i\uparrow} + c_{i\uparrow} c_{i\downarrow} \right)$ (38)

$(P_i = P_0 \, e^{-i\vec{q}\vec{R}_i})$

⇒ H_1 describes the generation (or annihilation) of a bound pair of an spin-↑ and a spin-↓ electron (singlet pairing). (→ violates particle number conservation)

⇒ Since these pairs of electrons correspond to Bosons, they can Bose-condensate to a superfluid, i.e., a superconducting state, where the pairs move without friction ⇒ electrical resistivity $R = 0$!

→ SUPERCONDUCTIVITY (Note: $R=0$ is not condition for superconductivity → also MEISSNER effect is needed, which is actually the defining property of a SC!)

↳ external magnetic field cannot enter the SC ⇔ perfect diamagnetism!

⇒ Question: How can electrons, which repel each other due to the repulsive Coulomb interaction form bound pairs?

⇒ An effective attractive interaction is necessary: There are several mechanisms which generate such effective attractive interactions between electrons: Phonons („standard" superconductivity), spin-fluctuations (high-temperature SC), ...

On the level of the Hubbard model: We simply consider $U<0$!

The observable O, in whoes response on the pairing field H_1 we are interested in, is the local **pair density** $\Delta_i = \Delta = c^+_{i\downarrow} c^+_{i\uparrow} + c_{i\uparrow} c_{i\downarrow}$!

$$\frac{\partial \langle \Delta \rangle}{\partial P_0}\Big|_{P_0=0} = -\sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \left\langle \left(c^+_{j\downarrow}(\tau) c^+_{j\uparrow}(\tau) + c_{j\uparrow}(\tau) c_{j\downarrow}(\tau)\right)\left(c^+_{0\downarrow} c^+_{0\uparrow} + c_{0\uparrow} c_{0\downarrow}\right)\right\rangle$$

$$= -\sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \left\langle c^+_{j\downarrow}(\tau) c^+_{j\uparrow}(\tau) c_{0\uparrow} c_{0\downarrow}\right\rangle + \left\langle c_{j\uparrow}(\tau) c_{j\downarrow}(\tau) c^+_{0\downarrow} c^+_{0\uparrow}\right\rangle \quad (39)$$

($\langle c^+c^+c^+c^+\rangle = \langle cccc\rangle = 0$ since for $P_0=0$ the number of particles is conserved)

$\rightarrow \langle c_{j\uparrow}(\tau) c_{j\downarrow}(\tau) c^+_{0\downarrow} c^+_{0\uparrow}\rangle = \langle c^+_{\downarrow(-j)}(\beta-\tau) c^+_{\uparrow(-j)}(\beta-\tau) c_{0\uparrow} c_{0\downarrow}\rangle$ where $-j \hat{=} -\vec{R}_j$!

↳ This can be again seen by the cyclicity of the trace and shifting the entire lattice by $\vec{R}_j$

↳ Inside the $\sum_j$, $-\vec{R}_j \to +\vec{R}_j$, and inside $\int_0^\beta$, $\beta-\tau \to \tau$:

$$\boxed{\frac{\partial \langle \Delta \rangle}{\partial P_0}\Big|_{P_0=0} = -2 \sum_j e^{-i\vec{q}\vec{R}_j} \int_0^\beta d\tau \; G^{(2),M}_{j0j0,\uparrow\downarrow}(\tau,0,\tau) := -2\tilde{\chi}^{M}_{\vec{q},pp}(i\Omega=0) \quad (39)}$$

$\tilde{\chi}^M_{\vec{q},pp}(i\Omega)$ is the susceptibility in particle-particle channel, where the 3 frequencies and momenta are chosen according to the particle-particle notation (see chapter 3 on 2-particle Green's functions).

(b) Adiabatic response: Can be obtained from the isothermal response by thermodynamic identities:

For instance, for the response of the magnetization to a magnetic field:

$$\chi^A = \chi^I - \frac{T}{C_F}\left(\frac{\partial\langle m\rangle}{\partial T}\right)^2_F \quad (40)$$

, where C is the specific heat at constant field F

↪ derivative should be taken at constant field F!

(c) Isolated (Kubo) response

Let us consider a time dependent external perturbation $F(t)$:

⇒ The Hamiltonian up to linear order in $F(t)$ then reads: $H(F) = H + F(t)\cdot H_1 = H(t)$

⇒ Since the system is decoupled from the bath, the density operator ρ will undergo a time evolution $\rho(t)$ due to $F(t)$!

⇒ We need an equation of motion for $\rho(t)$!

General definition $\rho(t) = \sum_i \lambda_i(t) |\psi_i(t)\rangle\langle\psi_i(t)|$, $\sum_i \lambda_i(t) = 1$ (41)

⇒ Taking into account the Schrodinger Eq. $i\frac{\partial}{\partial t}|\psi_i(t)\rangle = H(t)|\psi_i(t)\rangle$
we can derive the following differential equation for $\rho(t)$:

$$\frac{d}{dt}\rho(t) = -i\,[H(t)\rho(t) - \rho(t)H(t)] + \sum_i \frac{d\lambda_i(t)}{dt} |\psi_i(t)\rangle\langle\psi_i(t)| \quad (42)$$

$$\Rightarrow \boxed{\frac{d}{dt}\rho(t) = -i\,[H(t), \rho(t)] + \frac{\partial\rho(t)}{\partial t}, \quad \frac{\partial\rho(t)}{\partial t} = \sum_i \frac{d\lambda_i(t)}{dt}|\psi_i(t)\rangle\langle\psi_i(t)| \quad (43)}$$

⇒ The total time derivative of the density matrix $\rho(t)$ consists of two terms:

→ $-i[H(t), \rho(t)]$: This contribution to $\frac{d}{dt}\rho(t)$ is due to the intrinsic dynamics of the system determined by the Hamiltonian $H(t)$.

→ $\frac{\partial\rho(t)}{\partial t} = \sum_i \frac{d\lambda_i(t)}{dt}|\psi_i(t)\rangle\langle\psi_i(t)|$: This contribution to $\frac{d}{dt}\rho(t)$ corresponds to the explicit time dependence of $\rho(t)$ given by the time dependence of the occupation number $\lambda_i(t)$.

⇒ In our case, we start from a grand canonical ensemble at $t=-\infty$ for which we have $\rho(t=-\infty)=\rho_0=\frac{1}{Z}e^{-\beta H}$ (where $H=H(t=-\infty)$):

⇒ In terms of an eigenbasis of H, i.e., $H|N\rangle=E_N|N\rangle$ we can write $\rho_0=\sum_N \frac{1}{Z}e^{-\beta E_N}|N\rangle\langle N|$ and for $\rho(t)=\sum_N \lambda_N(t)\,|N(t)\rangle\langle N(t)|$ $\left(\lambda_N(-\infty)=\frac{e^{-\beta E_N}}{Z}\right)$ (44)

⇒ We consider only the case where $\lambda_N(t)\equiv\lambda_N(t=-\infty)=e^{-\beta E_N}$ $\left(\text{i.e. } \frac{\partial\lambda(t)}{\partial t}=0\right)$:

⇒ To achieve this, we have to understand HOW $\lambda_N(t)$ can change with time (which also tells us how to avoid such change):

a) Scattering from $|N\rangle\to|M\rangle$: They can occur (and, hence, change the occupation number λ_M and λ_N) when the time dependent perturbation is very FAST. We can avoid this by assuming that the external perturbation $F(t)$ is switched on ADIABATICALLY (i.e. infinitesimaly slowly): $F(t)\propto e^{\varepsilon t}$, $\varepsilon\to 0+$. Then the adiabatic theorem states, that $|N\rangle$ adiabatically evolves to the eigenstate $|N(t)\rangle$ of $H(t)$, i.e., $H(t)|N(t)\rangle=E_N(t)|N(t)\rangle$ (and is not scattered into another state $|M\rangle$)!

b) Thermalization: In the adiabatic situation discussed in a), also the eigenvalues $E_\nu(t)$ evolve in time. If the system is coupled to an external bath, the occupation numbers will evolve according to $\lambda_\nu(t) = e^{-\beta E_\nu(t)}$. This, however, does NOT happen if the system is PERFECTLY ISOLATED!

Remark: In real experiments, a system cannot be perfectly isolated for infinitly long times. In this situation, the time scale of the perturbation $F(t)$, i.e. t_F, must be much larger than $\frac{\hbar}{E_\nu - E_n} = t_A$, so that the adiabatic assumption is still valid. On the other hand, t_F must be much smaller than the time scale t_{Therm} where thermalization processes set in:

$$t_A = \frac{\hbar}{E_n - E_\nu} \ll t_F \ll t_{Therm} \quad (45)$$

Under these assuptions we have:

$$\boxed{\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)] \quad , \quad \rho(t=-\infty) = \rho_0 = \frac{1}{Z} e^{-\beta H} \quad (46)}$$

$\Rightarrow$ We want to find a solution of Eq. (46) up to linear order in $F(t)$!
$(H(t) = H(F) = H + F(t) H_1)$

$\Rightarrow$ We expand $\rho(t)$ in terms of $F(t)$: $\rho(t) = \rho_0 + \underbrace{\rho_1(t)}_{\mathcal{O}(F(t))} + \mathcal{O}(F(t)^2)$ (47)

$$\Rightarrow \frac{d}{dt}\rho(t) = \frac{d}{dt}\rho_1(t) = -i\left[H + F(t) H_1, \rho_0 + \rho_1(t)\right] + \mathcal{O}(F(t)^2) \quad (48)$$

$$= -i\overbrace{[H, \rho_0]}^{0 \text{ since } \rho_0 \sim e^{-\beta H}} - i[H, \rho_1(t)] - iF(t)[H_1, \rho_0] - i\overbrace{F(t)[H_1, \rho_1(t)]}^{\mathcal{O}(F(t)^2)} + \mathcal{O}(F(t)^2)$$

$$\Rightarrow \boxed{\frac{d}{dt}\rho_1(t) = -i[H, \rho_1(t)] - iF(t)[H_1, \rho_0] + \mathcal{O}(F(t)^2), \quad \rho_1(t \to -\infty) = 0 \quad (49)}$$

Ansatz: $\rho_1(t) = e^{-iHt} G(t) e^{+iHt}$ $\Rightarrow \frac{d}{dt}\rho_1(t) = \cancel{-i[H, \rho_1(t)]} + e^{-itH}\frac{dG(t)}{dt}e^{itH}$
$= \cancel{-i[H, \rho_1(t)]} - iF(t)[H_1, \rho_0]$ (50)

$$\Rightarrow e^{-itH}\frac{dG(t)}{dt}e^{itH} = -iF(t)[H_1, \rho_0] \quad (51)$$

$$\Rightarrow \frac{dG(t)}{dt} = -i e^{itH}[H_1, \rho_0]e^{-itH}F(t) \overset{[H, \rho_0]=0}{=} -iF(t)\left[e^{itH}H_1 e^{-itH}, \rho_0\right] = -iF(t)[H_1(t), \rho_0] \quad (52)$$

$$\Rightarrow G(t) - \overset{0}{\overset{\parallel}{G(t\to-\infty)}} = -i\int_{-\infty}^{t} dt'\, F(t')\,[H_1(t'), \rho_0]\,,\quad H_1(t) = e^{itH} H_1 e^{-itH} \quad (53)$$

$$\Rightarrow \rho_1(t) = -i\, e^{-itH}\int_{-\infty}^{t} dt'\, F(t')\,[e^{it'H} H_1 e^{-it'H}, \rho_0] = -i\int_{-\infty}^{t} dt'\,[H_1(t'-t), \rho_0]\,F(t') \quad (54)$$

$$\rho(t) = \rho_0 + \rho_1(t) \Rightarrow \langle O\rangle_t(F(t)) = \mathrm{Tr}(\rho(t)\,O) = \underbrace{\mathrm{Tr}(\rho_0 O)}_{\text{independent of } F(t)} + \mathrm{Tr}(\rho_1(t)\,O) \quad (55)$$

$$\Rightarrow \text{Linear response: } \left.\frac{\partial\langle O\rangle_t(F(t''))}{\partial F(t'')}\right|_{F(t'')=0} = -i\,\mathrm{Tr}([H_1(t''-t), \rho_0]\,O)\,\Theta(t-t'') \text{ since } \frac{\partial F(t')}{\partial F(t'')} = \delta(t'-t'') \quad (56)$$

$$\underset{t''\to t'}{\Longrightarrow} \left.\frac{\partial\langle O\rangle_t(F(t'))}{\partial F(t')}\right|_{F(t')=0} = -i\,\mathrm{Tr}\left(e^{i(t'-t)H} H_1 e^{-i(t'-t)H}\rho_0 O - \rho_0 e^{i(t'-t)H} H_1 e^{-i(t'-t)H} O\right)\Theta(t-t')$$

$$\overset{\text{cyclicity of Tr and } [\rho_0, H]=0}{=} -i\,\mathrm{Tr}\Big(\rho_0 \underbrace{e^{itH} O e^{-itH}}_{O(t)}\, \underbrace{e^{it'H} H_1 e^{-it'H}}_{H_1(t')} - \rho_0 \underbrace{e^{it'H} H_1 e^{-it'H}}_{H_1(t')}\, \underbrace{e^{itH} O e^{-itH}}_{O(t)}\Big) \times \Theta(t-t') \quad (57)$$

$$\Rightarrow \boxed{\left.\frac{\partial\langle O\rangle_t(F(t'))}{\partial F(t')}\right|_{F(t')=0} = -i\,\langle [O(t), H_1(t')]\rangle\,\Theta(t-t') = G^R_{OH_1}(t-t') \quad (58)}$$

The isolated (Kubo) linear response corresponds to a (generalized) retarded Green's function for the operators O and H_1!

Fourier Transform: $\chi^{K}_{OH_1}(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t} \frac{\partial \langle O \rangle_A (F(A'))}{\partial F(A')}\Big|_{F(A')=0} = \tilde{G}^{R}_{OH_1}(\omega)$ (59)

Comparison to isothermal static response:

$\chi^{I}_{H_1 0} = \chi^{I}_{OH_1} = \tilde{G}^{M}_{OH_1}(i\Omega = 0)$

$\chi^{K}_{OH_1}(\omega) = \tilde{G}^{R}_{OH_1}(\omega) = \tilde{G}^{M}_{OH_1}(i\Omega \Rightarrow \omega + i\delta)$

The Matsubara Green's Function $\tilde{G}^{M}_{OH_1}$ contains both the static isothermal ($i\Omega = 0$) as well as the dynamic isolated (Kubo) ($i\Omega \Rightarrow \omega + i\delta$) response!

Note: $\chi^{I}_{OH_1}$ is a STATIC (frequency-independent) response function while $\chi^{K}_{OH_1}(\omega)$ DYNAMIC (frequency dependent) response function. If we consider $\omega = 0$ for $\chi^{K}_{OH_1}(\omega)$ it seems, that the two responses become equivalent since both correspond to evaluating $\tilde{G}_{OH_1}(z)$ at the origin of the complex plane $z = 0$. This is, however, not always the case since: $\chi^{I}_{OH_1} = \tilde{G}_{OH_1}(z=0)$ and $\chi^{K}_{OH_1}(\omega = 0) = \lim_{\delta \to 0+} \tilde{G}_{OH_1}(i\delta)$ and $\tilde{G}_{OH_1}(z)$

has a discontinuity at the real axis!