Linear Response Theory

System + external perturbation

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

$\mathcal{H}_0$ ↓ system

$\mathcal{H}_1$ ↓ perturbation (<u>weak</u>)

typical form: $\mathcal{H}_1 = - f B$

B → system observable

f → "field"

$B = B(\Gamma)$ $\quad \Gamma$ phasespace coordinate example: Ising model : $\mathcal{H} = \underbrace{-J \sum_{\langle ij \rangle} S_i S_j}_{\mathcal{H}_0} - \underbrace{H}_{f} \underbrace{\sum_i S_i}_{M = B}$

desired: "response" of some observable $A = A(\Gamma)$

to the external field, in the limit $f \to 0$

$$\chi_{AB} = \frac{\partial A}{\partial f}\bigg|_{f=0}$$

generalized susceptibility

"response function"

conjugate to f

example: $\chi_0 = \frac{\partial M}{\partial H}\Big|_{H=0}$

fluctuation relation : $\boxed{\chi_0 = \beta \underbrace{\{ \langle M^2 \rangle - \langle M \rangle^2 \}}_{= \beta \langle \delta M^2 \rangle}}$

property of the UNPERTURBED system!

Can we generalize this to the case of DYNAMICS when $f = f(t)$? <u>YES</u>

$$\mathcal{H} = \mathcal{H}_0 - f(t)\, B$$

time-independent (do not depend on time EXPLICITLY!)

<u>Statics</u>: $\bar{A} = \langle A \rangle + \chi_{AB} f + O(f^2)$

$f(t) = \text{const.}$

$\bar{A}$: average in the presence of the perturbation

$\langle A \rangle$: thermal average of A in the ABSENCE of the perturbation

Dynamics:

$$\bar{A}(t) = \underbrace{\langle A \rangle}_{\text{time-independent}} + \int_{-\infty}^{\infty} d\tau \, \underbrace{\chi_{AB}(t,\tau)}_{} f(\tau) + O(f^2)$$

most general linear relation

must again be a property of the UNPERTURBED system which is in EQUILIBRIUM!

In equilibrium: time translational invariance

$$\Rightarrow \chi_{AB}(t,\tau) = \chi_{AB}(t-\tau)$$

Causality: only the times in the PAST contribute

$$\bar{A}(t) = \langle A \rangle + \int_{-\infty}^{\infty} d\tau \, \chi_{AB}(t-\tau)\, f(\tau) + O(f^2)$$

$\tau > t \rightarrow$ no contribution $\quad t - \tau < 0$

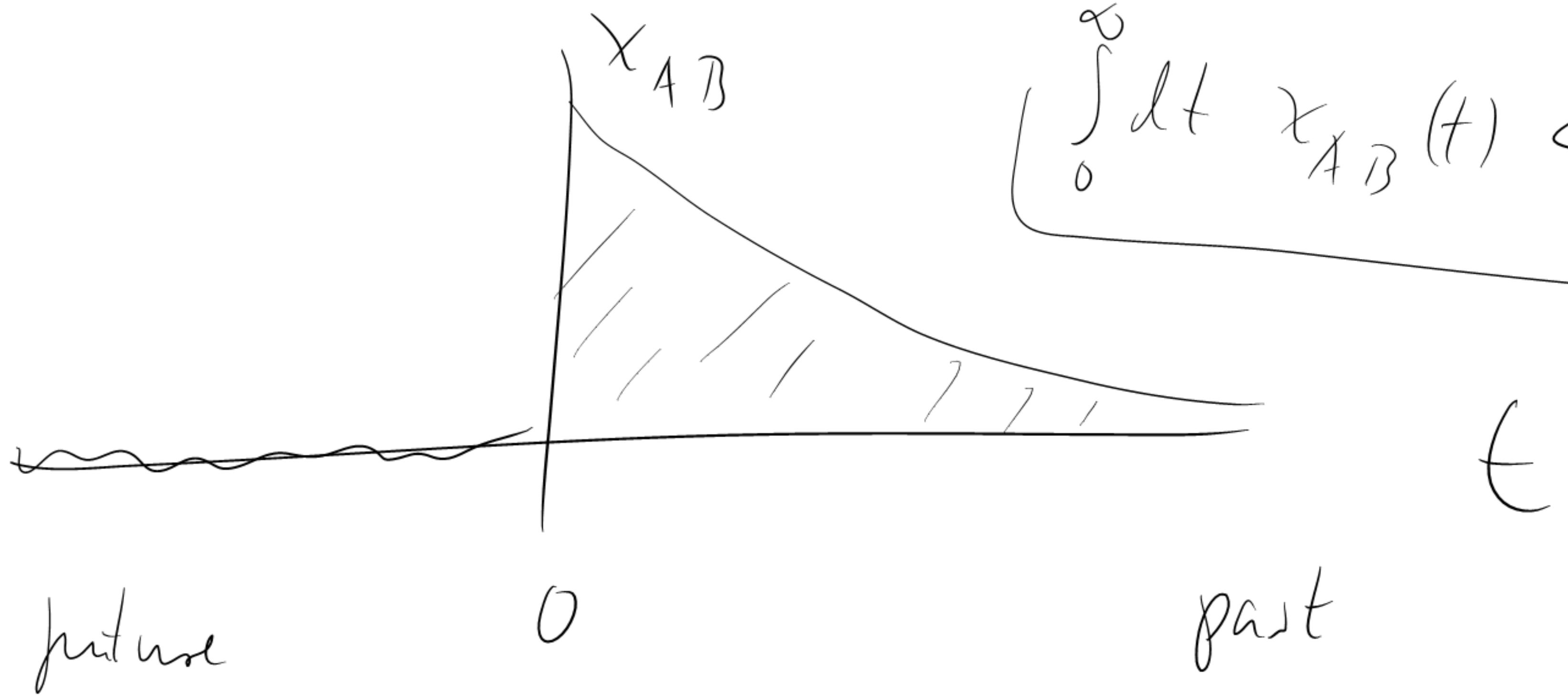
$$\Rightarrow \chi(t) = 0 \text{ for } t < 0$$

look at the far-reaching past → rather small contribution (typically)

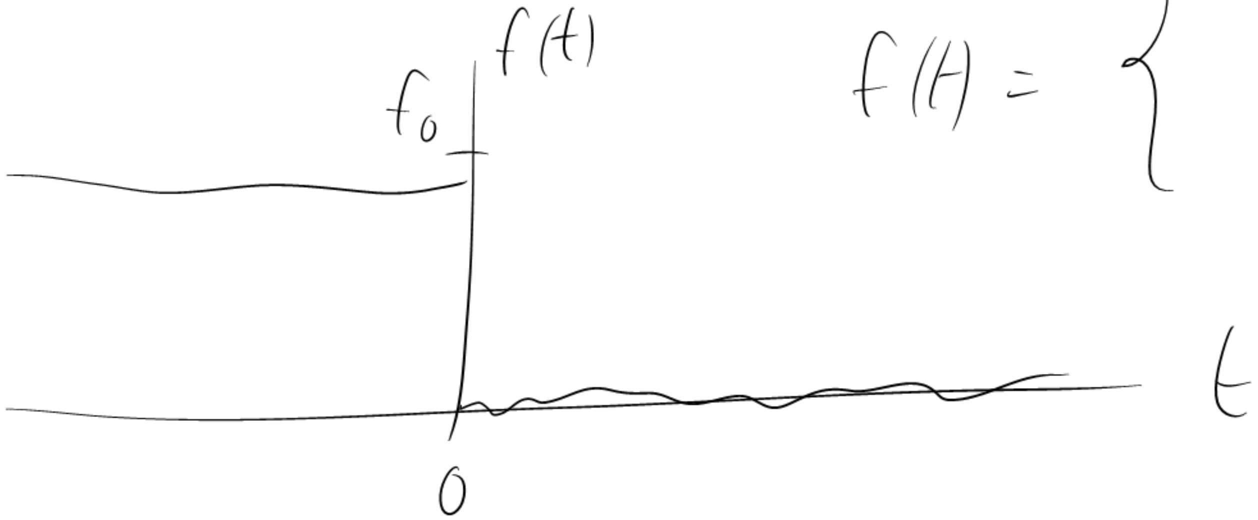
<u>typical</u> function

<u>also</u> typical:

$$\boxed{\int_0^\infty dt \, \chi_{AB}(t) < \infty}$$



Switch-off experiment



$$f(t) = \begin{cases} f_0 & t < 0 \\ 0 & t > 0 \end{cases}$$

$$\bar{A}(t) = \langle A \rangle + f_0 \int_{-\infty}^{0} d\tau \, \chi_{AB}(t-\tau) + O(f^2)$$

$$\tau = -\infty \qquad t - \tau = +\infty \qquad d(t-\tau) = -d\tau$$

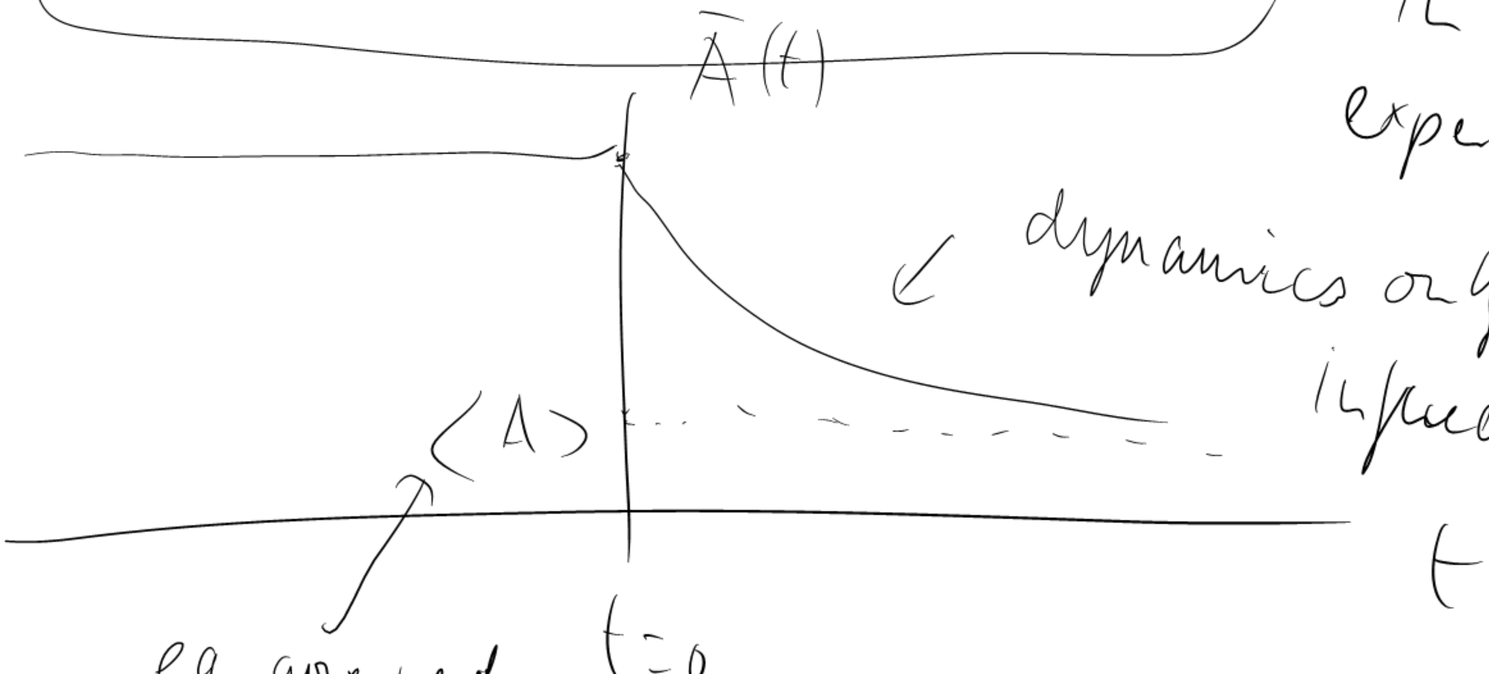
$$\tau = 0 \qquad t - \tau = t$$

$$\bar{A}(t) = \langle A \rangle - f_0 \int_{+\infty}^{t} d\tau \, \chi_{AB}(\tau) + O(f^2)$$

$$\frac{d}{dt}\bar{A}(t) = -f_0\,\chi_{AB}(t) + \mathcal{O}(f^2)$$

$$\chi_{AB}(t) = \lim_{f_0 \to 0}\left(-\frac{1}{f_0}\frac{d}{dt}\bar{A}(t)\right)$$

dynamics of A in the switch-off experiment



dynamics only under the influence of $\mathcal{H}_0$!

eq. governed by $\mathcal{H}_0$!

classical system

$$\underline{A(t)} = A(\Gamma(t))$$ phase space trajectory

average = average over the initial conditions!

for $t<0$ the system obeys a Boltzmann distribution with Hamiltonian

$$\underbrace{\mathcal{H}_0 - f_0 B}$$

$$\bar{A}(t) = \frac{\int d\Gamma \exp(-\beta \mathcal{H}_0 + \beta f_0 B) \; A(t)}{\int d\Gamma \exp(-\beta \mathcal{H}_0 + \beta f_0 B)}$$

$\langle \; \rangle$ = thermal average with $e^{-\beta \mathcal{H}_0}$

$$\bar{A}(t) = \frac{\langle e^{\beta f_0 B} A(t) \rangle}{\langle e^{\beta f_0 B} \rangle}$$

Taylor wrt f_0

$$\bar{A}(t) \simeq \frac{\langle (1+\beta f_0 B)\ A(t) \rangle}{\langle 1+\beta f_0 B \rangle} =$$

$$= \frac{\langle A \rangle + \beta f_0 \langle B\, A(t) \rangle}{1+\beta f_0 \langle B \rangle}$$

$$A(t) = \langle A \rangle + \delta A(t)$$

$$B = \langle B \rangle + \delta B$$

$$= \frac{1}{1+\beta f_0 \langle B \rangle} \left\{ \langle A \rangle + \beta f_0 \big\langle (\langle B \rangle + \delta B)(\langle A \rangle + \delta A(t)) \big\rangle \right\}$$

$$= \frac{1}{1+\beta f_0 \langle B \rangle} \left\{ \langle A \rangle + \beta f_0 \langle A \rangle \langle B \rangle + \cancel{\beta f_0 \langle B \rangle \underbrace{\langle \delta A(t) \rangle}_{=0}} + \beta f_0 \langle \delta B\, \delta A(t) \rangle + \cancel{\beta f_0 \underbrace{\langle \delta B \rangle}_{=0} \langle A \rangle} \right\}$$

$$= \langle A\rangle + \frac{\beta f_0}{1+\beta f_0 \langle B\rangle} \langle \delta B \, \delta A(t)\rangle$$

$$\underline{\underline{\cong \langle A\rangle + \beta f_0 \langle \delta B(0)\,\delta A(t)\rangle}} = \bar{A}(t)$$

$$\frac{d}{dt}\bar{A}(t) = \beta f_0 \langle \delta B(0)\, \delta \dot{A}(t)\rangle$$

$$\boxed{\chi_{AB}(t) = -\beta \langle \delta B(0)\, \delta \dot{A}(t)\rangle}$$

$$\delta \dot{A} \equiv \frac{d}{dt}\left(\delta A(t)\right)$$

time translational invariance $\Rightarrow$

$$\langle \delta B(t)\, \delta A(t+\tau) \rangle = \langle \delta B(0)\, \delta A(\tau) \rangle \quad \Big| \frac{d}{d\tau}$$

$$\langle \delta \dot{B}(t)\, \delta A(t+\tau) \rangle + \langle \delta B(t)\, \delta \dot{A}(t+\tau) \rangle = 0 \quad \Big| \tau = 0$$

$$\langle \delta \dot{B}(0)\, \delta A(t) \rangle + \underline{\langle \delta B(0)\, \delta \dot{A}(t) \rangle} = 0$$

$$\boxed{\chi_{AB} = +\beta \langle \delta \dot{B}(0)\, \delta A(t) \rangle}$$

dynamic correlation function

use this for transport coefficients

let $f(t) = f_0 = \text{const.}$ for all t

f_0 puts the system into a non-equilibrium steady state (NESS)

let A be a variable that becomes constant in NESS $\quad \bar{A}(t) = \bar{A}$

$$\bar{A} = \langle A \rangle + f_0 \int_{-\infty}^{\infty} d\tau \, \chi_{AB}(t-\tau) =$$

$$= \langle A \rangle + f_0 \int_{-\infty}^{t} d\tau \, \chi_{AB}(t-\tau) =$$

$$= \langle A \rangle + f_0 \int_{+\infty}^{0} (-d\tau) \, \chi_{AB}(\tau) =$$

$$= \langle A \rangle + f_0 \int_{0}^{\infty} dt \, \chi_{AB}(t) =$$

$$= \langle A \rangle + \beta f_0 \int_{0}^{\infty} dt \, \langle \delta A(t) \, \delta \dot{B}(0) \rangle$$

so-called Green-Kubo formula