

Kubo formula for response function [nl27]

Interaction representation for time evolution of $\mathcal{H}(t) = \mathcal{H}_0 - b(t)B$:

$$\begin{aligned}\frac{dA}{dt} &= \frac{i}{\hbar}[\mathcal{H}_0, A] \quad \Rightarrow \quad A(t) = e^{i\mathcal{H}_0 t/\hbar} A e^{-i\mathcal{H}_0 t/\hbar}, \\ \frac{dB}{dt} &= \frac{i}{\hbar}[\mathcal{H}_0, B] \quad \Rightarrow \quad B(t) = e^{i\mathcal{H}_0 t/\hbar} B e^{-i\mathcal{H}_0 t/\hbar}, \\ \frac{d\rho}{dt} &= -\frac{i}{\hbar}[-b(t)B, \rho] \quad \Rightarrow \quad \rho(t) = \rho_0 + \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') [B(t'), \rho(t')].\end{aligned}$$

Set $\rho(t) = \rho_0 + \rho_1(t)$ with $\rho_0 = Z_0^{-1} e^{-\beta\mathcal{H}_0}$.

Full response: $\langle A(t) \rangle - \langle A \rangle_0 = \text{Tr}\{\rho_1(t)A(t)\}$

Leading correction to ρ_0 : $\rho_1(t) \simeq \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') [B(t'), \rho_0]$

Linear response:

$$\begin{aligned}\langle A(t) \rangle - \langle A \rangle_0 &= \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') \text{Tr}\{[B(t'), \rho_0]A(t)\} \\ &= \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') \text{Tr}\{\rho_0[A(t), B(t')]\} \\ &= \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') \langle [A(t), B(t')] \rangle_0.\end{aligned}$$

Compare with definition of response function in [nl26].

Kubo formula:

$$\tilde{\chi}_{AB}(t - t') = \frac{i}{\hbar} \theta(t - t') \langle [A(t), B(t')] \rangle_0.$$

- Causality requirement is ensured by step function $\theta(t - t')$.
- Hermitian A, B imply Hermitian $i[A, B]$. Hence $\tilde{\chi}(t)$ is real.
- Linear response depends only on equilibrium quantities.
- Response function only depends on time difference $t - t'$.

The Kubo formula establishes a general link between

- the dynamical properties of a many-body system at equilibrium,
- the dynamical response of that system to experimental probes.