Equilibrium correlation functions

We derived that the linear response of an operator $\hat{B}$ to a perturbation $\hat{A}$ can be characterized by

$$\langle \hat{B} \rangle(t) - \langle \hat{B} \rangle_{eq} = \int_{-\infty}^{+\infty} dt' \, \chi_{BA}(t-t') \, f(t')$$

with the generalized susceptibility $\chi_{BA}(t-t')$ determined from an unequal time equilibrium correlation function by means of the Kubo relation

$$\chi_{BA}(t-t') = \frac{i}{\hbar} \left\langle \left[\hat{B}_I(t), \hat{A}_I(t') \right] \right\rangle_{eq} \theta(t-t')$$

We also showed that a general equilibrium correlation function can be expressed as

$$\langle \hat{B}_I(t)\, \hat{A}_I(t') \rangle_{eq} =$$

$$\frac{1}{Z(\beta)} \sum_{nn'} e^{-\beta E_n} e^{i(E_n - E_{n'})(t-t')/\hbar} \langle n|\hat{B}|n'\rangle \langle n'|\hat{A}|n\rangle$$

which immediately implies a formal expression for the generalized susceptibility $\chi_{BA}(t-t')$

Now in order to understand this better and obtain an intuition, we will look more generally at different two point correlation functions

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If we consider operators $\hat{B}_I(t)$, $\hat{A}_I(t')$ quantum theory, we can distinguish two operator orderings

<u>Wightman functions</u>

$$G^{>}_{BA}(t,t') = \langle \hat{B}_I(t)\,\hat{A}_I(t')\rangle_{eq}$$

$$G^{<}_{BA}(t,t') = \langle \hat{A}_I(t')\,\hat{B}_I(t)\rangle_{eq}$$

equivalently, one can consider a different basis

<u>Spectral function</u>: $$\rho_{BA}(t,t') = \frac{1}{\hbar}\langle [B_I(t), A_I(t')]\rangle_{eq}$$

<u>Statistical correlation function</u>: $$F_{BA}(t,t') = \frac{1}{2}\langle \{B_I(t), A_I(t')\}_+\rangle_{eq}$$

where the pre-factors are conventional and different conventions exist in the literature

Based on ρ_{BA}, F_{BA} we can construct any two point correlation function of the operator $\hat{B}$ and $\hat{A}$. However at first sight it appears as if ρ_{BA} is the relevant correlation function that determines the generalized susceptibility

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Now to get a physical understanding of the different correlation functions it is useful to consider the classical limit

Quantum theory	Classical theory
$\frac{-i}{\hbar}[\hat{B},\hat{A}] \longrightarrow$	$\{B,A\}_{PB}$
Commutator	Poisson Bracket
$\frac{1}{2}\{B,A\}_+ \longrightarrow$	BA
Anti-Commutator	Product

and consider a simple example of e.g. $\hat{B}=\hat{A}=\hat{x}$ denoting the position of a particle in 1D

$$\rho_{xx}^{cl}(t,t') = i \left\langle \{x(t), x(t')\}_{PB} \right\rangle_{eq}^{cl}$$

$$= i \left\langle \frac{\partial x(t)}{\partial x(t')} \frac{\partial x(t')}{\partial p(t')} - \frac{\partial x(t)}{\partial p(t')} \frac{\partial x(t')}{\partial x(t')} \right\rangle_{eq}^{cl}$$

$$= -i \left\langle \frac{\partial x(t)}{\partial p(t')} \right\rangle_{eq}^{cl}$$

which characterizes the response of the particles position $x(t)$ at time t to a change of the momentum of the particle $p(t')$ at time t'

→ Spectral function characterizes the structure of possible excitations of the system without actually measuring whether or not these modes are excited

$$F_{xx}^{cl}(t,t') = \langle x(t)\, x(t') \rangle_{eq}^{cl}$$

characterizes the correlation between the position $x(t)$ at time t and the position $x(t')$ at time t'

→ Statistical correlation function characterizes which excitations physically exist in a system

$\parallel$

Even though in general Γ and ρ characterize independent properties, in equilibrium systems they are related by a fluctuation dissipation relation

Kubo - Martin - Schwinger (KMS) relation

Starting from our previous result

$$\langle \hat{B}_I(t) \hat{A}_I(t') \rangle_{eq} =$$

$$\frac{1}{Z(\beta)} \sum_{nn'} e^{-\beta E_n} e^{i \underbrace{(E_n - E_{n'})}_{\equiv \hbar \omega_{nn'}} (t-t')/\hbar} \underbrace{\langle n | \hat{B} | n' \rangle}_{=B_{nn'}} \underbrace{\langle n' | \hat{A} | n \rangle}_{\equiv A_{n'n}}$$

we got

$$\langle \hat{B}_I(t) \hat{A}_I(t') \rangle_{eq} = \frac{1}{Z(\beta)} \sum_{nn'} e^{-\beta E_n} e^{i\omega_{nn'}(t-t')} B_{nn'} A_{n'n}$$

such that interchanging $B_I(t')$ and $A_I(t)$

$$\langle A_I(t') B_I(t) \rangle_{eq} = \frac{1}{Z(\beta)} \sum_{nn'} e^{-\beta E_n} e^{-i\omega_{nn'}(t-t')} A_{nn'} B_{n'n}$$

changes $n' \leftrightarrow n$

$$= \frac{1}{Z(\beta)} \sum_{nn'} e^{-\beta E_{n'}} e^{+i\omega_{nn'}(t-t')} B_{nn'} A_{n'n}$$

we get

$$\rho_{BA}(t,t') = \frac{1}{\hbar} \langle [B_I(t), A_I(t')] \rangle_{eq}$$

$$= \frac{1}{Z(\beta)} \sum_{nn'} \frac{1}{\hbar} \left(e^{-\beta E_n} - e^{-\beta E_{n'}} \right) e^{i\omega_{nn'}(t-t')} B_{nn'} A_{n'n}$$

$$F_{BA}(t,t') = \frac{1}{Z(\beta)} \sum_{nn'} \frac{1}{2} \left(e^{-\beta E_n} + e^{-\beta E_{n'}} \right) e^{i\omega_{nn'}(t-t')} B_{nn'} A_{n'n}$$

Now we see that up to the statistical factors ρ_{BA} and F_{BA} involve the same time evolution and operator matrix elements, so to make similarities more apparent go to Fourier space

$$\tilde{\rho}_{BA}(\omega) = \int_{-\infty}^{+\infty} d(t-t')\, \rho_{BA}(t,t')\, e^{i\omega(t-t')}$$

$$= \frac{2\pi}{Z(\beta)} \sum_{nn'} \frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{\hbar} B_{nn'} A_{n'n}\, \delta(\omega + \omega_{nn'})$$

$$\tilde{F}_{BA}(\omega) = \frac{2\pi}{Z(\beta)} \sum_{nn'} \frac{e^{-\beta E_n} + e^{-\beta E_{n'}}}{2} B_{nn'} A_{n'n}\, \delta(\omega + \omega_{nn'})$$

Now we notice that

$$\frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{\hbar} = \frac{e^{-\beta E_n}}{\hbar}\left(1 - e^{-\beta(E_{n'} - E_n)}\right)$$

$$= \frac{e^{-\beta E_n}}{\hbar}\left(1 - e^{-\beta\hbar\omega_{n'n}}\right)$$

and similarly

$$\frac{e^{-\beta E_n} + e^{-\beta E_{n'}}}{2} = \frac{e^{-\beta E_n}}{2}\left(1 + e^{-\beta\hbar\omega_{n'n}}\right)$$

since we have $\delta(\omega + \omega_{nn'})$ we know that $\omega_{n'n} = -\omega_{nn'} = \omega$ so

$$\tilde{\rho}_{BA}(\omega) = \frac{2\pi}{Z(\beta)}\left(\frac{1 - e^{-\beta\hbar\omega}}{\hbar}\right)\sum_{nn'} e^{-\beta E_n} B_{nn'} A_{n'n}\, \delta(\omega + \omega_{nn'})$$

$$\tilde{F}_{BA}(\omega) = \frac{2\pi}{Z(\beta)}\left(\frac{1 + e^{-\beta\hbar\omega}}{2}\right)\sum_{nn'} e^{-\beta E_n} B_{nn'} A_{n'n}\, \delta(\omega + \omega_{nn'})$$

Now we see that

$$\tilde{F}_{BA}(\omega) = \frac{\hbar}{2} \frac{1+e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} \tilde{\rho}_{BA}(\omega)$$

yielding the KMS relation

$$\boxed{\tilde{F}_{BA}(\omega) = \frac{\hbar}{2} \coth\left(\frac{\beta\hbar\omega}{2}\right) \tilde{\rho}_{BA}(\omega)}$$

We note that the factor relating F and ρ has a rather intuitive understanding as

$$\frac{\hbar}{2} \coth\left(\frac{\beta\hbar\omega}{2}\right) = \hbar\left(\underbrace{n_{BE}(\hbar\omega)}_{\text{Bose Einstein distribution describing thermal fluctuations}} + \underbrace{\frac{1}{2}}_{\text{Vacuum quantum fluctuations}}\right)$$

such that in equilibrium all possible excitations as characterized by $\tilde{\rho}(\omega)$ are populated by thermal and quantum fluctuations

Similarly, we can derive an analogous relation for classical systems by taking the limit $\hbar \to 0$ (or directly working in the classical theory)

using $\coth(x) \simeq \frac{1}{x} + O(x)$

$$\tilde{F}^{cl}_{BA}(\omega) = \frac{1}{\beta\omega} \tilde{\rho}_{BA}(\omega)$$

where now $n_{RJ}(\omega) = \frac{k_B T}{\omega} = \frac{1}{\beta\omega}$ is the Rayleigh-Jeans distribution and there are no vacuum fluctuations in the classical theory

Similar to the relation between F_{BA} and ρ_{BA} we can also express the general susceptibility χ_{BA} in terms of the spectral function (or vice versa)

$$\chi_{BA}(t-t') = \frac{i}{\hbar} \left\langle \left[\hat{B}_I(t), A_I(t') \right] \right\rangle_{eq} \theta(t-t')$$

where now to define the Fourier transform we consider

$$\tilde{\chi}_{BA}(\omega) = \lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} d(t-t')\, \chi_{BA}(t,t')\, e^{i\omega(t-t')} e^{-\varepsilon(t-t')}$$

evaluating the operator expectation values by performing the usual insertions of eigenstates etc. we arrive at

$$= \frac{1}{Z(\beta)} \sum_{nn'} i \frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{\hbar} B_{nn'} A_{n'n}$$

$$\int_{-\infty}^{+\infty} d(t-t') \, \Theta(t-t') e^{i\omega_{nn'}(t-t')} e^{i\omega(t-t')} e^{-\varepsilon(t-t')}$$

performing the integral, only the $(t-t')=0$ boundary contributes

$$= \frac{1}{Z(\beta)} \sum_{nn'} i \frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{\hbar} B_{nn'} A_{n'n} \frac{-1}{i\omega + i\omega_{nn'} - \varepsilon}$$

$$= \frac{1}{Z(\beta)} \sum_{nn'} \frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{\hbar} B_{nn'} A_{n'n} \frac{1}{\omega_{n'n} - \omega - i\varepsilon}$$

Now comparing this to the spectral function

$$\tilde{\rho}_{BA}(\omega) = \frac{1}{Z(\beta)} \sum_{nn'} \frac{e^{-\beta E_n} - e^{-\beta E_{n'}}}{\hbar} B_{nn'} A_{n'n} \, 2\pi \, \delta(\omega + \omega_{nn'})$$

We see that the structure is identical except that for $\tilde{\rho}(\omega)$ we have $\omega = \omega_{n'n}$, such that

$$\tilde{\chi}_{BA}(\omega) = \lim_{\varepsilon \to 0} \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega' \; \frac{\tilde{\rho}_{BA}(\omega')}{\omega' - \omega - i\varepsilon}$$

which is called <u>spectral</u> or <u>Lehmann representation</u> of the generalized susceptibility

Similarly by measuring $\tilde{\chi}_{BA}(\omega)$ and $\tilde{\chi}_{AB}(\omega)$ one can re-construct the spectral function $\rho_{AB}(\omega)$ as is easily seen in the time domain where

$$\rho_{AB}(t) = -\rho_{BA}(-t)$$

with

$$\chi_{BA}(t) = i\,\rho_{BA}(t)\,\theta(t)$$

$$\chi_{AB}(t) = i\,\rho_{AB}(t)\,\theta(t) = -i\,\rho_{BA}(-t)\,\theta(t)$$

so we got

$$\rho_{BA}(t) = -i\,\chi_{BA}(|t|)\,\theta(t) + i\,\chi_{AB}(|t|)\,\theta(-t)$$

such that by measuring the linear response for a perturbation of an equilibrium system, one can learn about its equilibrium spectral function.

Green-Kubo relations

Now the phenomenological transport coefficients encountered in chapter I can be defined in terms of operator expectation values in the underlying microscopic theory

Generally, the form of our phenomenological constitutive relations was of the form

$$\langle \hat{B} \rangle = \langle \hat{B} \rangle_{eq} + L_{BA} \langle \hat{A} \rangle$$

where $\hat{B}$ measures the flux of some quantity, in response to an affinity $\hat{A}$

Now from our linear response analysis we have

$$\langle \hat{B}(\omega) \rangle - \langle \hat{B}(\omega) \rangle_{eq} = \tilde{\chi}_{BA}(\omega) \langle \hat{A}(\omega) \rangle$$

from which the coefficient L_{BA} is obtained in the zero frequency limit

$$L_{BA} = \lim_{\omega \to 0} \tilde{\chi}_{BA}(\omega)$$

Exploiting the result

$$\chi_{BA}(t-t') = \frac{i}{\hbar} \langle [\hat{B}_I(t), A_I(t')] \rangle_{eq} \, \theta(t-t')$$

we get

$$L_{BA} = \frac{i}{\hbar} \int_0^{\infty} d(t-t') \, \langle [B_I(t), A_I(t')] \rangle_{eq}$$

Note that beyond the real time correlation functions discussed here, there are also so called Euclidean correlation functions, involving imaginary time evolution. Such objects play an important role in practical calculations e.g. in thermal field theory, or in Monte Carlo calculations of transport coefficients.

Basic properties and relations can be derived from the spectral representation as discussed e.g. in Borghini's lecture notes