Symmetries of response function:–

We start by assuming that A, B (or m's) are self-adjoint operators, and that we also know how they transform under time reversal.

We defined: $\chi''_{AB}(t-t') = \frac{1}{2\hbar}\langle [A(t), B(t')]\rangle$

a) $\rightarrow \quad \chi''_{AB}(t-t') = -\chi''_{BA}(t'-t)$
$\rightarrow \quad \chi''_{AB}(\omega) = -\chi''_{BA}(-\omega)$
} anti-symmetry including reversal of A and B.

b) In fact, χ'' is imaginary (hence the $''$)

$$\chi''^{*}_{AB}(t-t') = \frac{1}{2\hbar}\langle [A(t), B(t')]\rangle^{*} =$$

$$= \frac{1}{2\hbar}\sum_{i} \frac{e^{-\beta E_i}}{Z}\langle i | [A(t), B(t')] | i\rangle^{*}$$

$$\cancel{= \frac{1}{2\hbar}\sum_{i,f} \frac{e^{-\beta E_i}}{Z}\langle i | [A(t), B(t')] | f\rangle^{*}\langle f | [A(t), B(t')] | i\rangle}$$

$$= \frac{1}{2\hbar}\sum_{i} \frac{e^{-\beta E_i}}{Z}\left\{\langle i | A(t) B(t') | i\rangle^{*} - \langle i | B(t') A(t) | i\rangle^{*}\right\}$$

$$= \frac{1}{2\hbar}\sum_{i,j} \frac{e^{-\beta E_i}}{Z}\left\{\langle i | A(t) | j\rangle^{*}\langle j | B(t') | i\rangle^{*} - \langle i | B(t') | j\rangle^{*}\langle j | A(t) | i\rangle^{*}\right\}$$

Hence: $\langle i | A(t) | j\rangle^{*} = \langle j | A^{+}(t) | i\rangle = \langle j | A(t) | i\rangle$
if self-adjoint.

$$\Rightarrow \chi''^{*}_{AB}(t-t') = \frac{1}{2\hbar}\sum_{i,j} \frac{e^{-\beta E_i}}{Z}\left\{\langle j | A(t) | i\rangle\langle i | B(t') | j\rangle - \langle j | B(t') | i\rangle\langle i | A(t) | j\rangle\right\}$$

$$= \frac{1}{2\hbar} \sum_{i,j} \frac{e^{-\beta E_i}}{Z} \left\{ \underbrace{\langle i | B(t') | \underbrace{j\rangle\langle j}_{=1} | A(t) | i\rangle - \langle i | A(t) | \underbrace{j\rangle\langle j}_{=1} | B(t') | i\rangle}_{\& \; [B(t'), A(t)]} \right\}$$

$$= \chi''_{BA}(t'-t)$$

Therefore: $\chi^{*}_{AB}(t-t') = \chi''_{BA}(t'-t) = -\chi''_{AB}(t-t')$ (1)

symmetry derived above.

$\Rightarrow$ $\chi''_{AB}(t-t')$ is a purely imaginary quantity.

From the equality in (1) we also have:

$$\chi''_{AB}(\omega)^{*} = -\chi''_{AB}(-\omega)$$

which is general for the Fourier transform of a purely imaginary function.

Time reversal properties.

Let T be the time reversal operator. In a Hamiltonian system, the density matrix is invariant under time reversal:

[Given a linear operator A, ~~...~~$^{-1}$ the transformed operator A_G under a symmetry transformation G implemented by a unitary operator U_G gives:

$$|\langle \phi_G | A_G | \psi_G\rangle| = |\langle \phi | A | \psi\rangle|$$ for any two states $|\phi\rangle$ and $|\psi\rangle$.

To satisfy this, define $A_G = U_G A U_G^{+}$

since $|\langle \phi_G | U_G A U_G^{+} | \psi_G\rangle| = |\langle U_G^{+}\phi_G | A U_G^{+} | \psi_G\rangle = \langle \phi | A | \psi\rangle$

Quantum Mechanics follows the classical rules for the invariance under time transformation:

$$U_T \hat{r}_i U_T^+ = \hat{r}_i$$

$$U_T \hat{p}_i U_T^+ = -\hat{p}_i$$

$$U_T \hat{S}_i U_T^+ = -\hat{S}_i$$

the transformation of spin follows the transformation of angular momentum as induced by the transformation of position and momentum.

We denote in general:

$$U_T A(t) U_T^+ = \epsilon_A A(-t)$$

where $\epsilon_A = \pm 1$ depending on whether the operator is even or odd under time reversal.

~~Note 2 ... equilibrium~~,

Symmetry of the dynamic susceptibility. Since the density matrix is invariant under time reversal:

$$\hat{\rho}(-t) = U_T \hat{\rho}(t) U_T^+ = \hat{\rho}(t)$$

So for any self adjoint operator $\langle A \rangle = \langle A^+ \rangle = \langle (\underbrace{U_T A U_T^+}_{A(-t)})^+ \rangle$

(in particular $\langle A \rangle = 0$ if $\epsilon_A = -1$ for a purely Hamiltonian system).

This is a tricky comment. I think it is best to restrict it to equilibrium.

We have defined:

$$\chi''_{AB}(t-t') = \frac{1}{2\hbar} \langle [A(t), B(t')] \rangle_{eq} =$$

identity above

$$\stackrel{\downarrow}{=} \frac{1}{2\hbar} \langle (U_T [A(t), B(t')] U_T^+)^+ \rangle_{eq},$$

$$= \frac{1}{2\hbar}\left\langle \left(U_T A(t) U_T^{-1} U_T B(t') U_T^{+} - U_T B(t') U_T^{-1} U_T A(t) U_T^{+} \right)^{+} \right\rangle_{eq}$$

U is unitary $U^{-1} = U^{+}$

$$\overset{?}{=} \frac{1}{2h}\left\langle \left(\epsilon_A A(-t)\, \epsilon_B B(-t') - \epsilon_B B(-t')\, \epsilon_A A(-t) \right)^{+} \right\rangle_{eq} =$$

$$\cancel{= \frac{1}{2\hbar}\epsilon_A \epsilon_B \langle [A(-t), B(-t')] \rangle_{eq}}$$

$$\cancel{\Rightarrow \chi''_{AB}(t-t') =}$$

$$= \frac{1}{2\hbar}\epsilon_A \epsilon_B \left\langle B^{+}(-t') A^{+}(-t) - A^{+}(-t) B^{+}(-t') \right\rangle$$

$$= \frac{1}{2h}\epsilon_A \epsilon_B \left\langle B(-t') A(-t) - A(-t) B(-t') \right\rangle_{eq}$$

$$= -\frac{\epsilon_A \epsilon_B}{2h}\left\langle [A(-t), B(-t')] \right\rangle_{eq} \Rightarrow \boxed{\chi''_{AB}(t-t') = -\epsilon_A \epsilon_B \chi''_{AB}(t'-t)}$$

$$\Downarrow$$

$$\boxed{\chi''_{AB}(\omega) = -\epsilon_A \epsilon_B \chi''_{AB}(-\omega)}$$

From these equations, we can derive the symmetry of the fluctuations.

Recall:

$$S_{AB}(\omega) = \hbar \coth\left(\frac{\beta\hbar\omega}{2}\right) \chi''_{AB}(\omega)$$

a) $\chi''_{AB}(\omega) = -\epsilon_A \epsilon_B \chi''_{AB}(-\omega) = \epsilon_A \epsilon_B \chi''_{BA}(\omega)$

$$\Rightarrow \boxed{S_{AB}(\omega) = \epsilon_A \epsilon_B S_{BA}(\omega)}$$

b) $\chi''^{*}_{AB}(\omega) = -\chi''_{AB}(-\omega) = \epsilon_A \epsilon_B \chi''_{AB}(\omega)$

$$\Rightarrow \boxed{S^{*}_{AB}(\omega) = \epsilon_A \epsilon_B S_{AB}(\omega)}$$

Real if $\epsilon_A \epsilon_B = 1$

c) $\coth(-x) = -\coth(x)$

$$\chi''_{AB}(\omega) = -\epsilon_A \epsilon_B \chi''_{AB}(-\omega)$$

$$\Rightarrow \boxed{S_{AB}(\omega) = \epsilon_A \epsilon_B S_{AB}(-\omega)}$$