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Universal Properties of Nonlinear Response Functions of Nonequilibrium Steady States

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Universal properties of response functions

Response of equilibrium states

- linear response function : completed (Nyquist, Callen, Kubo, ...)
- higher-order response function : completed (Kubo, Blömbergen, ...)

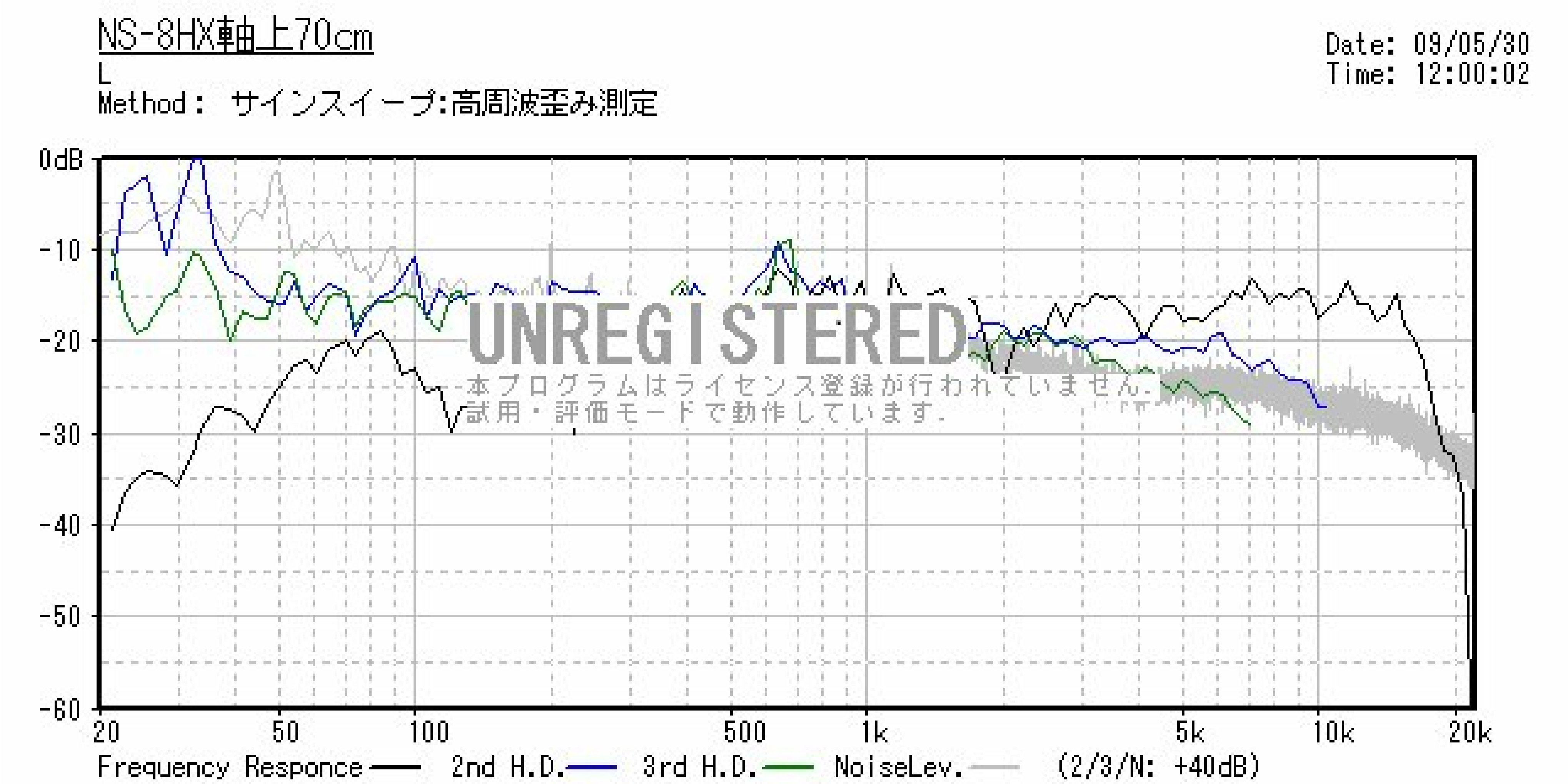
Response of nonequilibrium steady states

- linear response function : completed (AS and T. Yuge (2010))
- higher-order response function : this talk

1次、2次、3次応答係数の実測例

清水の愛用スピーカー measured by 清水

（2次、3次は+40dB してプロット）



Response function of a NESS of macroscopic quantum systems

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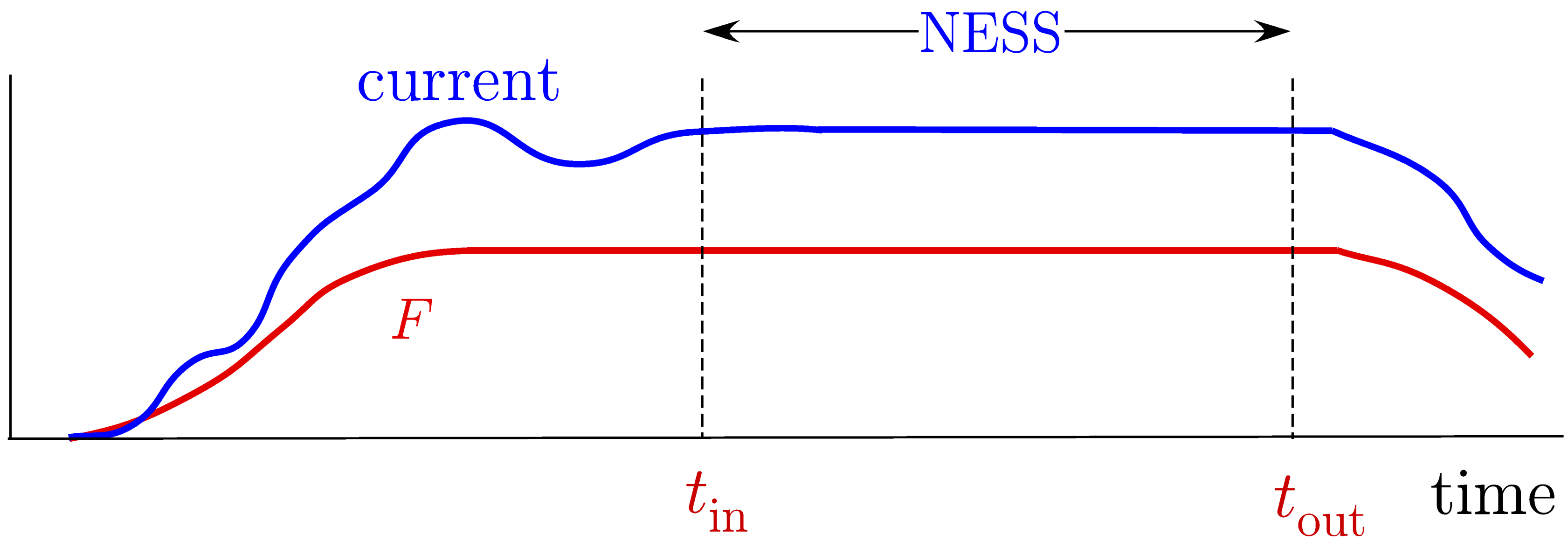
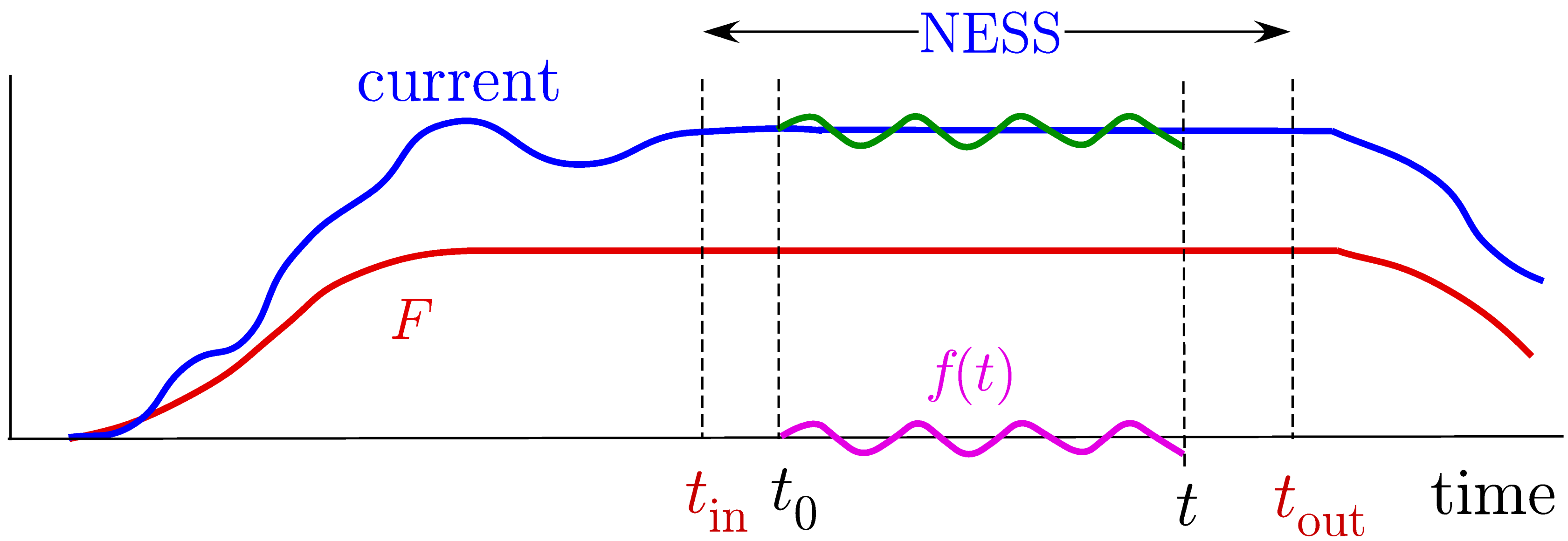


A nonequilibrium steady states (NESS) is realized for a macroscopic interval $[t_{\text{in}}, t_{\text{out}}]$.

- Further apply a weak and time-dependent probe fields for $t \geq t_0$,

$$F_{\text{total}}(t) \;=\; F + f_1(t) + f_2(t) + \cdots + f_m(t)$$



- Response of the NESS to $\boldsymbol{f}(t)$: see the response,

$$\Delta A(t) \equiv \langle A \rangle_{F+\boldsymbol{f}}^{t} - \langle A \rangle_F$$

of a macroscopic variable A.

ex. $A = M_z = \mu_B \sum_{\boldsymbol{r}} \sigma_z(\boldsymbol{r})$: total magnetic moment

- Assume that the NESS is stable : If $\boldsymbol{f}$ is small, ΔA is small.

$$\Delta A(t) = A^{(1)}(t) + A^{(2)}(t) + \cdots ,$$

where n-th order response

$$\Delta A^{(n)}(t) = \frac{1}{n!} \sum_{\alpha_1=1}^{m} \cdots \sum_{\alpha_n=1}^{m} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \times \Phi^{(n)F}_{\alpha_1\cdots\alpha_n}(t-t_1, \cdots, t-t_n) f_{\alpha_1}(t_1) \cdots f_{\alpha_n}(t_n).$$

- The n-th order response function is defined by this and the causality relation,

$$\Phi^{(n)F}_{\alpha_1\cdots\alpha_n}(\tau_1, \cdots, \tau_n) = 0 \text{ for either of } \tau_j < 0,$$

and the symmetrization,

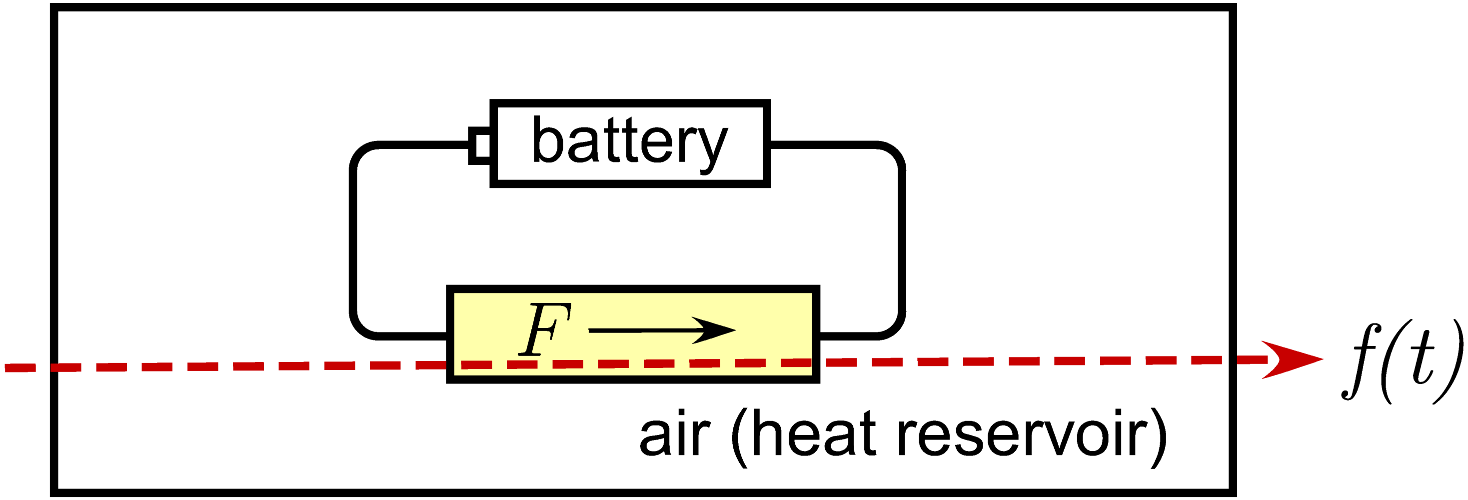
$\Phi^{(n)F}_{\alpha_1\cdots\alpha_n}(\tau_1, \cdots, \tau_n)$ is invariant under permutaions of $\alpha_1\tau_1, \cdots, \alpha_n\tau_n$.

General and universal properties of $\Phi^{(n)F}_{\alpha_1\cdots\alpha_n}$?

General formula — a microscopic expression of $\Phi^{(n)F}$

- A large system

  targ



$\boldsymbol{f}(t) = f_1(t) + \cdots + f_m(t)$ is treated as external fields.

- Hamiltonian

$$\hat{H}^{\mathrm{tot}} - \sum_{\alpha=1}^{m} \hat{B}_\alpha f_\alpha(t) \quad (\hat{B}_\alpha \in \text{target system}).$$

- Density operator of the total system: $\hat{\rho}^{\rm tot}_{F+\boldsymbol{f}}(t)$, or $\hat{\rho}^{\rm tot}_{F}(t)$ for $\boldsymbol{f}=0$.

  $\to$ density operator of the NESS of the target system is

$$\hat{\rho}_F \equiv \mathrm{Tr}'\left[\hat{\rho}^{\rm tot}_F(t)\right] \quad (\mathrm{Tr}' \equiv \text{trace over out of the target system}).$$

- From these eqs.,

a microscopic expression of $\Phi^{(n)F}_{\alpha_1\cdots\alpha_n}$

$$\Phi^{(n)F}_{\alpha_1\cdots\alpha_n}(\tau_1,\cdots,\tau_n) \quad \text{for } \tau_1,\cdots,\tau_n \geq 0$$
$$= \underset{\alpha_1\tau_1,\cdots,\alpha_n\tau_n}{\mathcal{S}} \frac{1}{(i\hbar)^n}\mathrm{Tr}\left(\hat{\rho}^{\rm tot}_F\left[\breve{B}_{\alpha_n}(-\tau_n)^\times\cdots\breve{B}_{\alpha_1}(-\tau_1)^\times\hat{A}\right]\right).$$

Here,

$$\begin{aligned}
\mathcal{S} &\equiv \text{symmetrizing operation},\\
\breve{X}(\tau) &\equiv e^{\frac{i}{\hbar}\hat{H}^{\rm tot}\tau}\hat{X}\,e^{\frac{-i}{\hbar}\hat{H}^{\rm tot}\tau},\\
X^\times Y &\equiv [X,\ Y].
\end{aligned}$$

Response to sinusoidal fields

Sinusoidal probe fields

$$\begin{aligned} f_\alpha(t) &= f_\alpha^{+} e^{-i\omega_\alpha t} + f_\alpha^{-} e^{+i\omega_\alpha t} \qquad ([f_\alpha^-]^* = f_\alpha^+) \\ &= \sum_{\sigma=\pm 1} f_\alpha^\sigma e^{-i\sigma\omega_\alpha t} \end{aligned}$$

n-th order response

$$\begin{aligned} \Delta A^{(n)}(t) &= \frac{1}{n!} \sum_{\alpha_1,\sigma_1} \cdots \sum_{\alpha_n,\sigma_n} \Xi^{(n)F}_{\alpha_1\cdots\alpha_n}(\sigma_1\omega_{\alpha_1}, \cdots, \sigma_n\omega_{\alpha_n}) \\ &\quad \times f_{\alpha_1}^{\sigma_1} \cdots f_{\alpha_n}^{\sigma_n} \, e^{-i(\sigma_1\omega_{\alpha_1}+\cdots+\sigma_n\omega_{\alpha_n})t} \end{aligned}$$

Here, $\Xi^{(n)F}$ is the Fourier tr. of $\Phi^{(n)F}$;

$$\begin{aligned} &\Xi^{(n)F}_{\alpha_1\cdots\alpha_n}(\sigma_1\omega_{\alpha_1}, \cdots, \sigma_n\omega_{\alpha_n}) \\ &\quad = \int_{-\infty}^{+\infty} d\tau_1 \cdots \int_{-\infty}^{+\infty} d\tau_n \, \Phi^{(n)F}_{\alpha_1\cdots\alpha_n}(\tau_1, \cdots, \tau_n) \, e^{i(\sigma_1\omega_{\alpha_1}\tau_1+\cdots+\sigma_n\omega_{\alpha_n}\tau_n)}. \\ &\quad = \Xi^{(n)F*}_{\alpha_1\cdots\alpha_n}(-\sigma_1\omega_{\alpha_1}, \cdots, -\sigma_n\omega_{\alpha_n}) \end{aligned}$$

Example: $n = 2, m = 2$

$$f_1(t) = f_1^+ e^{-i\omega_1 t} + f_1^- e^{+i\omega_1 t} \qquad ([f_1^-]^* = f_1^+)$$

$$f_2(t) = f_2^+ e^{-i\omega_2 t} + f_2^- e^{+i\omega_2 t} \qquad ([f_2^-]^* = f_2^+)$$

$$\Delta A^{(2)}(t) = \frac{1}{2!} \sum_{\alpha_1,\sigma_1} \sum_{\alpha_2,\sigma_2} \Xi^{(2)F}_{\alpha_1\alpha_2}(\sigma_1\omega_{\alpha_1}, \sigma_2\omega_{\alpha_2}) f_{\alpha_1}^{\sigma_1} f_{\alpha_2}^{\sigma_2}\, e^{-i(\sigma_1\omega_{\alpha_1}+\sigma_2\omega_{\alpha_2})t}$$

$$= \frac{1}{2}\,\Xi^{(2)F}_{11}(\omega_1,\omega_1)\left(f_1^+\right)^2\, e^{-2i\omega_1 t} + c.c. \quad \rightarrow \omega = 2\omega_1$$

$$+ \; \frac{1}{2}\,\Xi^{(2)F}_{22}(\omega_2,\omega_2)\left(f_2^+\right)^2\, e^{-2i\omega_2 t} + c.c. \quad \rightarrow \omega = 2\omega_2$$

$$+ \; \Xi^{(2)F}_{12}(\omega_1,\omega_2) f_1^+ f_2^+\, e^{-i(\omega_1+\omega_2)t} + c.c. \quad \rightarrow \omega = \omega_1 + \omega_2$$

$$+ \; \Xi^{(2)F}_{12}(\omega_1,-\omega_2) f_1^+ f_2^-\, e^{-i(\omega_1-\omega_2)t} + c.c. \quad \rightarrow \omega = \omega_1 - \omega_2$$

$$+ \; \frac{1}{2}\,\Xi^{(2)F}_{11}(\omega_1,-\omega_1)\left|f_1^+\right|^2 + c.c. \quad \rightarrow \omega = 0$$

$$+ \; \frac{1}{2}\,\Xi^{(2)F}_{22}(\omega_2,-\omega_2)\left|f_2^+\right|^2 + c.c. \quad \rightarrow \omega = 0$$

These $\Xi^{(2)F}$'s take different values, and are basically independent of each other.

Found several universal relations as we have found for $\Xi^{(1)F}(\omega)$ in
AS and T. Yuge, J. Phys. Soc. Jpn. 79 (2010) 013002.

One of the universal relations: Sum rule for $\mathrm{Re}\,\Xi^{(n)F}$

$$\int_{-\infty}^{\infty}\frac{d\omega_1}{\pi}\cdots\int_{-\infty}^{\infty}\frac{d\omega_n}{\pi}\,\mathrm{Re}\,\Xi^{(n)F}_{\alpha_1\cdots\alpha_n}(\sigma_1\omega_{\alpha_1},\cdots,\sigma_n\omega_{\alpha_n})$$
$$=\underset{\alpha_1,\cdots,\alpha_n}{\mathcal{S}}\frac{1}{(i\hbar)^n}\left\langle \hat{B}^{\times}_{\alpha_n}\cdots\hat{B}^{\times}_{\alpha_1}\hat{A}\right\rangle_F \quad \text{for all } F \text{ and } \sigma_1,\cdots,\sigma_n$$

$\hat{A}$: observable of interest

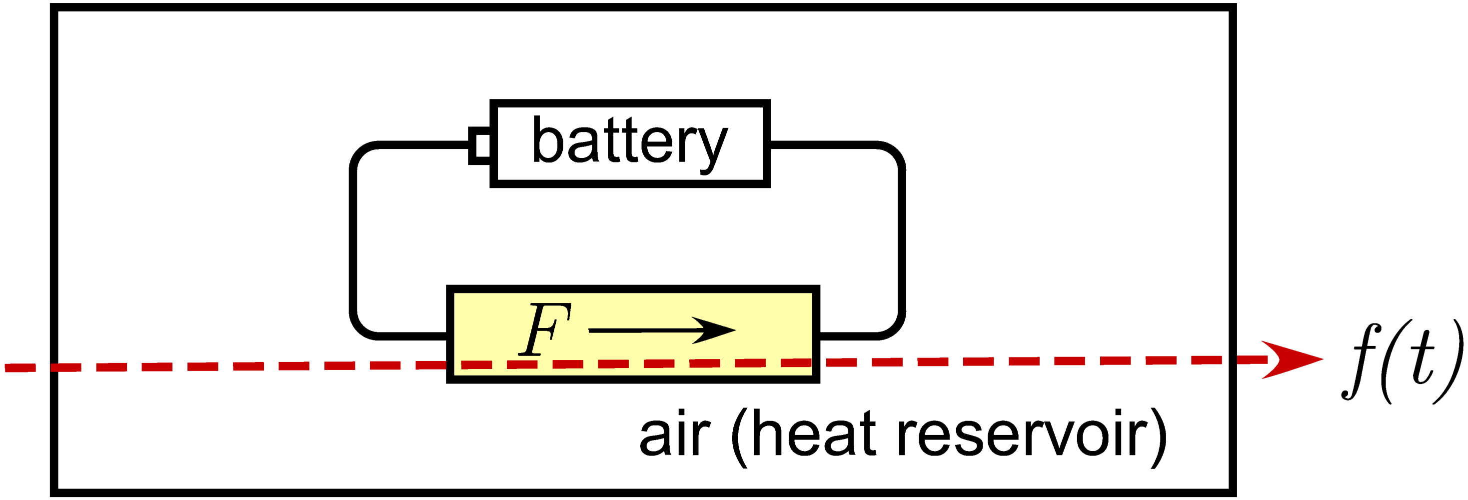
$\hat{B}_\alpha$: observable that couples to $f_\alpha(t)$ via the interaction term, $-\hat{B}_\alpha f_\alpha(t)$

$\langle\cdot\rangle_F \equiv \mathrm{Tr}\,(\hat{\rho}_F\,\cdot\,)$: expectation value in the NESS $\quad\left(\hat{\rho}_F \equiv \mathrm{Tr}'\left[\hat{\rho}^{\mathrm{tot}}_F(t)\right]\right)$

Example: $n = 2$

$$\int_{-\infty}^{\infty} \frac{d\omega_1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega_2}{\pi} \,\mathrm{Re}\, \Xi^{(2)F}_{\alpha_1 \alpha_2}(\sigma_1 \omega_{\alpha_1}, \sigma_2 \omega_{\alpha_2})$$
$$= \frac{1}{2(i\hbar)^2} \left\langle \left[\hat{B}_{\alpha_1}, \left[\hat{B}_{\alpha_2}, \hat{A} \right] \right] + (1 \leftrightarrow 2) \right\rangle_F \quad \text{for all } F \text{ and } \sigma_1, \sigma_2$$

- Generalization of that for $\Xi^{(1)F}(\omega)$ by AS and T. Yuge (2010).
- Unlike some formal relations,
  - all terms can be measured experimentally.
  - predictions on two or more independent experiments.
- Almost no assumption is made except that the NESS is stable
  $\rightarrow$ applicable to diverse physical systems



When $A = I$ (electric current averaged over the x direction),

$$\begin{aligned}\Delta I(t) &\equiv \langle I\rangle^t_{F+\boldsymbol{f}} - \langle I\rangle_F \\ &= \sum_\alpha \int_{t_0}^t dt_1\, \Phi^{(1)F}_\alpha(t-t_1) f_\alpha(t_1) \\ &\quad + \frac{1}{2!}\sum_{\alpha_1,\alpha_2}\int_{t_0}^t dt_1 \int_{t_0}^t dt_2\, \Phi^{(2)F}_{\alpha_1\alpha_2}(t-t_1, t-t_2) f_{\alpha_1}(t_1) f_{\alpha_2}(t_2) \\ &\quad + \cdots\end{aligned}$$

The sum rule says;

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \,\mathrm{Re}\,\Xi_{\alpha}^{(1)F}(\omega) = \frac{e^2 N_e}{mL} \quad : \text{ independent of } F,$$

$$\int_{-\infty}^{\infty} \frac{d\omega_1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega_2}{\pi} \,\mathrm{Re}\,\Xi_{\alpha_1\alpha_2}^{(2)F}(\omega_1, \omega_2) = 0 \quad : \text{ independent of } F,$$

$$\int_{-\infty}^{\infty} \frac{d\omega_1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega_2}{\pi} \int_{-\infty}^{\infty} \frac{d\omega_3}{\pi} \,\mathrm{Re}\,\Xi_{\alpha_1\alpha_2\alpha_3}^{(3)F}(\omega_1, \omega_2, \omega_3) = 0 \quad : \text{ independent of } F,$$

although $\mathrm{Re}\,\Xi^{(n)F}$'s at individual values of ω_α's depend strongly on F at low frequencies.

Discussions and Summary

非平衡定常状態の高次応答関数の普遍的性質、特に総和則

- The sum rule is a prediction on the collection of the results of many separate experiments.
- ハミルトン系でなくても、まともなモデルなら、sum ruleは成立
  → 成立しなければ、そのモデルはダメ！
- いわば、電荷保存則のようなもの
  - きわめて広い範囲で成立
  - 計算や測定に便利
    * まだ測ってない部分を予言できる
    * 誤りを検出できる
  - 知っているといないのとでは、大きく違う
  - まともなモデル・計算の満たすべき必要条件
    → 非平衡系のリトマス試験紙！
    計算や測定のチェックにも使ってください