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Quantum measurement theory and micro-macro consistency in nonequilibrium statistical mechanics

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In nonequilibrium statistical mechanics,

- quantum measurement theory
- requirement of micro-macro consistency

have been implicitly used.

This talk

- Where they are used.
- They actually play crucial roles.
- Recent results on universal properties of response functions of nonequilibrium steady states (NESSs).

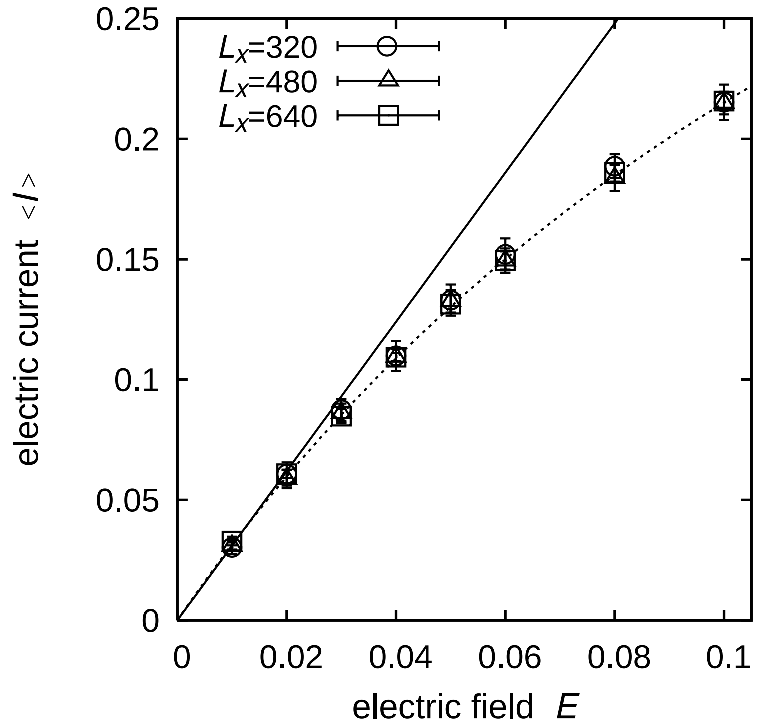
CONTENTS

1. **linear nonequilibrium regime**

   Kubo formula revisited.

2. **nonlinear nonequilibrium regime**

   universal properties of response functions of NESSs.



$\langle I \rangle$ versus F $(= eE)$ of a conductor

1. linear nonequilibrium regime — Kubo formula revisited

Derivation by R. Kubo (1957)

- For $t < t_0$ (later taken as $-\infty$), the target system contacts with a reservoir;

$$\hat{\rho}(t_0) = \hat{\rho}_{\rm eq} = (1/Z)\exp[-\beta \hat{H}]$$

- Detach the reservoir at $t = t_0$

  $\Rightarrow$ the target system becomes an isolated system.

- For $t > t_0$, apply a weak external field $f(t)$ adiabatically, so

$$i\hbar \frac{\partial}{\partial t}\hat{\rho}(t) = \left[\hat{H} - \hat{B} f(t), \hat{\rho}(t)\right] \quad : \text{ von Neumann eq.}$$

- To the linear order in $f(t)$, an observable A of interest changes by

$$\begin{aligned} \Delta A(t) &\equiv \mathrm{Tr}[\hat{\rho}(t)\hat{A}] - \mathrm{Tr}[\hat{\rho}_{\rm eq}\hat{A}] \\ &= \int_{t_0}^{t} \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}_{\rm eq}\left[\hat{B},\ \breve{A}(t-t')\right]\right) f(t')dt', \end{aligned}$$

Here,

$$\breve{A}(\tau) \equiv e^{\frac{i}{\hbar}\hat{H}\tau}\hat{A}\, e^{\frac{-i}{\hbar}\hat{H}\tau}.$$

- On the other hand, macroscopic physics says

$$\Delta A(t) = \int_{t_0}^{t} \Phi_{\mathrm{eq}}(t-t')f(t')dt',$$

which defines the linear response function of equilibrium states Φ_{eq}.

- By comparing the two eqs., one obtains a microscopic expression of Φ_{eq};

$$\Phi_{\mathrm{eq}}(\tau) = \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}_{\mathrm{eq}}\left[\hat{B},\ \breve{A}(\tau)\right]\right)$$

- Using $\hat{\rho}_{\mathrm{eq}} = (1/Z)\exp[-\beta\hat{H}]$, one can recast the RHS as the canonical correlation;

$$\Phi_{\mathrm{eq}}(\tau) = \frac{1}{k_B T}\langle\dot{\breve{B}}(0);\breve{A}(\tau)\rangle_{\mathrm{eq}}: \text{Kubo formula}$$

- The response function (in the linear nonequilibrium regime) is related to 'fluctuation' in the equilibrium state : fluctuation-dissipation relation

Reconsideration — 1

Q1. Does the canonical correlation represent fluctuation, i.e., time correlation of measurement outcomes?

In the classical regime $k_B T \gg \hbar\omega$, the answer is **yes** (in most cases):

$$\Phi_{\mathrm{eq}}(\tau) = \frac{1}{k_B T}\langle \dot{\breve{B}}(0); \breve{A}(\tau)\rangle_{\mathrm{eq}}\text{: canonical correlation (Kubo formula)}$$

$$\overset{[i]}{=} \frac{1}{k_B T}\left\langle \frac{\dot{\breve{B}}(0)\breve{A}(\tau) + \breve{A}(\tau)\dot{\breve{B}}(0)}{2} \right\rangle_{\mathrm{eq}} \quad \text{for } k_B T \gg \hbar\omega$$

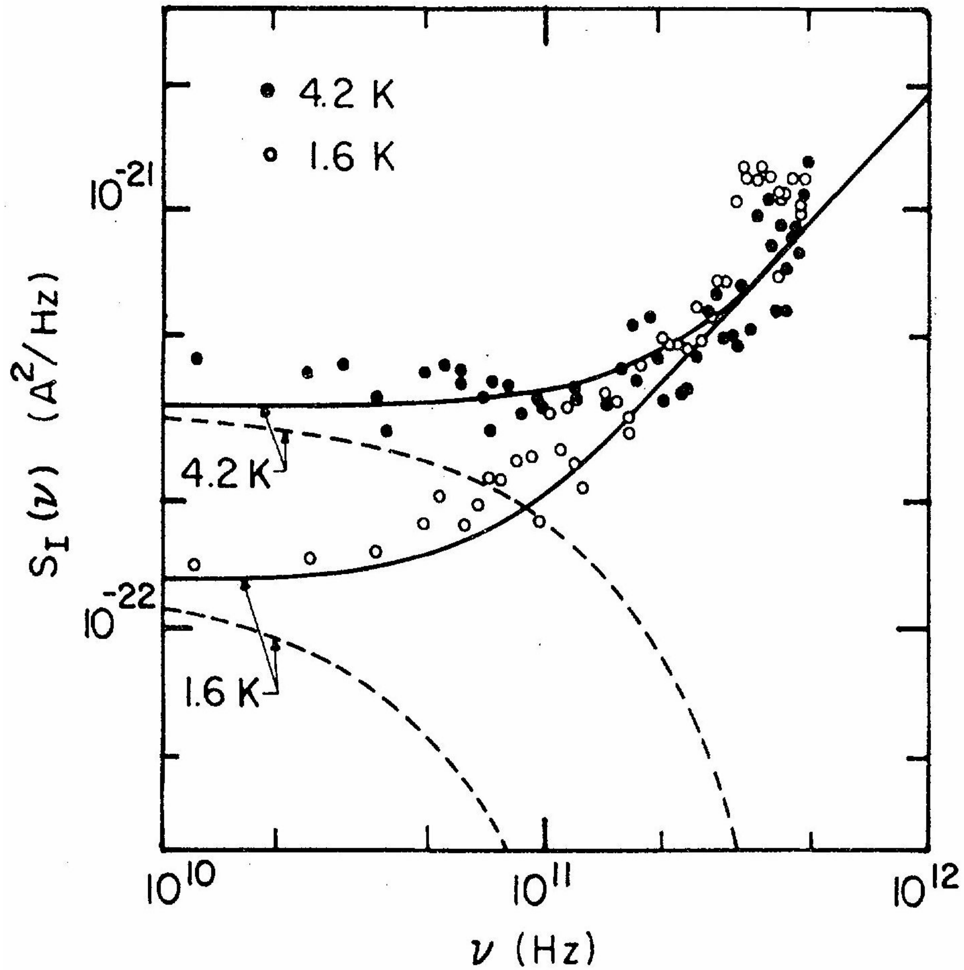
: symmetrized time correlation

$$= \text{FT of fluctuation for } k_B T \gg \hbar\omega$$

$\rightarrow$ fluctuation-dissipation relation

[i] Kubo, Toda, Hashitsume, Statistical Physics part II.

In the quantum regime $k_B T \lesssim \hbar\omega$, the answer depends on what apparatus you use. See, e.g., Sec. 4 of K. Koshino and A. Shimizu, Physics Reports 412 (2005) 191.



R. H. Koch, et al., Phys. Rev. B26 (1982) 74.

Q1. Does the canonical correlation represent fluctuation, i.e., time correlation of measurement outcomes?

A1. In the classical regime, **yes**. In the quantum regime, **yes or no** depending on what apparatus you use.

Reconsideration — 2

In order to measure

$$\Xi_{\text{eq}}(\omega) \equiv \int_0^\infty \Phi_{\text{eq}}(\tau) e^{i\omega\tau} d\tau,$$

one has to measure the observable continuously for a long time $\gg 1/\omega$.

Q2. Then, you cannot use the von Neumann eq., can you? But, it was used in deriving Kubo formula! (H. Takahashi (1957))

This could be resolved by the results on stability of general quantum states of macroscopic systems by A. Shimizu and T. Miyadera, Phys. Rev. Lett. 89 (2002) 270403.

skip .....

Reconsideration — 3

One obtains the same result also for other statistical ensembles.

ex. canonical ensemble $\to$ microcanonical ensemble

$$\hat{\rho}_{\rm eq}(T,V,N) \to \hat{\rho}_{\rm eq}(U,V,N)$$

$$(1/Z)\exp[-\beta \hat{H}] \to (1/W) \sum_{U-\delta U<E\le U} \sum_{\nu} |E,\nu\rangle\langle E,\nu|$$

Equilibrium states can also be represented by non-standard ensembles.

ex. Classical statistical mechanics

Almost every state on an equi-energy surface is the same equilibrium state.

$\to$ one can take either of the following as the equilibrium state:

(i) mixture of all states on the equi-energy surface of finite thickness δU

(ii) mixture of a part of states on the equi-energy surface of thickness δU

(iii) a single pure state in these mixed states (MD simulations use such a state)

Q3. What happens if we take (ii) or (iii) as $\hat{\rho}(t_0) = \hat{\rho}_{\rm eq}$?

Then, in general, $\hat{\rho}(t)$ evolves by the equilibrium Hamiltonian $\hat{H}$.

ex. $\hat{\rho}(t_0)$ = a coherent state

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = \left[\hat{H}, \hat{\rho}(t)\right] \neq 0 \ \Rightarrow\ \hat{\rho}(t) \neq \hat{\rho}(t_0).$$

Hence, microscopic observables vary in this equilibrium state;

$$\langle a \rangle^t \neq \langle a \rangle^{t_0}$$

However, every macroscopic variable A takes a constant value $\langle A \rangle_{\mathrm{eq}}$ in the sense that

$$\langle A \rangle^t = \langle A \rangle_{\mathrm{eq}} + o\left(\langle A \rangle_{\mathrm{tp}}\right).$$

Here, $\langle A \rangle_{\mathrm{tp}}$ denotes a typical value of A.

ex. Total magnetization: $\langle M_z \rangle_{\mathrm{tp}} = O(V)$,

$$\langle M_z \rangle^t = \langle M_z \rangle_{\mathrm{eq}} + o(V).$$

These are natures of real equilibrium states!

Then, we obtain

$$\Delta A(t) \equiv \mathrm{Tr}[\hat{\rho}(t)\hat{A}] - \mathrm{Tr}[\hat{\rho}_{\mathrm{eq}}\hat{A}]$$
$$= \int_{t_0}^{t} \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}(t')\left[\hat{B},\ \breve{A}(t-t')\right]\right) f(t')dt' \ \leftarrow \ \text{microscopic physics}$$

which apparently contradicts with

$$\Delta A(t) = \int_{t_0}^{t} \Phi_{\mathrm{eq}}(t-t') f(t')dt' \ \leftarrow \ \text{macroscopic physics}$$

The micro-macro consistency requires

- t' in $\hat{\rho}(t')$ should be irrelavant to the integral.
  $\rightarrow$ $\hat{\rho}(t')$ can be replaced with $\hat{\rho}(t_0)$.
- All possible forms of $\hat{\rho}_{\mathrm{eq}}$ give identical results for (correlations of) macroscopic variables, if we neglect $o\left(\langle A\rangle_{\mathrm{tp}}\right)$ terms.
  $\rightarrow$ $\hat{\rho}(t_0)$ (such as a coherent state) can be replaced with $(1/Z)\exp[-\beta\hat{H}]$.

If you accept these assumtions, you recover the Kubo formula.

These assumptions have never been proved for general models.
Presumably, the proof is impossible for general models.
These assumptions are restrictions imposed by Nature on physical models, rather than statements to be proved.

Similar restriction:
According to thermodynamics, entropy S increases with increasing U.
This cannot be true for general Hamiltonians.
Hence, this is a restriction imposed by Nature on physical models.
ex. S of spin Hamiltonians decreases with increasing U for $U > 0$.
In real physical systems, many modes (other than spin degrees of freedom) are excited for $U > 0$, and S does increase with increasing U.
$\rightarrow$ Spin models are physically valid only for $U < 0$.

Q3. What happens if we take (ii) or (iii) as $\hat{\rho}(t_0) = \hat{\rho}_{\mathrm{eq}}$?
A3. If you accept the restrictions imposed by Nature, then you recover the Kubo formula.

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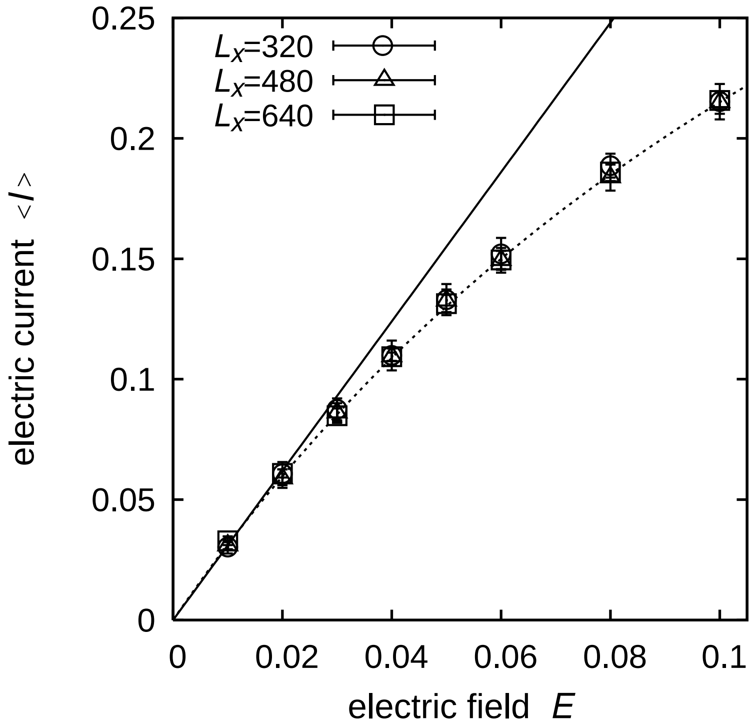
   universal properties of response functions of NESSs.



$\langle I \rangle$ versus F $(= eE)$ of a conductor

Universal properties of response functions

Equilibrium states

Response to a weak force $f(t)$

$\rightarrow$ linear response function $\Phi_{\rm eq}$

$\rightarrow$ $\Phi_{\rm eq}$ = [Kubo formula]

$\rightarrow$ many universal properties

$\rightarrow$ all important results in the 'linear nonequilibrium regime'!

Nonequilibrium steady states (NESSs) driven by a (strong) force F

Response to a weak force $f(t)$

$\rightarrow$ linear response function Φ_F

$\rightarrow$ $\Phi_F \neq$ [Kubo formula]

$\rightarrow$ any universal properties in the 'nonlinear nonequilibrium regime' ?

F : pump, $f(t)$: probe $\rightarrow$ pump-probe experiment

This talk:

Universal properties of Φ_F.

- common to diverse physical systems ($\Leftrightarrow$ limited to specific systems)
- relations between measurable quantities ($\Leftrightarrow$ merely formal relations)
- relevant to macroscopic systems ($\Leftrightarrow$ only to mesoscopic or smaller systems)

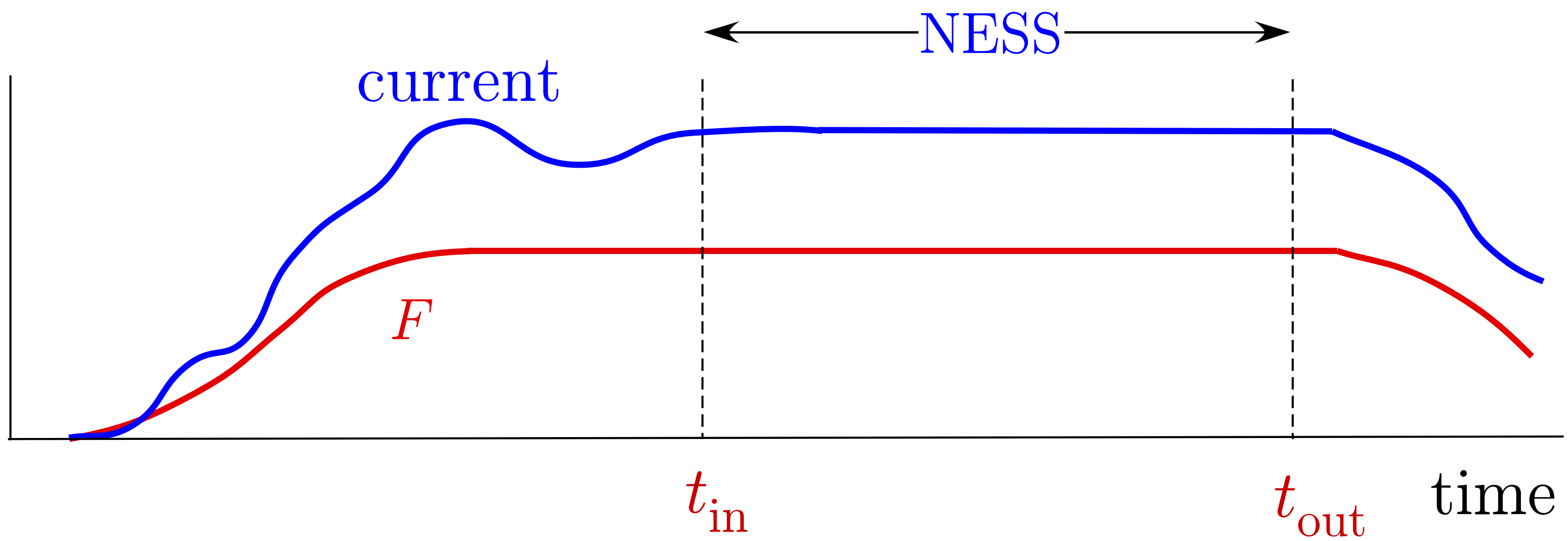
Further in this talk:

Universal properties of nonlinear response functions $\Phi_F^{(2)}, \Phi_F^{(3)}, \cdots$ of NESSs.

c.f. Those of eq. states, $\Phi_{\rm eq}^{(2)}, \Phi_{\rm eq}^{(3)}, \cdots$, are well-known.

Response function of a NESS of macroscopic quantum systems

- Apply a strong static field F (pump field).



A nonequilibrium steady states (NESS) is realized for $[t_{\mathrm{in}}, t_{\mathrm{out}}]$

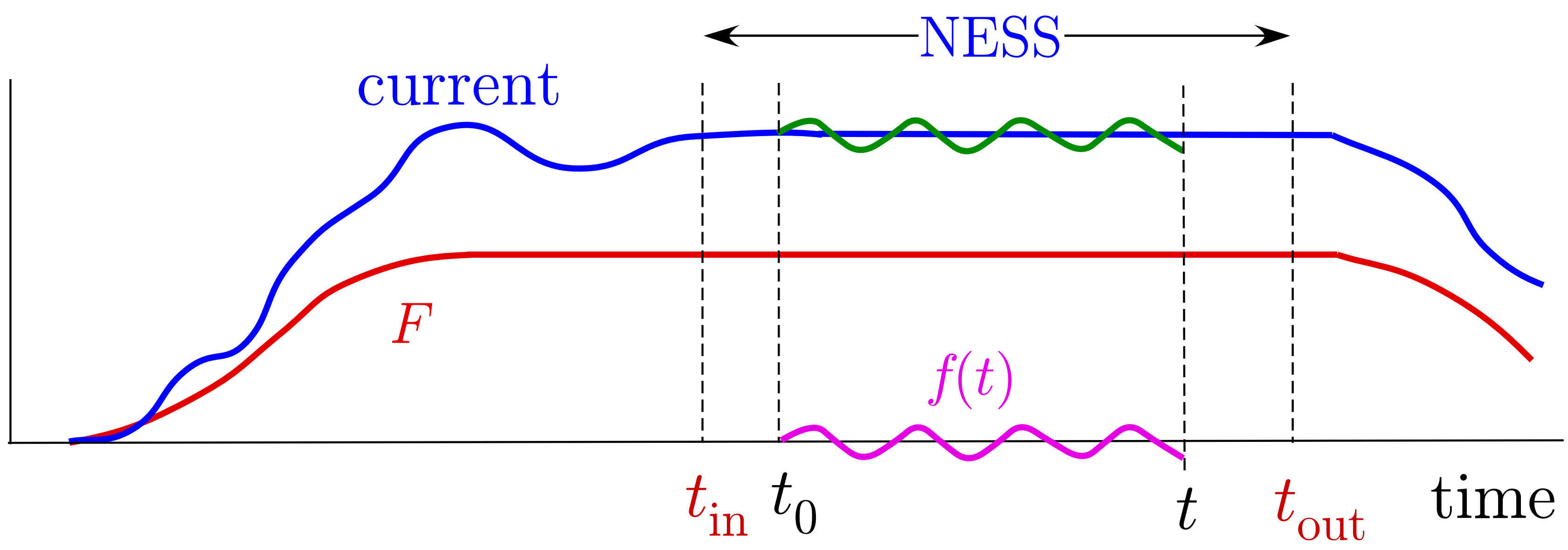
Every macroscopic variable A takes a constant value $\langle A \rangle_F$, i.e.,

$$\langle A \rangle_F^t = \langle A \rangle_F + o\left(\langle A \rangle_{\mathrm{tp}}\right).$$

Here, $\langle A \rangle_{\mathrm{tp}}$ denotes a typical value of A.

- Further apply a weak and time-dependent probe field $f(t)$ for $t \geq t_0$,

$$F(t) = F + f(t).$$



- Response of the NESS to $f(t)$: see the response,

$$\Delta A(t) \equiv \langle A \rangle^t_{F+f} - \langle A \rangle_F,$$

of a macroscopic variable A.

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

- To the linear order in f,

$$\Delta A(t) = \int_{t_0}^{t} \Phi_F(t-t') f(t') dt'$$

- This and the causality relation

$$\Phi_F(\tau) = 0 \text{ for } \tau < 0$$

define the (linear) response function $\Phi_F(\tau)$ of the NESS.

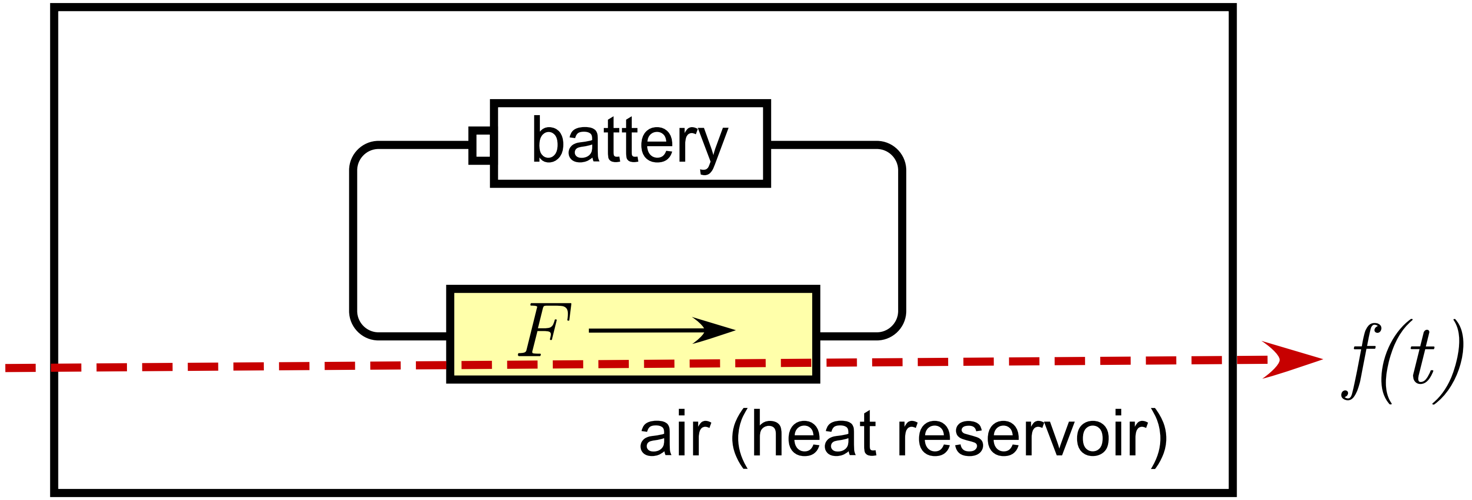
General and universal properties of Φ_F?

A. Shimizu and T. Yuge, J. Phys. Soc. Jpn. 79 (2010) 013002.

General formula — a microscopic expression of Φ_F

- A large system

  target system + driving source + heat reservoir + $\cdots$ $\equiv$ total system



  $f(t)$ is treated as an external field.

- Hamiltonian

$$\hat{H}^{\rm tot} - \hat{B} f(t) \quad (\hat{B} \in \text{target system}).$$

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

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

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

- To the linear order in f;

$$\begin{aligned} \Delta A(t) &\equiv \mathrm{Tr}[\hat{\rho}_{F+f}^{\mathrm{tot}}(t)\hat{A}] - \mathrm{Tr}[\hat{\rho}_F^{\mathrm{tot}}(t_0)\hat{A}] \\ &= \int_{t_0}^{t} \frac{1}{i\hbar} \mathrm{Tr}\left(\hat{\rho}_F^{\mathrm{tot}}(t') \left[\hat{B},\ \breve{A}(t-t') \right] \right) f(t') dt', \end{aligned}$$

Here,

$$\breve{A}(\tau) \equiv e^{\frac{i}{\hbar}\hat{H}^{\mathrm{tot}}\tau} \hat{A}\, e^{\frac{-i}{\hbar}\hat{H}^{\mathrm{tot}}\tau}.$$

- This must be consistent with the macroscopic physics,

$$\Delta A(t) = \int_{t_0}^{t} \Phi_F(t-t') f(t') dt'.$$

Hence, t' in $\hat{\rho}_F^{\mathrm{tot}}(t')$ must be irrelevant. We write

$$\hat{\rho}_F^{\mathrm{tot}} \equiv \hat{\rho}_F^{\mathrm{tot}}(t'),$$

where t' is an arbitrary time (such as t_0) in $[t_{\mathrm{in}}, t_{\mathrm{out}}]$.

• We thus obtain a microscopic expression of Φ_F;

response-correlation relation (RCR)

$$\Phi_F^{AB}(\tau) = \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}_F^{\mathrm{tot}}\left[\hat{B},\ \breve{A}(\tau)\right]\right) \qquad \text{for } \tau \geq 0.$$

Note: The RHS is not fluctuation because correlation does not necessarily represent fluctuation (as will be shown shortly).

Violation of fluctuation-dissipation and reciprocal relations

When $F = 0$ (equilibrium states),

$$
\begin{aligned}
\Phi_F^{AB}(\tau) &= \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}_F^{\mathrm{tot}}\left[\hat{B},\ \breve{A}(\tau)\right]\right) : \text{response-correlation relation} \\
&\downarrow \\
\Phi_{\mathrm{eq}}^{AB}(\tau) &= \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}_{\mathrm{eq}}\left[\hat{B},\ \breve{A}(\tau)\right]\right) \\
&= \frac{1}{k_B T}\langle \dot{\breve{B}}(0); \breve{A}(\tau)\rangle_{\mathrm{eq}} : \text{canonical correlation (Kubo formula)} \\
&\quad \to \text{reciprocal relations} \\
&\overset{[i]}{=} \frac{1}{k_B T}\left\langle \frac{\dot{\breve{B}}(0)\breve{A}(\tau) + \breve{A}(\tau)\dot{\breve{B}}(0)}{2} \right\rangle_{\mathrm{eq}} \quad \text{for } k_B T \gg \hbar\omega \\
&\quad : \text{symmetrized time correlation} \\
&\overset{[ii]}{=} \text{FT of fluctuation for } k_B T \gg \hbar\omega \\
&\quad \to \text{fluctuation-dissipation relation}
\end{aligned}
$$

[i] Kubo, Toda, Hashitsume, Statistical Physics part II.

[ii] Sec. 4 of K. Koshino and A. Shimizu, Physics Reports 412 (2005) 191.

When $F \neq 0$ (NESSs),

$$\Phi_F^{AB}(\tau) = \frac{1}{i\hbar}\mathrm{Tr}\left(\hat{\rho}_F^{\mathrm{tot}}\left[\hat{B},\ \breve{A}(\tau)\right]\right) : \text{response-correlation relation}$$

$$\neq \frac{1}{k_B T}\langle \dot{\breve{B}}(0); \breve{A}(\tau)\rangle_F : \text{canonical correlation}$$

$$\not\to \text{reciprocal relations}$$

$$\not\to \text{fluctuation-dissipation relation}$$

- The response-correlation relation holds both for equilibrium states and for NESSs.
- But, it is equivalent to the Kubo formula only for the former.
- As a result, the FDR and the reciprocal relations are violated in NESSs.

General properties of $\Phi_F^{AB}(\tau)$

$$\Xi_F^{AB}(\omega) \equiv \int_0^\infty \Phi_F^{AB}(\tau) e^{i\omega\tau} d\tau$$

(i) From the causality alone (rather obvious relations)

- dispersion relations;

$$\begin{aligned} \mathrm{Re}\,\Xi_F^{AB}(\omega) &= \int_{-\infty}^{\infty} \frac{\mathcal{P}}{\omega' - \omega} \mathrm{Im}\,\Xi_F^{AB}(\omega') \frac{d\omega'}{\pi}, \\ \mathrm{Im}\,\Xi_F^{AB}(\omega) &= -\int_{-\infty}^{\infty} \frac{\mathcal{P}}{\omega' - \omega} \mathrm{Re}\,\Xi_F^{AB}(\omega') \frac{d\omega'}{\pi}. \end{aligned}$$

- moment sum rules

- etc.

These are exactly same as those for $\Xi_{\mathrm{eq}}^{AB}(\omega)$.

- **Sum rules**

$$\int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{AB}(\omega) \frac{d\omega}{\pi} = \left\langle \frac{1}{i\hbar} \left[\hat{B}, \hat{A} \right] \right\rangle_F ,$$

$$\int_{-\infty}^{\infty} \left\{ \omega\, \mathrm{Im}\, \Xi_F^{AB}(\omega) - \left\langle \frac{1}{i\hbar} \left[\hat{B}, \hat{A} \right] \right\rangle_F \right\} \frac{d\omega}{\pi} = \left\langle \frac{1}{i\hbar} \left[\hat{B}, \dot{\check{A}}(0) \right] \right\rangle_F ,$$

where

$\hat{A}$: observable of interest

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

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

$$\boxed{\text{These are generalization of those for } \Xi_{\mathrm{eq}}^{AB}(\omega).}$$

Unlike some formal relations,

– all terms can be measured experimentally.

– predictions on two or more independent experiments.

- **Asymptotic behaviors** $(|\omega| \to \infty)$
  - $\Xi_F^{AB}(\omega)$ should decay quickly s.t. the integrals of the sum rules converge.
  - In particular,

$$\lim_{\omega \to \infty} \omega \, \mathrm{Im}\, \Xi_F^{AB}(\omega) = \left\langle \frac{1}{i\hbar} \left[\hat{B}, \hat{A} \right] \right\rangle_F .$$

$$\boxed{\text{These are generalization of those for } \Xi_{\mathrm{eq}}^{AB}(\omega).}$$

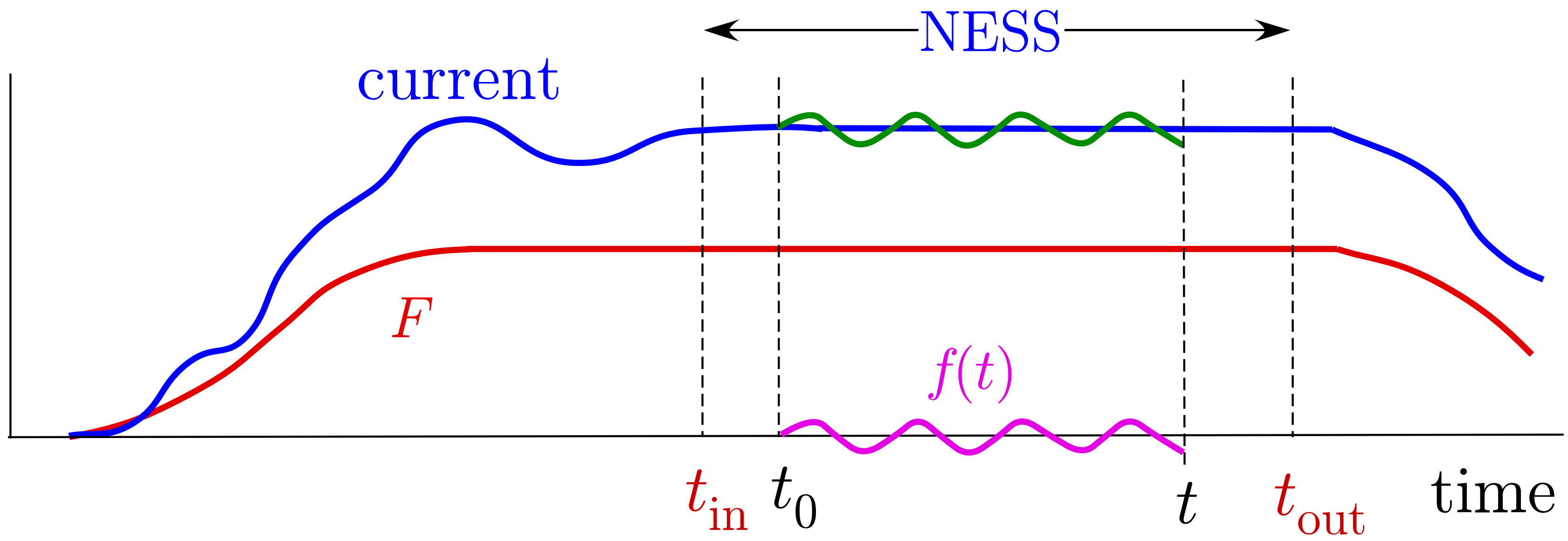
- **Reciprocal relation for the integrated values**

$$\int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{AB}(\omega) d\omega = - \int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{BA}(\omega) d\omega,$$

although reciprocal relations *for each* ω are violated for $F \neq 0$.

All of these properties are general and universal!

- No assumption except that NESSs are stable against small perturbations.



$$\forall \epsilon > 0, \exists f_\epsilon, |\Delta A| < \epsilon \text{ for } |f(t)| < f_\epsilon.$$

- Applicable to diverse physical systems.

  ex. electrical conductors, magnetic materials, dielectric materials, nonlinear optical materials, fluids, stars, biological systems, $\cdots$.

- Hold for any value of F.

Universal properties, which hold for any value of F, of response functions: The complete list

	eq. states ($F=0$)	NESSs ($F \neq 0$)
dispersion relations	Yes	Yes
moment sum rules	Yes	Yes
sum rules	Yes	Yes, if $\langle\cdot\rangle_{\mathrm{eq}} \to \langle\cdot\rangle_F$
asymptotic behaviors	Yes	Yes, if $\langle\cdot\rangle_{\mathrm{eq}} \to \langle\cdot\rangle_F$
reciprocal rels. for integrated values	Yes	Yes

Universal properties which hold only for $F=0$ (eq. states)

	eq. states ($F=0$)	NESSs ($F \neq 0$)
reciprocal relatoins for each ω	Yes	No
fluctuation-dissipation relations	Yes	No

Impossible universal properties, which hold for any value of F.

	eq. states ($F=0$)	NESSs ($F \neq 0$)
(impossible)	No	Yes

Implications of the sum rules and asymptotic behaviors

We focus on

$$\int_{-\infty}^{\infty} \mathrm{Re}\,\Xi_F^{AB}(\omega)\frac{d\omega}{\pi} = \lim_{\omega\to\infty} \omega\,\mathrm{Im}\,\Xi_F^{AB}(\omega) = \left\langle \frac{1}{i\hbar}\left[\hat{B},\hat{A}\right]\right\rangle_F .$$

Implication (1) – fundamental limits

- large positive response in some range of ω

  $\rightarrow$ small or large negative response in another range

- At high ω, response is small and independent of what you devise.

Implication (2) – operational meaning

- $\displaystyle\int_{-\infty}^{\infty} \mathrm{Re}\,\Xi_F^{AB}(\omega)\frac{d\omega}{\pi} = \Phi_F^{AB}(\tau \to +0)$: not measurable experimentally!
- $\mathrm{Re}\,\Xi_F^{AB}(\omega)$: measurable in a certain finite range of ω.
- For higher ω, $\mathrm{Re}\,\Xi_F^{AB}(\omega)$ decays quickly.

  $\rightarrow$ measurement at higher ω is not necessary.

The sum rule should be considered as a prediction on $\mathrm{Re}\,\Xi_F^{AB}(\omega)$ in a certain finite range of ω.

Implication (3) – usefulness

$$\int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{AB}(\omega) \frac{d\omega}{\pi} = \lim_{\omega\to\infty} \omega\, \mathrm{Im}\, \Xi_F^{AB}(\omega) = \left\langle \frac{1}{i\hbar} \left[\hat{B}, \hat{A}\right] \right\rangle_F$$

holds universally. So,

- Can estimate data in some range of ω from existing data in another range.
- Can detect errors in data.
- Reveal equivalence between independently-derived relations.
  (An example will be given later)
- Can check theoretical models and results against these relations.
  (Examples will be given later)

Implication (4) – the sum value (or asymptotic value)

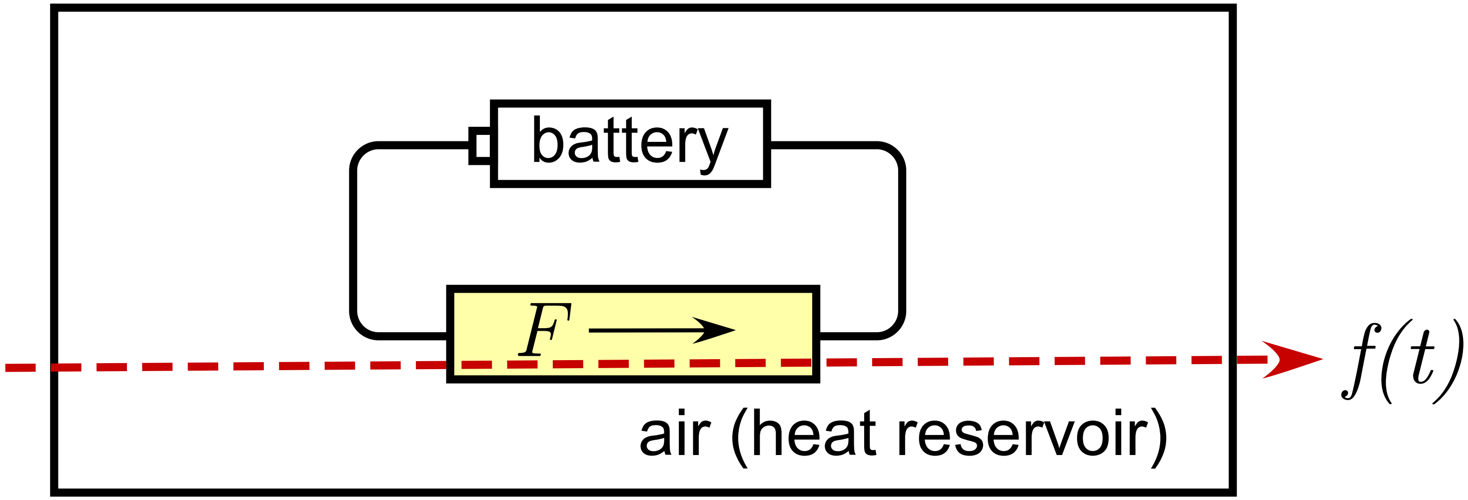
$$\int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{AB}(\omega) \frac{d\omega}{\pi} = \lim_{\omega\to\infty} \omega\, \mathrm{Im}\, \Xi_F^{AB}(\omega) = \left\langle \hat{C} \right\rangle_F, \text{ where } \hat{C} \equiv \frac{1}{i\hbar}\left[\hat{B}, \hat{A}\right].$$

- $\hat{C}$ depends neither on the Hamiltonian nor on the state.
- Only through $\hat{\rho}_F$ the sum value can be affected by these factors.
- When $\hat{A}$ and $\hat{B}$ are linear functions of canonical variables, in particular,

  $\to$ $\hat{C} \propto \hat{1}$

  $\to$ the sum takes the same value for *every* state.

Example: electrical conductor



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

$$\Delta I(t) \equiv \langle I \rangle^t_{F+f} - \langle I \rangle_F$$
$$= \int_{t_0}^{t} \Phi_F^{IB}(t-t') f(t') dt' + o(f),$$

$$\int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{IB}(\omega) \frac{d\omega}{\pi} = \lim_{\omega \to \infty} \omega\, \mathrm{Im}\, \Xi_F^{IB}(\omega)$$
$$= \frac{e^2 N_e}{mL} \quad : \text{ independent of } F\text{ !}$$

The sum rule for NESSs is rather counterintuitive

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

Low ω : $\mathrm{Re}\,\Xi_F^{IB}(\omega)$ depends strongly on F for large $|F|$.

High ω : $\mathrm{Re}\,\Xi_F^{IB}(\omega)$ would be insensitive to F.

$\rightarrow$ the integral would depend on F ?

$\rightarrow$ **No !**

An example: MD simulation of an electrical conductor

MD simulation of a model of a classical electrical conductor

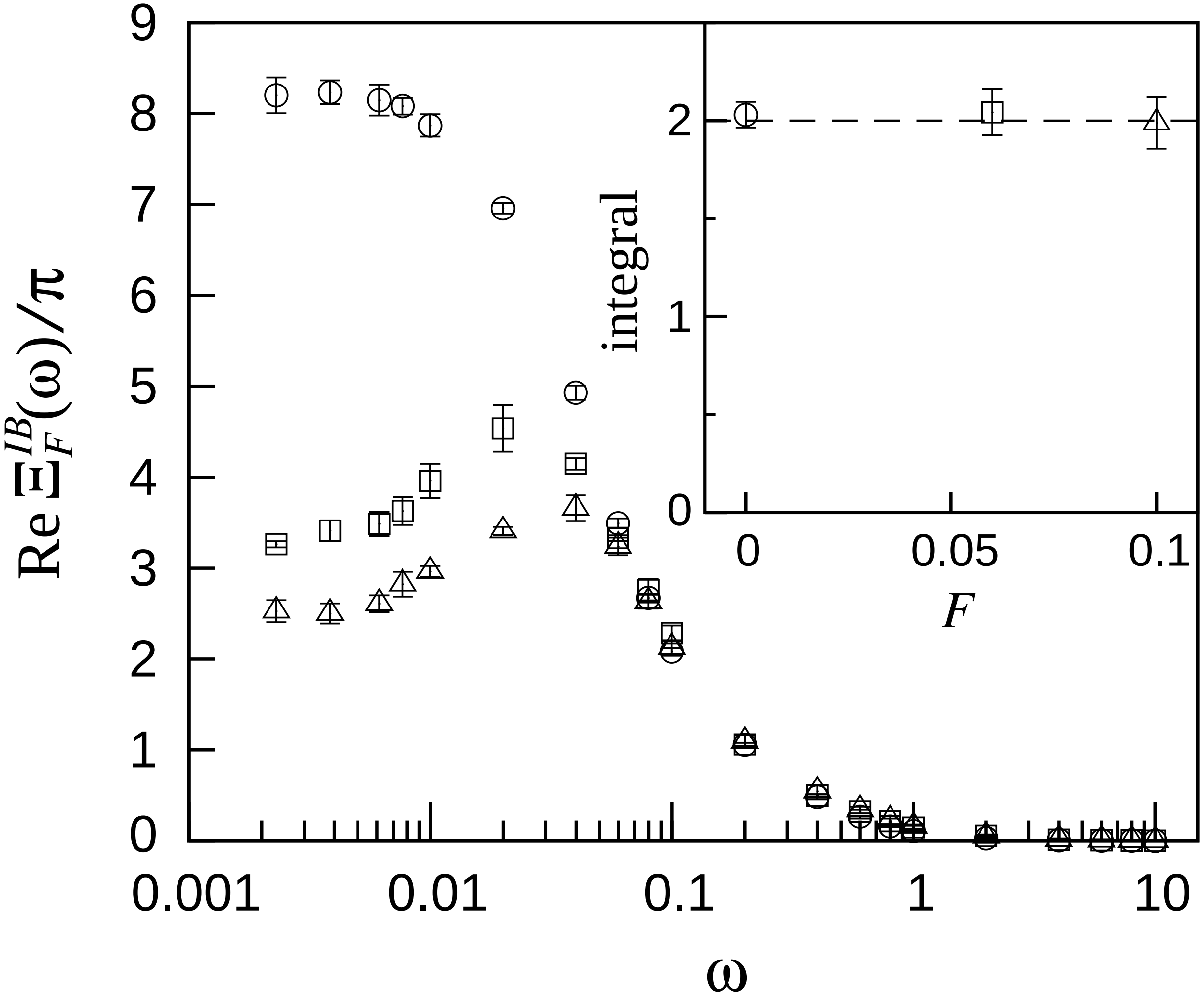
(For classical systems: commutators $\rightarrow$ Poisson brackets)

We have previously shown ...

- small F
  1. linear response [1]
  2. FDR and dispersion relations are satisfied [1]
  3. negative long-time tail $\propto 1/t^2$ [2]
- NESSs at large $|F|$
  1. nonlinear response [1]
  2. long-time tail is strongly modified [2]
  3. fluctuation-dissipation relation is violated due to reduced shot noise [3]

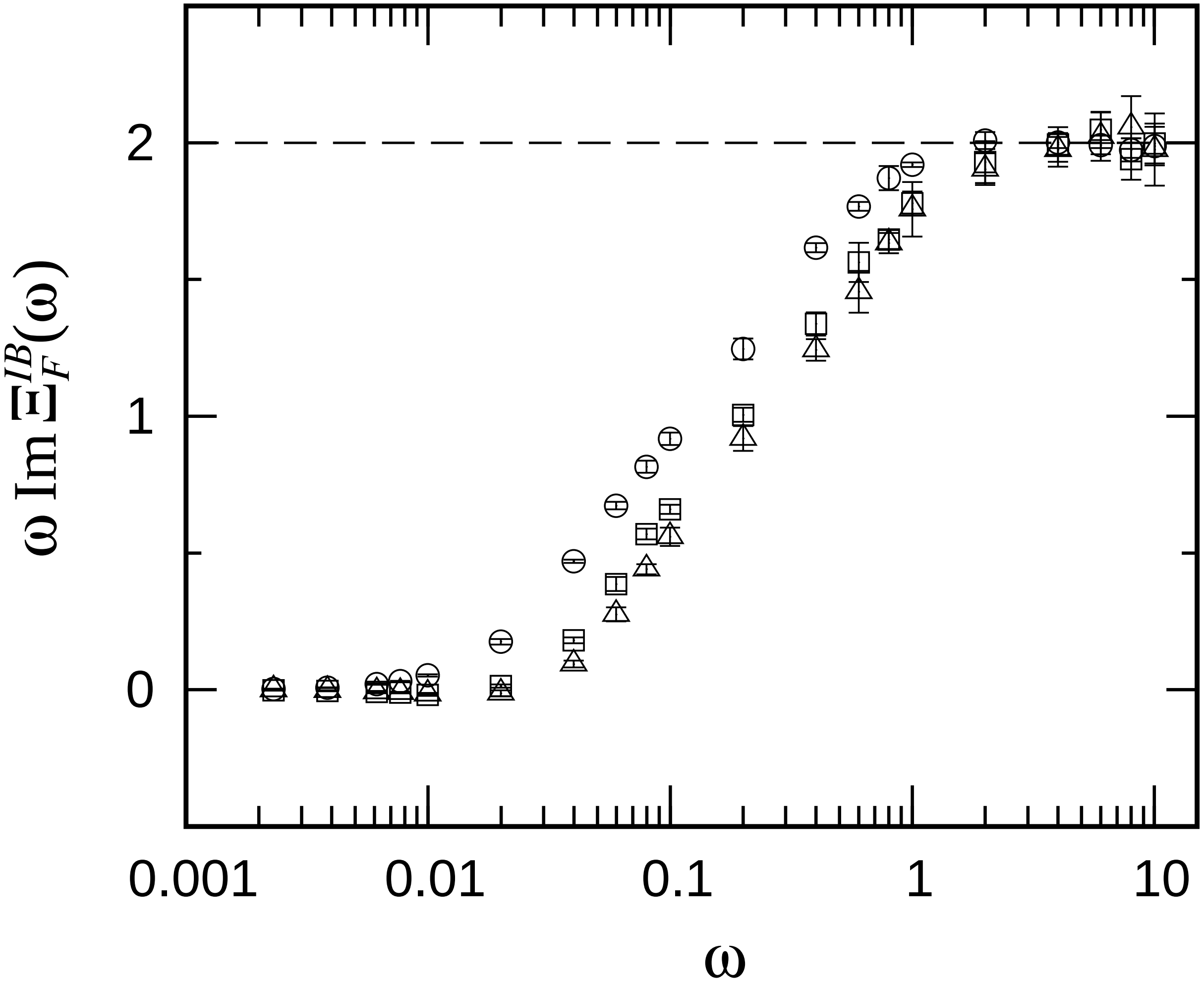
[1] T. Yuge, N. Ito and AS, J. Phys. Soc. Jpn. 74 (2005) 1895.
[2] T. Yuge and AS, J. Phys. Soc. Jpn. 76 (2007) 093001.
[3] T. Yuge and AS, J. Phys. Soc. Jpn. 78 (2009) 083001.

$$\textbf{Sum rule:} \quad \int_{-\infty}^{\infty} \mathrm{Re}\,\Xi_F^{IB}(\omega)\frac{d\omega}{\pi} = \frac{e^2 N_e}{mL} \ : \ \text{indepdendent of } F$$



$F = 0$ (circles), 0.06 (squares) and 0.1 (triangles).

Asymptotic behavior: $\displaystyle\lim_{\omega\to\infty}\omega\,\mathrm{Im}\,\Xi^{IB}_F(\omega)=\frac{e^2N_e}{mL}$: independent of F



$F=0$ (circles), 0.06 (squares) and 0.1 (triangles).

Confirmed:

- Correctness of the theoretical results.

Conversely: checked this particular model and results:

- The model is a good model.
- Our MD simulation correctly describes NESSs and their responses.

Is the sum always independent of F ?

No. It depends on the observable of interest.

Example: When $A = I^2$,

$$\int_{-\infty}^{\infty} \mathrm{Re}\, \Xi_F^{I^2 B}(\omega) \frac{d\omega}{\pi} = \lim_{\omega \to \infty} \omega\, \mathrm{Im}\, \Xi_F^{I^2 B}(\omega)$$

$$= \frac{2e^2 N_e}{mL} \langle I \rangle_F \quad : \text{strongly depends on } F \;!$$

Although the *forms* of the sum rules are similar to those for Ξ_{eq}, the sum *values* can be much different from those of Ξ_{eq}.

Do the above results hold in non-Hamiltonian systems? – Yes

All real physical systems are Hamiltonian systems
$\rightarrow$ the above results (such as the sum rule) hold

Non-Hamiltonian models (such as stochastic models) are introduded for the sake of convenience (of theoreticians).
$\rightarrow$ If modeled properly, the above results (such as the sum rule) hold.
If not hold, the model is NG.

Example: projection

Original Hamiltonian system sum rule: **yes**
$\downarrow$ projection
An equation whose γ, ξ are complicated functions sum rule: **yes**
$\downarrow$ approximations
Approx. A: underdamped Langevin eq. sum rule: **yes**
Approx. B : overdamped Langevin eq. sum rule: **no** !
Approx. C : unphysical approximation sum rule: **no** !

Our results (such as the sum rule) are something like the charge conservation

- hold in diverse physical systems
- convenient for calculations and experiments
- Sometimes very powerful

  ex. : Equivalence of identities in underdamped Langevin eq.

  Harada-Sasa (2006) $\Longleftarrow$ (identical) $\Longrightarrow$ Hasegawa et al. (1979)

$$\langle J \rangle_F = (\gamma/m)(\langle p^2 \rangle_F / m - k_B T)$$

- A necessary condition for good models and calculations

  ex.: justification of results of MD simulations

  Note: not a sufficient condition

  ex. underdamped Langevin eq. sum rule: **yes**, but good only for **small** F.

Extension to nonlinear response functions

AS, in preparation

$$\Delta A(t) \equiv \langle A \rangle^t_{F+f_1+f_2+\cdots} - \langle A \rangle_F = \sum_{n=1}^{\infty} \Delta A^{(n)}(t)$$

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

Relations similar to those for Φ_F $(= \Phi_F^{(1)})$ can be derived for $\Phi_F^{(n)}$.

ex. $n = 2$:

$$\int\int_{-\infty}^{\infty} \Xi_F^{(2)AB_{\alpha_1}B_{\alpha_2}}(\sigma_1\omega_1, \sigma_2\omega_2) \frac{d\omega_1}{\pi}\frac{d\omega_2}{\pi}$$
$$= \frac{1}{2(i\hbar)^2} \left\langle \left[\hat{B}_{\alpha_1}, \left[\hat{B}_{\alpha_2}, \hat{A} \right] \right] + (1 \leftrightarrow 2) \right\rangle_F .$$

Summary

In nonequilibrium statistical mechanics,

- quantum measurement theory
- requirement of micro-macro consistency

have been implicitly used.

In the linear nonequilibrium regime

- Where they are used.
- They actually play crucial roles.

In the nonlinear nonequilibrium regime

- The complete list of universal properties of response functions of nonequilibrium steady states (NESSs).

非平衡定常状態の応答関数の一般的性質、特に総和則と漸近的性質

- 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
  $\rightarrow$ 成立しなければ、そのモデルは要注意！
- 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
    $\rightarrow$ 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

Extension to microscopic systems

So far: NESS of macroscopic systems:

Every macroscopic observable $A =$ 'constant';

$$\frac{\text{fluctuation of } A}{\text{typical value of } A} \to 0 \quad \text{as } V \to \infty.$$

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

$$\frac{\text{fluctuation of } M_z}{\text{typical value of } M_z} = \frac{o(V)}{O(V)} \to 0.$$

We have assumed that $\hat{\rho}_F^{\mathrm{tot}}(t)$ satisfies this condition.

- Not steady microscopically, in general.
- Microscopic observables can vary (as in eq. states);

$$\langle \sigma_z(\boldsymbol{r}) \rangle \text{ evolves with } t, \text{ whereas } \langle M_z \rangle = \text{'constant'}.$$

Extension : Steady states of microscopic systems:

For every observable A (such as $\sigma_z(\boldsymbol{r})$),

$$\langle A \rangle = \text{constant}.$$

$\rightarrow$ $\hat{\rho}_F$ is independent of t.

Our results are applicable if

- Both F and $f(t)$ can be treated as external fields acting on the target system.
- Density operator $\hat{\rho}_F$ of the target system for $f = 0$ is independent of t.

What are 'macroscopic systems'?

Theory of macroscopic systems (thermodynamics, statistical mechanics, $\cdots$) is an asymptotic theory:

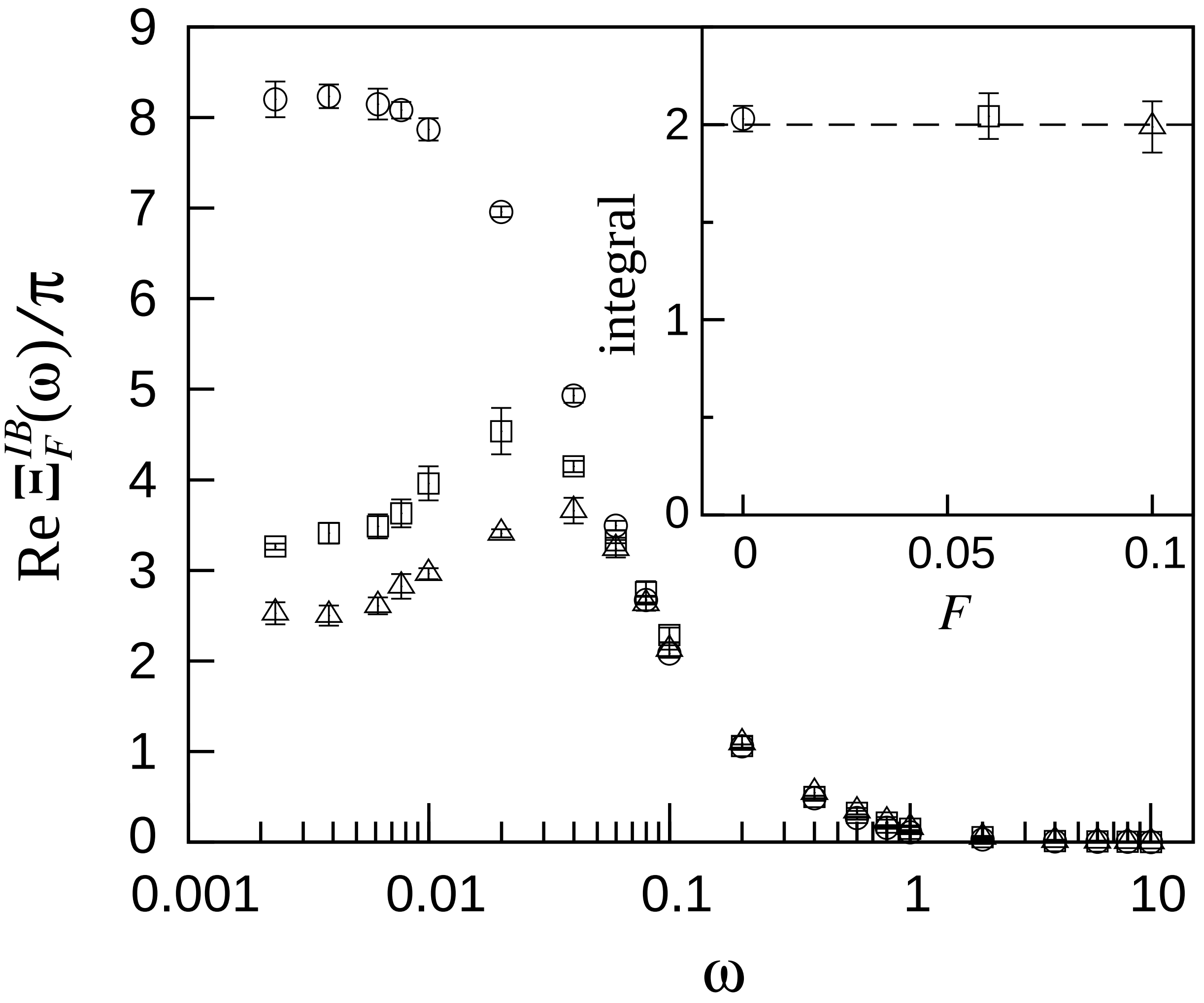
$$
\begin{aligned}
&\forall \epsilon > 0, \exists V_\epsilon \text{ such that} \\
&\big|[\text{theoretical value}] - [\text{experimental value}]\big| < \epsilon \text{ for } \forall V > V_\epsilon \\
&\text{for all intensive variables (such as the energy density).}
\end{aligned}
$$

If you require precision ϵ and if $V > V_\epsilon$, then the system is a macroscopic system (for this theory).

- If you require $\epsilon = 0.1$ and if $V > V_{0.1}$, then the system is macroscopic.
- If you require $\epsilon = 0.01$ but if $V_{0.1} < V < V_{0.01}$, then the system is *not* macroscopic.

A given system is a macroscopic system or not depending on the precision you require.

$$\textbf{Sum rule:} \quad \int_{-\infty}^{\infty} \mathrm{Re}\,\Xi_F^{IB}(\omega)\frac{d\omega}{\pi} = \int_{-\infty}^{\infty} \omega \mathrm{Re}\,\Xi_F^{IB}(\omega)\frac{d\ln\omega}{\pi} = \frac{e^2 N_e}{mL}$$



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