Quantum Violation of Fluctuation-Dissipation Theorem

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K. Fujikura and AS, Phys. Rev. Lett. **117**, 010402 (2016).
AS and K. Fujikura, J. Stat. Mech. (2017) 024004.

Fluctuation-Dissipation Theorem (FDT)

$$\begin{aligned}\text{linear response function} &= \beta \times \text{equilibrium fluctuation}\\ &= \beta \times \text{time correlation in equilibrium}\end{aligned}$$

Many *experimental evidences* for real symmetric parts of response functions (e.g., $\mathrm{Re}\,\sigma_{xx}$) in the "classical regime" $\hbar\omega \ll k_B T$.

Question : *Does the FDT really hold in other cases?*

Our answer : *No*, as relations between observed quantities.

- holds only in the above case.
- violated at all ω (including $\omega = 0$) for real antisymmetric parts (e.g., $\mathrm{Re}\,\sigma_{xy}$).

Motivation

Nothing moves in Gibbs states.

In the thermal pure quantum states, macrovariables do not move, whereas microvariables move.

To calculate fluctuation of macrovariables, we must calculate time correlation.

But, when we look at an equilibrium state, macrovariables do move (fluctuate).

My question: What is the quantum state in which macrovariables fluctuate?

Kyota Fujikura (M1 at that time) got interested in this question.
$\Rightarrow$ He constructed a 'squeezed equilibrium state' (shown later).

Such a state should be found, e.g., just after measurement.

My question: Is it a universal result?

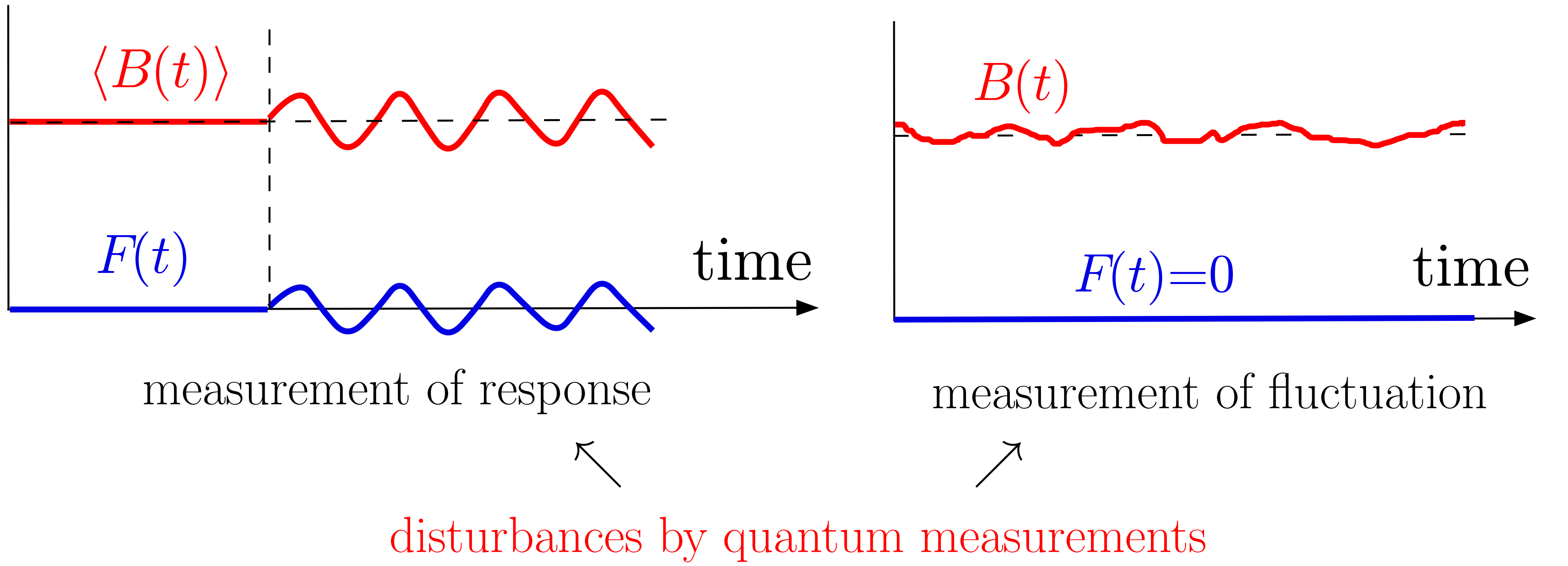
He answered yes.
$\Rightarrow$ I was upset because I realized it implies universal violation of FDT!
$\Rightarrow$ Detailed analysis.

Contents

What's wrong with derivations of the FDT?

H. Takahashi (J. Phys. Soc. Jpn. 7, 439 (1952))

- derived the FDT for classical systems.
- About its translation to quantum systems:
  "*profound difficulty that every observation disturbs the system.*"



What's wrong with derivations of the FDT? (continnued)

Callen and Welton (1951) and Kubo (1957)

- "Derived" the FDT for quantum systems from the Schrödinger equation.
- Neglected the disturbances by measurements.

Nevertheless, 'Kubo formula' is often regarded as a proof of the FDT.

Kubo: linear response function $=$ $\beta \times$ canonical time correlation*

disturbance → ||? disturbance → ||?

FDT: linear response function $=$ $\beta \times$ time correlation in equilibrium

observed one observed one

* canonical time correlation:

$$\langle \hat{X} ; \hat{Y}(t) \rangle_{\rm eq} \equiv \frac{1}{\beta} \int_0^\beta \langle e^{\lambda \hat{H}} \hat{X} e^{-\lambda \hat{H}} \hat{Y}(t) \rangle_{\rm eq} d\lambda$$

What's wrong with derivations of the FDT? (continnued)

Question: Are macrovariables so affected by quantum disturbance?

Our answer:

- No, when response is measured.

  $\Rightarrow$ Kubo formula may be correct as a recipe to obtain response functions.

- Yes, when fluctuarion is measured.

  $\Rightarrow$ canonical time correlation $\neq$ observed time correlation.

Kubo: linear response function $=$ $\beta \times$ canonical time correlation

disturbance $\not\to$ $\|$ disturbance $\to$ $\nparallel$

FDT: linear response function $\neq$ $\beta \times$ time correlation in equilibrium

observed one observed one

FDT is violated as relations between observed quantities.

Contents

Assumptions on the system and its equilibrium states

$\boldsymbol{d}$-dimensional macroscopic system ($d = 1, 2, 3, \cdots$) of size $\boldsymbol{N}$ (e.g., # of spins)

- **Equilibrium state** of temperature $\boldsymbol{T}$ $(= 1/\beta)$

  thermal pure quantum state $|\boldsymbol{\beta}\rangle$ (same results as the Gibbs state)

  S. Sugiura ans AS, PRL **108**, 240401 (2012); PRL **111**, 010401 (2013).

  $\langle \cdot \rangle_{\mathrm{eq}} = \langle \beta | \cdot | \beta \rangle$

- **Assumption**

  Correlation between local observables decays faster than $1/r^{d+\epsilon}$ $(\epsilon > 0)$.

  ♣ holds generally, except at citical points.

  $\Rightarrow$ For all **additive observable** $\hat{A}$ $(= \sum_{\boldsymbol{r}}$ same local observable$)$,

$$\boldsymbol{\delta A}_{\mathrm{eq}} \equiv \sqrt{\langle (\Delta \hat{A})^2 \rangle_{\mathrm{eq}}} = O(\sqrt{N}).$$

  $\Delta \hat{A} \equiv \hat{A} - \langle \hat{A} \rangle_{\mathrm{eq}}$; throughout this talk $\boldsymbol{\Delta}$ denotes deviation from the equilibrium value.

- **Additional reasonable assumptions**

  $\Rightarrow$ **Q**uantum **C**entral **L**imit **T**heorem (D. Goderis and P. Vets (1989); T. Matsui (2002).)

  ♣ We do not write $\displaystyle\lim_{N \propto V \to \infty}$ explicitly, except when we want to stress it.

Contents

Assumptions on measurements

If a violent detector,

$\Rightarrow$ completely destroys the state by the 1st measurement

$\Rightarrow$ meaningless result for the 2nd measurement

$\Rightarrow$ wrong result for the correlation

To measure the time correlation correctly, "ideal" detectors should be used.

Classical systems

ideal detector $\equiv$ a detector that does not disturb the state at all.

Quantum systems

Such a detector is impossible!

$\Rightarrow$ Use a detector that simulates the classical ideal one as closely as possible.
"quasiclassical measurement"

To examine the validity of the FDT in quantum systems, we must assume quasiclassical measurements.

Assumptions on measurements (continued)

quasiclassical measurement should have a moderate magnitude of error:

- $\delta A_{\rm err} < \delta A_{\rm eq}$.
- $\delta A_{\rm err} \searrow \Rightarrow$ disturbance $\nearrow \;\Rightarrow\;$ $\delta A_{\rm err}$ should not be too small.

We require

$$\delta A_{\rm err} = \varepsilon \delta A_{\rm eq} \quad (\varepsilon : \text{ a small positive onstant}).$$

♣ Our results hold also for larger ε.

Since $\delta A_{\rm eq} = O(\sqrt{N})$,

$$\delta A_{\rm err} = O(\sqrt{N}).$$

To formulate measurements of equilibrium fluctuations, use

$$\hat{a} = \hat{A}/\sqrt{N}$$

$$\Rightarrow \;\; \delta a_{\rm eq} = O(1), \delta a_{\rm err} = O(1).$$

Assumptions on measurements (continued)

General framework of quantum measurement (adapted to our problem)

Pre-measurement state $= |\psi\rangle$ (uniform macroscopically)

Measurement of an additive observable $\hat{A} \to$ outcome $A_\bullet$ (real valued variable)

♣ $\delta A_{\rm err} > 0 \;\; \Rightarrow \;\; A_\bullet$ is not necessarily one of eigenvalues.

♣ $a_\bullet \equiv A_\bullet/\sqrt{N}$ can be regarded as a continuous variable.

Probability density of getting $a_\bullet$:

$$p(a_\bullet) = \langle \psi | \hat{E}_{a_\bullet} | \psi \rangle$$

$\hat{E}_{a_\bullet}$: probability operator (Hermitian, positive semidefinite, integral $= \hat{1}$)

$\hat{E}_{a_\bullet}$ can be decomposed as

$$\hat{E}_{a_\bullet} = \hat{M}^\dagger_{a_\bullet} \hat{M}_{a_\bullet}$$

$\hat{M}_{a_\bullet}$: measurement operator (not unique for a given $\hat{E}_{a_\bullet}$)

Post-measurement state $= \dfrac{1}{\sqrt{p(a_\bullet)}} \hat{M}_{a_\bullet} |\psi\rangle$

Assumptions on measurements (continued)

$$a_\bullet : \text{ outcome}, \quad p(a_\bullet) = \langle \psi | \hat{E}_{a_\bullet} | \psi \rangle, \quad \hat{E}_{a_\bullet} = \hat{M}^\dagger_{a_\bullet} \hat{M}_{a_\bullet}$$

Definiton: quasiclassical measurement of additive observables

(i) *unbiased* : $\overline{a_\bullet} = \langle \hat{a} \rangle_{\text{eq}}$ $\quad$ ($\overline{\cdots}$ = average over many runs of experiments)

$\because$ Otherwise, the FDT would look more violated.

(ii) For $|\beta\rangle$, $p_{\text{shifted}}(\Delta a_\bullet) \equiv p(a_\bullet)$ *converges* as $N \to \infty$.

$\Rightarrow$ e.g., measurement error $\delta A_{\text{err}} = \varepsilon \delta A_{\text{eq}}$, as required.

(iii) $\hat{M}_{a_\bullet}$ is *minimally disturbing* among $\hat{E}_{a_\bullet} = \hat{M}^\dagger_{a_\bullet} \hat{M}_{a_\bullet} = \hat{N}^\dagger_{a_\bullet} \hat{N}_{a_\bullet} = \cdots$.

$\Rightarrow$ $\hat{M}_{a_\bullet} = \sqrt{\hat{E}_{a_\bullet}}$

(iv) *homogeneous*, i.e., $\hat{E}_{a_\bullet}$ depends on $\hat{a}$ and $a_\bullet$ only through $\hat{a} - a_\bullet$.

$\Rightarrow$ e.g., δa_{err} = independent of $a_\bullet$.

From (i)-(iv), $\hat{M}_{a_\bullet} = f(\hat{a} - a_\bullet)$, where $f(x) \geq 0$.

(v) $f(x)$ *behaves well enough.*

e.g., it vanishes quickly as $|x| \to \infty$ (see paper for details)

Assumptions on measurements (continued)

Roughly speaking, quasiclassical measeurment is

- unbiased
- homogeneous
- minimally-disturbing
- moderate magnitudes of error (small enough to measure fluctuations, but not too small in order to avoid strong disturbances.)

ex. Gaussian measurement operator

$$f(x) = \frac{1}{(2\pi w^2)^{1/4}} \exp\left(-\frac{x^2}{4w^2}\right), \quad w = O(1) > 0.$$

$$\hat{M}_{a_\bullet} = f(\hat{a} - a_\bullet) = \frac{1}{(2\pi w^2)^{1/4}} \exp\left[-\frac{(\hat{a} - a_\bullet)^2}{4w^2}\right],$$

$$\delta a_{\mathrm{err}} = w = O(1) \qquad (\delta A_{\mathrm{err}} = w\sqrt{N} = O(\sqrt{N})).$$

Contents

Measurement of time correlation

$t = 0^-$: equilibrium state $= |\beta\rangle$ (thermal pure quantum state)

$\downarrow$

$t = 0$: measurement of $\hat{A} = \hat{a}\sqrt{N}$ $\Rightarrow$ outcome $A_\bullet = a_\bullet\sqrt{N}$

post-measurement state $= |\beta; a_\bullet\rangle = \dfrac{1}{\sqrt{p(a_\bullet)}} f(\hat{a} - a_\bullet)|\beta\rangle$

$\downarrow$ free evolution

$t > 0$: $e^{-i\hat{H}t/\hbar}|\beta; a_\bullet\rangle$

measurement of $\hat{A}$ (or another additive operator $\hat{B}$) $\Rightarrow$ outcome

$\Downarrow$ From the two outcomes ....

Obtain : correlation of $\hat{A}(0)$ and $\hat{A}(t)$ (or $\hat{B}(t)$)

- 1st measurement should be quasiclassical (to minimize disturbance)
- 2nd measurement can be either quasiclassical or error-less.
  (Because its post-measurement state will not be measured.)

Post-measurement state of 1st measurement

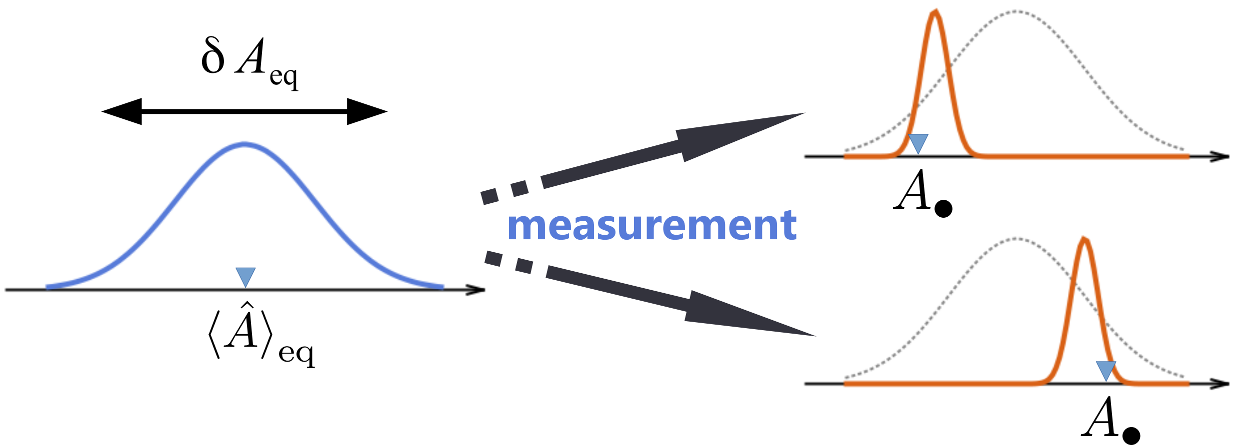
$t = 0$: measurement of $\hat{A} = \hat{a}\sqrt{N}$ $\Rightarrow$ outcome $A_\bullet = a_\bullet\sqrt{N}$

▶ post-measurement state $= |\beta; a_\bullet\rangle = \dfrac{1}{\sqrt{p(a_\bullet)}} f(\hat{a} - a_\bullet)|\beta\rangle$

Gaussian f $\quad \langle \cdot \rangle_{a_\bullet} \equiv \langle \beta; a_\bullet | \cdot | \beta; a_\bullet \rangle$, $\delta a_{\text{eq}}^2 \equiv \delta A_{\text{eq}}/\sqrt{N}$, $\Delta a_\bullet \equiv a_\bullet - \langle \hat{a} \rangle_{\text{eq}}$.

$$\langle \hat{a} \rangle_{a_\bullet} - \langle \hat{a} \rangle_{\text{eq}} = \frac{\delta a_{\text{eq}}^2}{\delta a_{\text{eq}}^2 + \delta a_{\text{err}}^2} \Delta a_\bullet \quad : \text{ shifted toward the outcome}$$

$$\langle (\hat{a} - \langle \hat{a} \rangle_{a_\bullet})^2 \rangle_{a_\bullet} = \left[1 - \frac{\delta a_{\text{eq}}^2}{\delta a_{\text{eq}}^2 + \delta a_{\text{err}}^2} \right] \delta a_{\text{eq}}^2 \quad : \text{ squeezed along } \hat{a}$$



Post-measurement state of 1st measurement (continued)

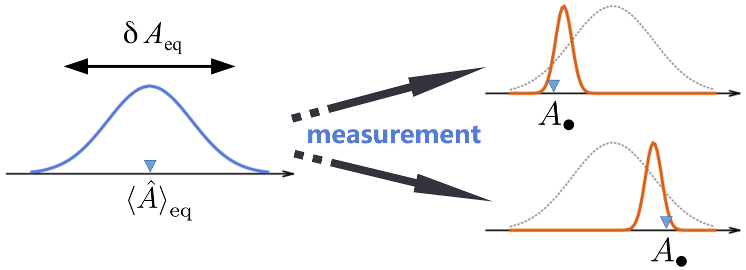
For another additive operator $\hat{B} = \hat{b}\sqrt{N}$,

$$\langle(\hat{b} - \langle\hat{b}\rangle_{a_\bullet})^2\rangle_{a_\bullet} = \delta b_{\rm eq}^2 - \frac{\langle\frac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}\}\rangle_{\rm eq}^2}{\delta a_{\rm eq}^2 + \delta a_{\rm err}^2} + \frac{\langle\frac{1}{2i}[\hat{a}, \hat{b}]\rangle_{\rm eq}^2}{\delta a_{\rm err}^2}$$

squeezing — squeezing is disturbed

All the above quantities are O(equilibrium fluctuations)

$\Rightarrow$ $|\beta; a_\bullet\rangle$ is *macroscopically* identical to $|\beta\rangle$ (equilibrium state).



"We are macroscopically identical to $|\beta\rangle$."

squeezed equilibrium state

<u>general f</u>

Similar results, which depend on f. (see K. Fujikura and AS, 2016)

- Disturbances on additive operators $\hat{A}, \hat{B}, \ldots$ by quasiclassical measurements are $O(\sqrt{N})$.
- The post-measurement state $|\beta; a_\bullet\rangle$ is a 'squeezed equilibrium state'.

2nd measurement

$t = 0$: measurement of $\hat{A} = \hat{a}\sqrt{N}$ $\Rightarrow$ outcome $A_\bullet = a_\bullet\sqrt{N}$

post-measurement state $= |\beta; a_\bullet\rangle$

$\downarrow$ free evolution

$t > 0$: $e^{-i\hat{H}t/\hbar}|\beta; a_\bullet\rangle$

▶ measurement of $\hat{A}$ (or another additive operator $\hat{B}$) $\Rightarrow$ outcome

Gaussian f

For any additive observable $\hat{B} = \hat{b}\sqrt{N}$,

$$\langle \Delta\hat{b}(t)\rangle_{a_\bullet} = \Theta(t)\langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\rm eq} \frac{\Delta a_\bullet}{\delta a_{\rm eq}^2 + \delta a_{\rm err}^2}$$

Here,

$$\Theta(t) = \text{step function (vanishes for } t < 0)$$

$$\langle \tfrac{1}{2}\{\hat{X}, \hat{Y}(t)\}\rangle_{\rm eq} \equiv \langle \tfrac{1}{2}(\hat{X}\hat{Y}(t) + \hat{Y}(t)\hat{X})\rangle_{\rm eq} : \text{symmetrized time correlation}$$

general f

$$\langle \Delta\hat{b}(t)\rangle_{a_\bullet} = \Theta(t)\langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\rm eq} \cdot \left(-\frac{p'(a_\bullet)}{p(a_\bullet)}\right) \quad : \text{depends on } f$$

Obtained time correlation

$t = 0$: measurement of $\hat{A} = \hat{a}\sqrt{N}$ $\Rightarrow$ outcome $A_\bullet = a_\bullet\sqrt{N}$

$\downarrow$ free evolution

$t > 0$: measurement of $\hat{B}$ $\Rightarrow$ $\langle$outcome$\rangle = \langle \hat{b}(t) \rangle_{a_\bullet}$

$\Downarrow$ From the two outcomes ....

▶ Obtain : correlation of $\hat{A}(0)$ and $\hat{B}(t)$

Correlation between $\Delta a_\bullet$ and $\langle \Delta\hat{b}(t) \rangle_{a_\bullet}$:

$$\text{For } t \geq 0, \quad \Xi_{ba}(t) \equiv \overline{\Delta a_\bullet \langle \Delta\hat{b}(t) \rangle_{a_\bullet}}$$

$$= \int \Delta a_\bullet \langle \Delta\hat{b}(t) \rangle_{a_\bullet} \, p(a_\bullet) da_\bullet$$

$$= \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\} \rangle_{\rm eq} \int \Delta a_\bullet \cdot \left[-p'(a_\bullet)\right] da_\bullet$$

$$= \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\} \rangle_{\rm eq} \int p(a_\bullet) da_\bullet$$

$$= \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\} \rangle_{\rm eq} \quad \text{for all } f.$$

Obtained time correlation (continued)

Universal result:

$$\text{For } t \geq 0, \quad \Xi_{ba}(t) = \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\mathrm{eq}} \quad \text{for all } f$$

If we combine the case where the role of $\hat{A}$ and $\hat{B}$ is interchanged,

$$\begin{aligned}\tilde{\Xi}_{ba}(t) &\equiv \text{correlation of } \hat{a} \text{ and } \hat{b}(t) \\ &= \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\mathrm{eq}} \quad \text{for all } t \text{ and all } f.\end{aligned}$$

♣ Throughout this talk, " ˜ " denotes some extension to all t.

When equilibrium fluctuations of macrovariables are measured in an ideal way that simulates classical ideal measurements as closely as possible, the symmetrized time correlation is always obtained (among many quantum correlations that reduce to the same classical correlation as $\hbar \to 0$).

Contents

Violation of FDT

Linear response of an additive observable $\hat{B}$ to an external field $F(t)$:

$$\frac{\langle \hat{B} \rangle_t}{N} - \frac{\langle \hat{B} \rangle_{\rm eq}}{N} = \int_{-\infty}^{t} \Phi_{ba}(t-t') F(t') dt' \quad (\Phi_{ba}(t) : \text{response function}).$$

When $F(t)$ interacts the system via

$$\hat{H}_{\rm ext}(t) = -F(t)\hat{C} \quad (\hat{C} : \text{an additive observable of the system}),$$

Kubo (1957) showed

$$\text{Kubo formula :} \quad \Phi_{ba}(t) = \Theta(t) \lim_{N \propto V \to \infty} \beta \langle \Delta \hat{a}; \Delta \hat{b}(t) \rangle_{\rm eq}$$

$$\Theta(t) \equiv \text{step function} \quad \Leftarrow \text{causality}$$

$$\hat{a} \equiv \hat{A}/\sqrt{N}, \ \hat{b} \equiv \hat{B}/\sqrt{N}$$

$$\hat{A} \equiv \frac{d}{dt}\hat{C}(t)\Big|_{t=0} = \frac{1}{i\hbar}[\hat{C}, \hat{H}] \quad : \text{velocity of } \hat{C},$$

$$\langle \hat{X}; \hat{Y}(t) \rangle_{\rm eq} \equiv \frac{1}{\beta} \int_0^{\beta} \langle e^{\lambda \hat{H}} \hat{X}^\dagger e^{-\lambda \hat{H}} \hat{Y}(t) \rangle_{\rm eq} d\lambda \quad : \text{canonical time correlation.}$$

Violation of FDT (continued)

Kubo formula : $\Phi_{ba}(t) = \Theta(t) \lim_{N \propto V \to \infty} \beta \langle \Delta \hat{a}; \Delta \hat{b}(t) \rangle_{\text{eq}}$

Some necessary conditions :

- $\hat{H}$ should be taken in such a way that $\lim_{N \propto V \to \infty} \langle \Delta \hat{a}; \Delta \hat{b}(t) \rangle_{\text{eq}}$ converges.
- $\lim_{t \to \infty} \lim_{N \propto V \to \infty} \langle \Delta \hat{a}; \Delta \hat{b}(t) \rangle_{\text{eq}} = 0.$
- This implies, e.g., $[\hat{A}, \hat{H}] \neq 0$ and $[\hat{B}, \hat{H}] \neq 0$.
- Consistency with equilibrium statistical mechanics:

$$\lim_{\epsilon \searrow 0} \lim_{N \propto V \to \infty} \epsilon \int_0^\infty \langle \hat{C}/N; \hat{B}(t)/N \rangle_{\text{eq}} e^{-\epsilon t} dt = \lim_{N \propto V \to \infty} \langle \hat{C}/N \rangle_{\text{eq}} \langle \hat{B}/N \rangle_{\text{eq}}.$$

A consequence: In general, Kubo formula is *inapplicable* to integrable systems.

We henceforth assume that the above conditions are all satisfied.

♣ Do not write $\lim_{N \propto V \to \infty}$ and $\lim_{\epsilon \searrow 0}$ explicitly, except when we want to stress it.

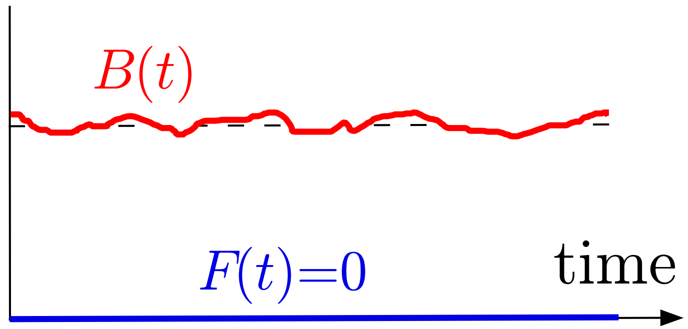
Violation of FDT (continued)

Kubo neglected disturbances by measurements.

Our results: Even if measurements are "ideal" (i.e., quasiclassical),

$$\text{disturbances on additive observables} = O(\sqrt{N}).$$

Measurement of temporal fluctuation :



$$\langle \Delta\hat{a}; \Delta\hat{b}(t)\rangle_{\rm eq} \qquad (\hat{a} = \hat{A}/\sqrt{N},\ \hat{b}(t) = \hat{B}(t)/\sqrt{N})$$

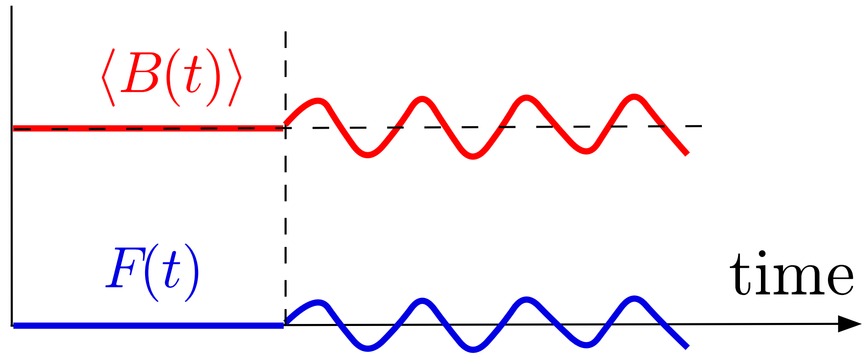
$$\text{disturbances on } \Delta\hat{a} \text{ and } \Delta\hat{b} = O(\sqrt{N})/\sqrt{N} = O(1).$$

> For measurements of temporal fluctuations, disturbances are significant.

In fact, observed time correlation $= \langle \frac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\rm eq} \neq \langle \Delta\hat{a}; \Delta\hat{b}(t)\rangle_{\rm eq}$.

Violation of FDT (continued)

Measurement of response function :



$$\frac{\langle \hat{B} \rangle_t}{N} - \frac{\langle \hat{B} \rangle_{\rm eq}}{N} = \int_{-\infty}^{t} \Phi_{ba}(t-t')F(t')dt'$$

There is a method with which disturbances are completely irrelevant.
But, in ordinary experiments, one will perform *multi-time* measurements.
Do they agree with each other?

$$\text{disturbance on } \hat{B}/N = O(\sqrt{N})/N = O(1/\sqrt{N}) \to 0.$$

For measurements of response functions, disturbances are negligible.

$\Rightarrow$ The result agrees with that of the disturbance-irrelevant method.

Violation of FDT (continued)

$$\begin{array}{rcl}
\textsf{Kubo:} \quad \Phi_{ba}(t) & = & \Theta(t)\beta\langle\Delta\hat{a};\Delta\hat{b}(t)\rangle_{\rm eq} \\
\text{disturbance} \not\to \quad \| & & \nparallel \leftarrow \text{disturbance} \\
\textsf{FDT:} \quad \Phi_{ba}(t) & \neq & \beta \times \text{time correlation in equilibrium}
\end{array}$$

- Kubo formula may be correct* as a recipe to obtain Φ_{ba}.
- But, observed time correlation $= \langle \frac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\rm eq} \neq \langle\Delta\hat{a};\Delta\hat{b}(t)\rangle_{\rm eq}$.

FDT is violated as relations between observed quantities.

* For other possible problems of Kubo formula, see, e.g., AS and H. Kato, Springer Lecture Notes in Physics, 54 (2000) pp.3-22. arXiv:cond-mat/9911333.

But, many experiments have confirmed FDT...?
To resolve this point, we must analyze FDT in the frequency domain!

Violation of FDT at ω

In experiments, one normally measures (generalized) admittance :

$$\chi_{ba}(\omega) \equiv \int_{\mathbf{0}}^{\infty} \Phi_{ba}(t)\, e^{i\omega t} dt$$
$$= \int_{\mathbf{0}}^{\infty} \beta \langle \Delta\hat{a}; \Delta\hat{b}(t) \rangle_{\text{eq}}\, e^{i\omega t} dt.$$

The lower limit of integration comes from

$$\text{causality :} \quad \Phi_{ba}(t) = 0 \ \text{ for } t < 0.$$

This is crucial because

$$\tilde{\chi}_{ba}(\omega) \equiv \int_{-\infty}^{\infty} \beta \langle \Delta\hat{a}; \Delta\hat{b}(t) \rangle_{\text{eq}}\, e^{i\omega t} dt$$

contradicts with experiments:

- $\mathrm{Re}\, \epsilon(\omega) \equiv \epsilon_0$??? $\Rightarrow$ No dielectric material???
- $\mathrm{Im}\, \sigma(\omega) \equiv 0$??? $\Rightarrow$ No phase shift???

♣ Unfortunately, FDT is sometimes stated in terms of $\tilde{\chi}$ in the literature.

Violation of FDT at $\boldsymbol{\omega}$ (continued)

Fourier transform of time correlation:

$$S_{ba}(\omega) \equiv \int_{\mathbf{0}}^{\infty} \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\rm eq}, \; e^{i\omega t} dt$$

$$\tilde{S}_{ba}(\omega) \equiv \int_{-\infty}^{\infty} \langle \tfrac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\rm eq} \, e^{i\omega t} dt.$$

Both are measurable.

$\Rightarrow$ Which should be compared with the observed admittance $\chi_{ba}(\omega)$?

In the classical limit $\hbar \to 0$, we will show

$\chi_{ba}(\omega) = \beta S_{ba}(\omega)$ holds for all ω,

$\chi_{ba}(\omega) = \beta \tilde{S}_{ba}(\omega)$ violated partially even at $\omega = 0$

= superficial violation coming from inappropriate comparison!

FDT in this talk

Relation between the observed admittance and observed fluctuation,

$$\chi_{ba}(\omega) = \beta S_{ba}(\omega).$$

We will inspect whether it holds in quantum systems.

Violation of FDT at ω (continued)

symmetric/antisymmetric parts

$\chi_{ba}(\omega)$ = response of $\hat{B}$ to $Fe^{-i\omega t}$ that couples to $\hat{C}$ (where $\hat{A} = d\hat{C}/dt$).
$\chi_{ab}(\omega)$ = response of $\hat{A}$ to $Fe^{-i\omega t}$ that couples to $\hat{D}$ (where $\hat{B} = d\hat{D}/dt$).

If the system has the time-reversal symmetry,

$$\chi_{ba}(\omega) = \epsilon_a \epsilon_b \chi_{ab}(\omega) \;:\; \text{reciprocal relation}$$

ϵ_a, ϵ_b : parities ($= \pm 1$) of $\hat{a}$ and $\hat{b}$ under the time reversal.

To make this symmetry manifest, we introduce

$$\chi_{ba}{}^{\pm}(\omega) \equiv [\chi_{ba}(\omega) \pm \chi_{ab}(\omega)]/2,$$

called symmetric/antisymmetric parts.

> If the system has the time-reversal symmetry (i.e., if magnetic field $\boldsymbol{h} = \mathbf{0}$),
> *either one of* $\chi_{ba}^{\pm}(\omega)$ *vanishes for all* ω, depending on the sign of $\epsilon_a \epsilon_b$.

ex. Hall conductivity $\sigma_{xy}(\omega)$ vanishes when $\boldsymbol{h} = \mathbf{0}$.

Violation of FDT at $\boldsymbol{\omega}$ (continued)

Similarly, we define

$$S^{\pm}_{ba}(\omega) \equiv [S_{ba}(\omega) \pm S_{ab}(\omega)]/2,$$
$$\tilde{S}^{\pm}_{ba}(\omega) \equiv [\tilde{S}_{ba}(\omega) \pm \tilde{S}_{ab}(\omega)]/2.$$

Then we can show ....

Violation of FDT at ω (continued)

Relation between observed admittance and observed fluctuation

$$\mathrm{Re}\,\chi^{+}_{ba}(\omega) = \beta\,\mathrm{Re}\,S^{+}_{ba}(\omega)/I_\beta(\omega),$$

$$\mathrm{Re}\,\chi^{-}_{ba}(\omega) = \beta\,\mathrm{Re}\,S^{-}_{ba}(\omega) + \beta\int_{-\infty}^{\infty}\frac{\mathcal{P}}{\omega'-\omega}\left[1-\frac{1}{I_\beta(\omega')}\right] i\tilde{S}^{-}_{ba}(\omega')\,\frac{d\omega'}{2\pi},$$

and similarly for the imaginary parts.

$$I_\beta(\omega) \equiv \frac{\beta\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right) \sim \begin{cases} 1 & (\hbar\omega \ll k_{\mathrm{B}}T) \\ \beta\hbar\omega/2 & (\hbar\omega \gg k_{\mathrm{B}}T) \end{cases}$$

Does FDT $\chi^{\pm}_{ba}(\omega) = \beta S^{\pm}_{ba}(\omega)$ hold?

For real symmetric part $\mathrm{Re}\,\chi^{+}_{ba}(\omega)$

- holds in the 'classical regime' $\hbar\omega \ll k_{\mathrm{B}}T$.
- violated for $\hbar\omega \gtrsim k_{\mathrm{B}}T$.

For real antisymmetric part $\mathrm{Re}\,\chi^{-}_{ba}(\omega)$

- violated at all ω, even in the classical regime $\hbar\omega \ll k_{\mathrm{B}}T$.

Violation of FDT at $\boldsymbol{\omega}$ (continued)

Example: electrical conductivity tensor in $\boldsymbol{B} = (0, 0, B)$.

$$\sigma_{\mu\nu}(\omega) = \int_0^\infty \langle \hat{j}_\nu ; \hat{j}_\mu(t) \rangle_{\text{eq}} \, e^{i\omega t} dt \quad : \text{observed conductivity (admittance)}$$

$$S_{\mu\nu}(\omega) = \int_0^\infty \langle \tfrac{1}{2} \{ \hat{j}_\nu , \hat{j}_\mu(t) \} \rangle_{\text{eq}} \, e^{i\omega t} dt \quad : \text{observed fluctuation}$$

Symmetric part (= diagonal conductivity)

$$\mathrm{Re}\, \sigma_{xx}(\omega) = \beta \frac{\mathrm{Re}\, S_{xx}(\omega)}{I_\beta(\omega)} = \begin{cases} \beta\, \mathrm{Re}\, S_{xx}(\omega) & (\hbar\omega \ll k_{\mathrm{B}} T) : \text{ FDT holds} \\ \dfrac{2}{\hbar\omega} \mathrm{Re}\, S_{xx}(\omega) & (\hbar\omega \gg k_{\mathrm{B}} T) : \text{ violated} \end{cases}$$

($\simeq$ Callen and Welton (1951))

Antisymmetric part (= Hall conductivity)

FDT is violated at all ω, even at $\omega = 0$ because

$$\sigma_{xy}(0) = \beta S_{xy}(0) + \beta \int_{-\infty}^{\infty} \frac{\mathcal{P}}{\omega'} \left[1 - \frac{1}{I_\beta(\omega')} \right] i \tilde{S}_{xy}(\omega') \frac{d\omega'}{2\pi} \quad : \text{ violated}$$

odd   even   odd

Contents

Experiments on violation

For $\mathrm{Re}\,\boldsymbol{\sigma_{xx}(\omega)}$ at $\boldsymbol{\hbar\omega \ll k_{\mathrm{B}}T}$

our result (taking account of disturbance by quasiclassical measurement)
= previous results for quantum systems (Callen-Welton, Nakano, Kubo)
= previous results for classical systems (Nyquist, Takahashi, Green).

$\therefore$ FDT is relatively insensitive to the choice of measuring apparatuses for the real symmetric part in the classical regime $\hbar\omega \ll k_B T$.

Many experimental evidences for this case, although conventional measuring apparatuses (not necessarily quasiclassical!) were used. (Johnson, ...).

Experiments on violation (continued)

For other cases such as

- $\mathrm{Re}\,\sigma_{xx}(\omega)$ at $\hbar\omega \gtrsim k_{\mathrm{B}}T$
- $\mathrm{Re}\,\sigma_{xy}(\omega)$ at all ω (including $\omega = 0$)

Our results predict the violation.
⇒ Greater care is necessary when inspecting FDT.

If measurement is not quaiclassical, FDT would look violated *more greatly*.
⇒ One could not tell whether the FDT is really violated.

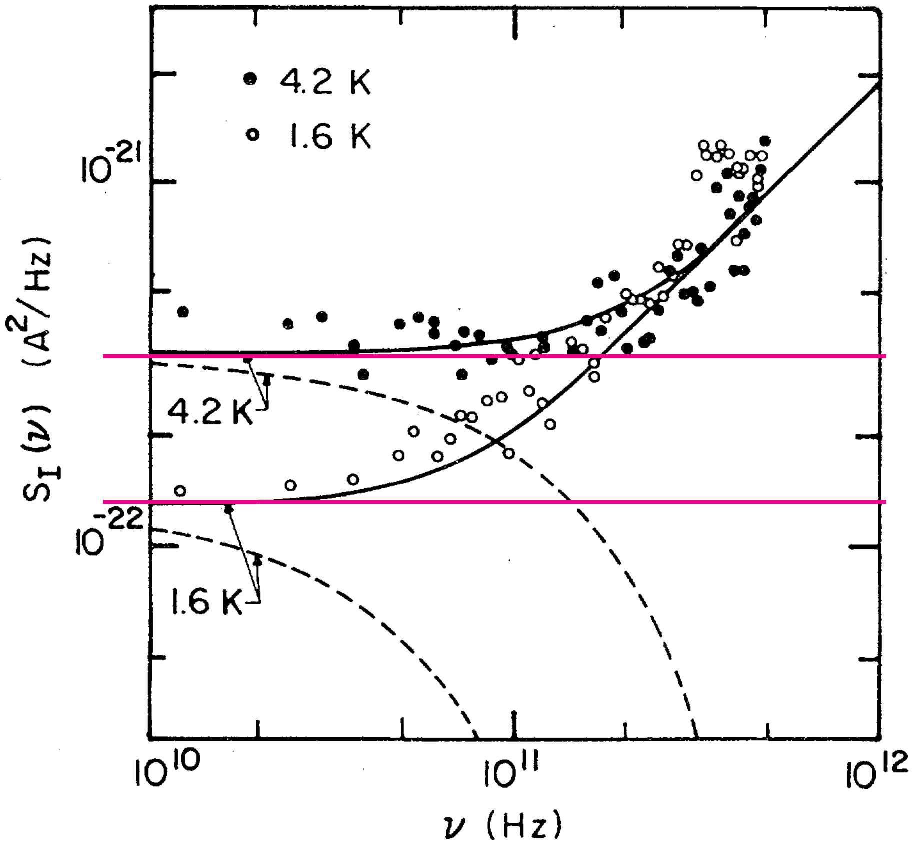
To inspect FDT in this case, quasiclassical measurements should be made.

Notice: Conventional measurements are not necessarily quasiclassical.
ex. measurement of electromagnetic fields (R. J. Glauber, PR 130, 2529 (1963))
⇒ conventional photodetectors destroy the state by absorbing photons.
⇒ cannot measure, e.g., the zero-point fluctuation
⇒ not quasiclassical
⇒ FDT looks violated more greatly.

Experiments on violation (continued)

Experiments using quasiclassical measurements

- $\sigma_{xx}(\omega)$: Koch et al. (1982) used the heterodyning technique $\simeq$ quasiclassical



Resisitiviy-shunted Josephson Junction.

$$\mathrm{Re}\, S_{xx}(\omega) \simeq I_\beta(\omega) k_\mathrm{B} T\, \mathrm{Re}\, \sigma_{xx}(\omega)$$

FDT is violated with increasing ω.

R. H. Koch et al., PR B **26**, 74 (1982).

- $\sigma_{xy}(\omega)$: Comparison with $S_{xy}(\omega)$ not reported $\Rightarrow$ experiments are welcome!

Contents

The violation is a genuine quantum effect

Antisymmetric part (such as σ_{xy}):

FDT is violated even in the "classical regime" $\hbar\omega \ll k_B T$. Why?

Two ways to reach the "classical regime"

1. hypothetical limit: $\hbar \to 0$

   $\Rightarrow$ system becomes classical

   $\Rightarrow$ violation disappears.

2. physical limit: $\omega \to 0$ while keeping $\hbar$ constant

   $\Rightarrow$ violation for antisymmetric parts.

Violation of the FDT is a genuine quantum effect, which appears on the macroscopic scale.

Relaxation of squeezed equilibrium state

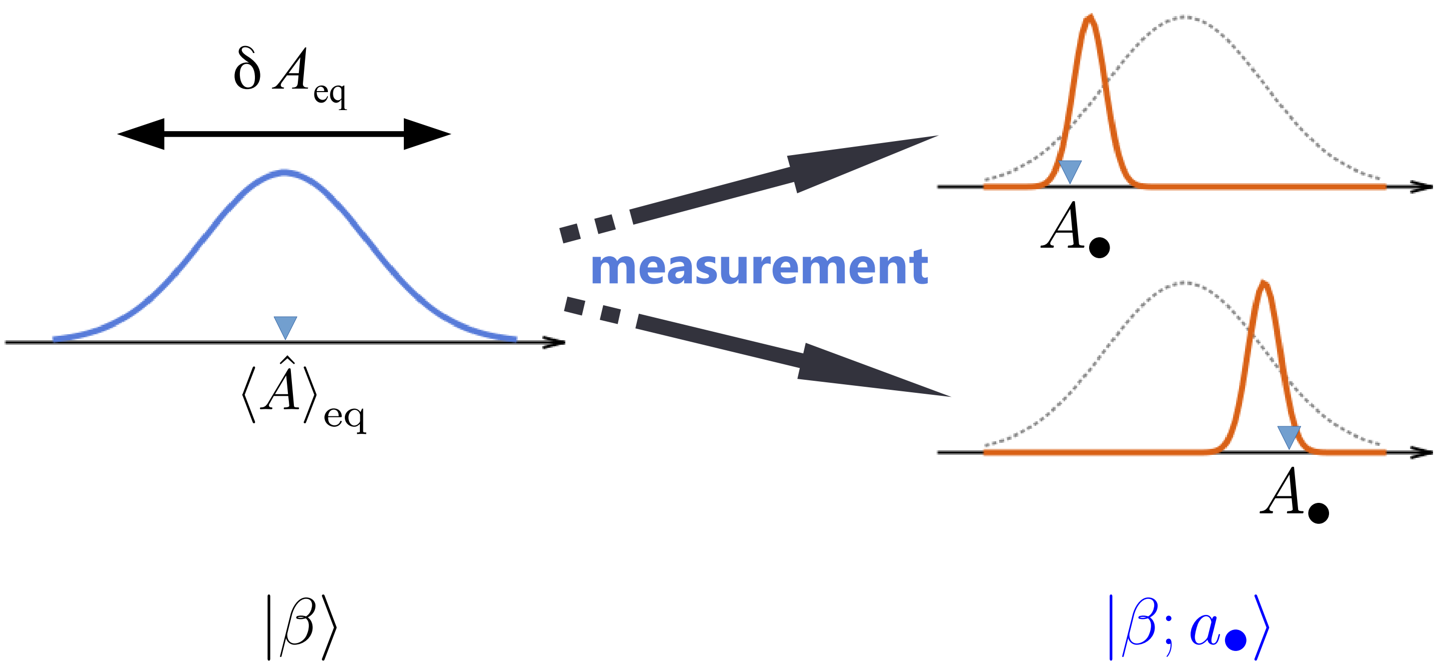
$t = 0^-$: equilibrium state $= |\beta\rangle$ (thermal pure quantum state)

$\downarrow$

$t = 0$: post-measurement state $= |\beta; a_\bullet\rangle = \dfrac{1}{\sqrt{p(a_\bullet)}} f(\hat{a} - a_\bullet)|\beta\rangle$

$\downarrow$ free evolution **squeezed equilibrium state**

$t > 0$: $e^{-i\hat{H}t/\hbar}|\beta; a_\bullet\rangle$



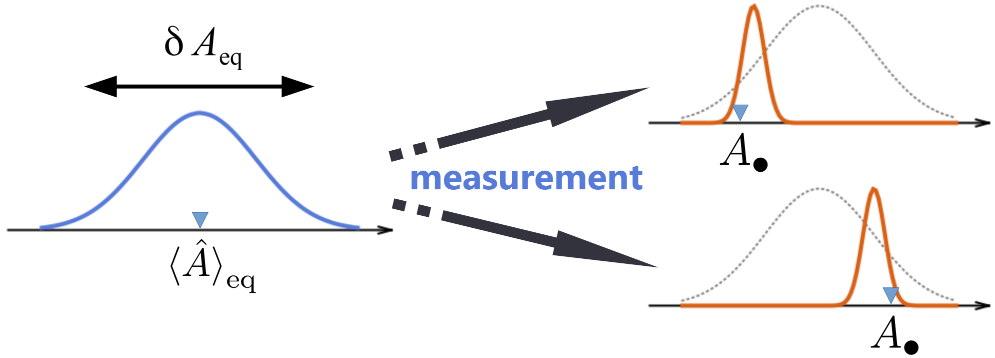
Relaxation of squeezed equilibrium state (continued)

Gaussian f (similar results for general f)

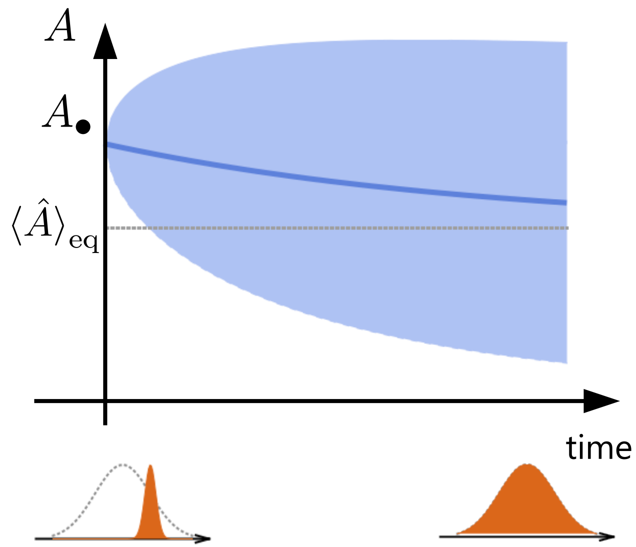
$$\langle \hat{b}(t)\rangle_{a_\bullet} - \langle \hat{b}\rangle_{\text{eq}} = \frac{\langle \frac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\text{eq}}}{\delta a_{\text{eq}}^2 + \delta a_{\text{err}}^2}\Delta a_\bullet$$

$$\langle (\hat{b}(t) - \langle \hat{b}(t)\rangle_{a_\bullet})^2\rangle_{a_\bullet} - \delta b_{\text{eq}}^2 = -\frac{\langle \frac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\text{eq}}^2}{\delta a_{\text{eq}}^2 + \delta a_{\text{err}}^2} + \frac{\langle \frac{1}{2i}[\hat{a}, \hat{b}(t)]\rangle_{\text{eq}}^2}{\delta a_{\text{err}}^2}$$

- Evolve with increasing t, unlike in $|\beta\rangle$ or $e^{-\beta\hat{H}}/Z$.
- Go to zero if $\langle \frac{1}{2}\{\Delta\hat{a}, \Delta\hat{b}(t)\}\rangle_{\text{eq}} \to 0$ and $\langle \frac{1}{2i}[\hat{a}, \hat{b}(t)]\rangle_{\text{eq}} \to 0$.



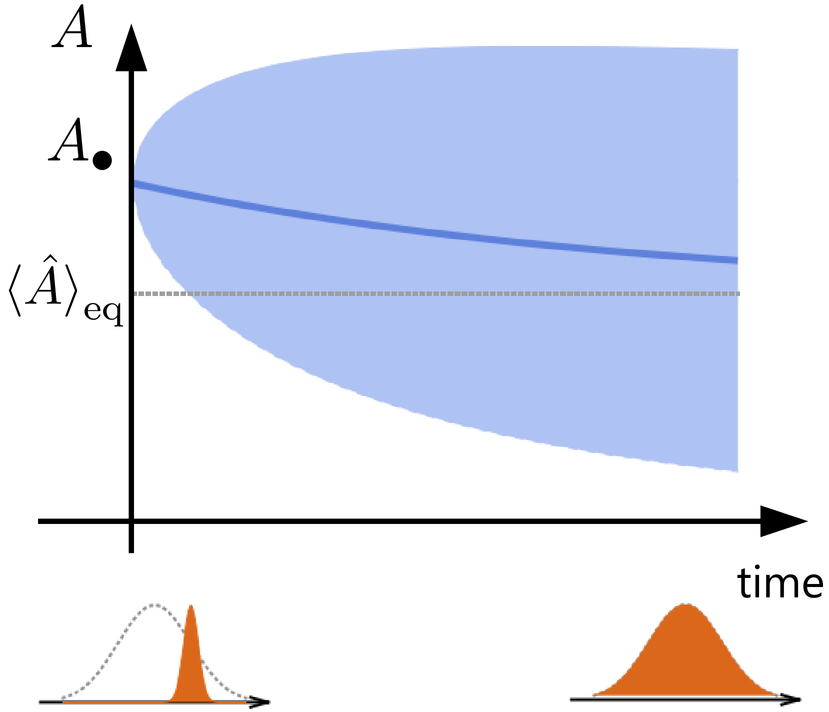
$\Rightarrow$



Relaxation of squeezed equilibrium state (continued)

The squeezed equilibrium state is a time-evolving state, in which macrovariables fluctuate and relax, unlike the Gibbs or thermal pure quantum state.

- Realized during quasiclassical measurements of equilibrium fluctuations.
- After the relaxation, one cannot distinguish $|\beta; a_\bullet\rangle$ from $|\beta\rangle$ by macroscopic observations. $\Rightarrow$ "thermalization"



Summary

- What is observed when equilibrium fluctuations are measured in an ideal way that simulates classical ideal measurements. "quasiclassical measurements"
- symmetrized time correlation is obtained quite generally.
- FDT is violated as a relation between observed quantities.
- Real symmetric parts of response functions: FDT is violated at $\hbar\omega \gtrsim k_B T$.

  $\Rightarrow$ A previous experiment on $\mathrm{Re}\,\sigma_{xx}(\omega)$ reported an evidence.
- Real antisymmetric parts: FDT is violated at all frequencies, even at $\omega = 0$.

  $\Rightarrow$ No experiments reported. Comprison of $\sigma_{xy}(0)$ with $S_{xy}(0)$ interesting.
- Violation is a genuine quantum effect, which survives on a macroscopic scale.
- Post-measurement state is a 'squeezed equilibrium state.'
- It is a time-evolving state, in which macrovariables fluctuate and relax, unlike the Gibbs or thermal pure quantum state.

  $\Rightarrow$ realized during quasiclassical measurements of equilibrium fluctuations.

Contents

1. What's wrong with derivations of the FDT?
2. Assumptions
   (a) on the system and its equilibrium states
   (b) on measurements
3. Measurement of time correlation
4. Violation of FDT
5. Experiments on violation
6. Discussions
7. Summary
8. Additional comments (if time allows)

Order of various limits and integral in Kubo formula

$$\chi_{ba}(\omega) = \int_0^\infty \lim_{N \propto V \to \infty} \beta \langle \Delta\hat{a}; \Delta\hat{b}(t) \rangle_{\text{eq}}\, e^{i\omega t} dt. \tag{1}$$

Not useful for studying properties of $\chi_{ba}(\omega)$.

Assuming the necessary conditons for the Kubo formula, we may rewrite (1) as

$$\chi_{ba}(\omega) = \lim_{\epsilon \searrow 0} \int_0^\infty \lim_{N \propto V \to \infty} \beta \langle \Delta\hat{a}; \Delta\hat{b}(t) \rangle_{\text{eq}}\, e^{i\omega t - \epsilon t} dt. \tag{2}$$

The recurrence time of $\langle \Delta\hat{a}; \Delta\hat{b}(t) \rangle_{\text{eq}}$ increases with increasing V. Hence,

$$\chi_{ba}(\omega) = \lim_{\epsilon \searrow 0} \lim_{N \propto V \to \infty} \int_0^\infty \beta \langle \Delta\hat{a}; \Delta\hat{b}(t) \rangle_{\text{eq}}\, e^{i\omega t - \epsilon t} dt. \tag{3}$$

$V < +\infty$ in this time integral $\Rightarrow$ useful for studying properties of $\chi_{ba}(\omega)$.

ex. One can express the integral using the energy eigenvalues and eigenstates.

Warning: $\lim_{\epsilon \searrow 0}$ should not be taken beofore $\lim_{N \propto V \to \infty}$.

Otherwise, unphysical results would be obtained (often found in the literature).

ex. magnetic susceptibility: $\chi_{\text{Kubo}} \le \chi_S \le \chi_T$ (Kubo-Toda-Hashitume-Saito, *Statistical Physics*)

Prof. Ken-ichi Asano said "Any ridiculous results can be derived."

Superficial violation of FDT in classical systems

Relations between χ_{ba} and $\tilde{S}_{ba}$ were previously known:

$$\mathrm{Re}\,\chi_{ba}^{+}(\omega) = \beta\,\mathrm{Re}\,\tilde{S}_{ba}^{+}(\omega)/[2I_{\beta}(\omega)],$$

$$\mathrm{Re}\,\chi_{ba}^{-}(\omega) = \beta \int_{-\infty}^{\infty} \frac{\mathcal{P}}{\omega' - \omega} \cdot \frac{1}{I_{\beta}(\omega')}\,\mathrm{Im}\,\tilde{S}_{ba}^{-}(\omega')\,\frac{d\omega'}{2\pi}.$$

As $\hbar \to 0$ they reduce to

$$\mathrm{Re}\,\chi_{ba}^{+}(\omega) = \beta\,\mathrm{Re}\,\tilde{S}_{ba}^{+}(\omega)/2,$$

$$\mathrm{Re}\,\chi_{ba}^{-}(\omega) = \beta \int_{-\infty}^{\infty} \frac{\mathcal{P}}{\omega' - \omega}\,\mathrm{Im}\,\tilde{S}_{ba}^{-}(\omega')\,\frac{d\omega'}{2\pi}.$$

FDT looks violated for $\mathrm{Re}\,\chi_{ba}^{-}(\omega)$ even in the classical limit; one would expect

$$\mathrm{Re}\,\chi_{ba}^{-}(\omega) = \beta\,\mathrm{Re}\,\tilde{S}_{ba}^{-}(\omega)/2.$$

♣ Actually, r.h.s. $\equiv 0$.

Multi-time measurements

time	0	t_1	$\cdots$	t_K
observable	$\hat{A}^0$	$\hat{A}^1$	$\cdots$	$\hat{A}^K$
measurement operator	f_0	f_1	$\cdots$	f_K
outcome	$\sqrt{N}a_\bullet^0$	$\sqrt{N}a_\bullet^1$	$\cdots$	$\sqrt{N}a_\bullet^K$

$$\begin{aligned}\overline{\Delta a_\bullet^j \Delta a_\bullet^k} &= \langle \tfrac{1}{2}\{\Delta \hat{a}^j(t_j), \Delta \hat{a}^k(t_k)\}\rangle_{\text{eq}} + \delta_{j,k}\delta a_{\text{err}}^{j\,2} \\ &\quad + \sum_{l=0}^{j-1} F_l \langle \tfrac{1}{2i}[\hat{a}^j(t_j), \hat{a}^l(t_l)]\rangle_{\text{eq}} \langle \tfrac{1}{2i}[\hat{a}^l(t_l), \hat{a}^k(t_k)]\rangle_{\text{eq}} \quad (0 \le j \le k),\end{aligned}$$

where $\delta a_{\text{err}}^{j\,2} = \int x^2 |f_j(x)|^2 dx$, $F_j = -4\int f_j''(x) f_j(x) dx$ ($= 1/w_j^2$ for Gaussian).

When $j = 0$ and $k \ge 1$, the backaction term is absent,

$$\overline{\Delta a_\bullet^0 \Delta a_\bullet^k} = \langle \tfrac{1}{2}\{\Delta \hat{a}^0, \Delta \hat{a}^k(t_k)\}\rangle_{\text{eq}} \text{ for } t_k > 0.$$

Analogous to the case of measuring twice, although other measurements may be performed for $0 < t < t_k$.

Quantum violation of Onsager's regression hypothesis

L. Onsager (1931):
"The average regression of equilibrium fluctuations will obey the same laws as the corresponding macroscopic irreversible processes." (classical systems)

Classical systems : H. Takahashi (1952) : "holds."

Quantum systems: contradictory claims from different assumptions.

- "violated, but something must be wrong" (assumed symmetrized time correlation)
  R. Kubo and M. Yokota (1955)
- "holds" (assumed a local equilibrium state for the state during fluctuation)
  S. Nakajima (1956), R. Kubo, M. Yokota and S. Nakajima (1957).
- "violated" (assumed symmetrized time correlation)
  P. Talkner (1986), G. W. Ford and R. F. O'Connel (1996)

We have proved: symmetrized time correlation is always obtained by quasiclassical measurements.

Onsager's hypothesis cannot be valid in quantum systems as relations between observed quantities.

Why quantum effects survive on the macroscopic scale?

Additive operators $= O(N)$:

$$\hat{A} = \sum_{\boldsymbol{r}} \hat{\xi}(\boldsymbol{r}), \quad \hat{B} = \sum_{\boldsymbol{r}} \hat{\zeta}(\boldsymbol{r}).$$

Their densities tend to commute as $N \to \infty$;

$$[\hat{A}/N, \hat{B}/N] = \frac{1}{N^2} \sum_{\boldsymbol{r}} [\hat{\xi}(\boldsymbol{r}), \hat{\zeta}(\boldsymbol{r})] = \frac{1}{N^2} O(N) \to 0$$

$\Rightarrow$ looks like a classical system

But, their fluctuations do not;

$$[\Delta\hat{A}/\sqrt{N}, \Delta\hat{B}/\sqrt{N}] = [\Delta\hat{a}, \Delta\hat{b}] = O(1)$$

$\Rightarrow$ quantum effects survive even for large N

Although $[\Delta\hat{a}, \Delta\hat{b}] = O(1) \propto \hbar$, a typical example shows

$$\text{FDT violation} \simeq \text{admittance} \times \frac{\hbar \times \text{microscopic parameters}}{\text{other microscopic parameters}}$$

$$\simeq \text{admittance} \times \text{not small} \;\Rightarrow\; \text{detectable enough!}$$

Different results for equilibrium fluctuation (time correlation)

	FT of $\langle j_x(0) j_x(t) \rangle_{\rm eq}$	FT of $\langle j_x(0) j_y(t) \rangle_{\rm eq}$
Nyquist PR 32, 110 (1928)	$k_{\rm B} T \sigma_{xx}(0) \dfrac{\beta\hbar\omega}{e^{\beta\hbar\omega}-1}$ FDT holds at **low** ω	not discussed
Callen-Welton PR 83, 34 (1951)	$k_{\rm B} T \sigma_{xx}(0) I_\beta(\omega)$ FDT holds at **low** ω	not discussed
Kubo JPSJ 12, 570 (1957)	$k_{\rm B} T \sigma_{xx}(\omega)$ FDT holds at **all** ω	$k_{\rm B} T \sigma_{xy}(\omega)$ FDT holds at **all** ω
Our results	$k_{\rm B} T \sigma_{xx}(\omega) I_\beta(\omega)$ FDT holds at **low** ω	$k_{\rm B} T \sigma_{xy}(\omega)$ $- \int_{-\infty}^{\infty} \dfrac{\mathcal{P}}{\omega' - \omega} \left[1 - \dfrac{1}{I_\beta(\omega')} \right] i \tilde{S}_{xy}(\omega') \dfrac{d\omega'}{2\pi}$ FDT **violated** at **all** ω

A rough estimate of magnitude of violation

Drude model in $\boldsymbol{B} = (0, 0, B)$.

$$\sigma_{xx}(\omega) = \sigma_0 \frac{1 - i\omega\tau}{(1 - i\omega\tau)^2 + (\omega_c\tau)^2}$$

$$\sigma_{xy}(\omega) = -\sigma_0 \frac{\omega_c\tau}{(1 - i\omega\tau)^2 + (\omega_c\tau)^2}$$

$$\sigma_0 = \frac{ne^2\tau}{m_*}, \quad \omega_c = \frac{eB}{m_*}$$

$$\langle \tfrac{1}{2}\{\hat{j}_\nu, \hat{j}_\mu(t)\}\rangle_{\mathrm{eq}} = \frac{\sigma_0}{\tau} e^{-|t|/\tau} \sin(\omega_c t) \quad \Rightarrow \quad \tilde{S}_{xy}(\omega) = \frac{2i}{\beta} \operatorname{Im} \sigma_{xy}(\omega).$$

$$\sigma_{xy}(0) - \beta S_{xy}(0) = 4\sigma_0 \int_{-\infty}^{\infty} \left[1 - \frac{1}{I_\beta(\omega)}\right] \frac{\omega_c\tau^2 d\omega/2\pi}{[1 + (\omega_c\tau)^2 - (\omega\tau)^2]^2 + 4(\omega\tau)^2}$$

ex. When $\omega_c\tau \ll 1$ and $k_{\mathrm{B}}T \sim \hbar/\tau$,

$$\sigma_{xy}(0) - \beta S_{xy}(0) \sim \sigma_0 \frac{\hbar\omega_c}{k_{\mathrm{B}}T}$$

$$\sim \sigma_0 \quad \text{when } \hbar\omega_c \sim k_{\mathrm{B}}T.$$

Phenomenology of Thermalization (macroscopic)

Equilibrium state: all additive variables take macroscopically definite values, i.e,

$$\text{fluctuations of additive variables} = o(N).$$

Non-equilibrium state:

$$|\text{value of some additive variable} - \text{its equilibrium value}| = O(N) > 0.$$

Relaxation from a non-equilibrium state:

$$\text{values of all additive variables} \to \text{their (new) equilibrium values}$$

Relaxation process:

$$\text{non-linear non-eq. regime} \to \text{linear non-eq. regime} \to \text{equilibrium}$$

$$\tau \text{ (relaxation time)} = \tau_{\mathrm{NL}} + \tau_{\mathrm{L}}$$

Relaxation (thermalization) time

$$\equiv \tau \text{ of an additive observable of slowest relaxation}$$
$$\geq \tau_{\mathrm{L}} \text{ of such an observable}$$

Thermalization in classical systems

An RC circuit, capaciter charged at $t = 0$

- Phenomenological theory

  Relaxation with time constant $\tau = RC$.

  $\Rightarrow$ admittance $(R + i/\omega C)^{-1}$ gives the time scale of thermalization

- Microscopic theory

  A sufficient condition for thermalization is

$$\text{mixing property : } \langle X(0)Y(t)\rangle_{\text{eq}} \to 0 \text{ as } t \to \infty$$

  $\Rightarrow$ time correlation $\langle X(0)Y(t)\rangle_{\text{eq}}$ gives the time scale of thermalization

- Linear response theory

$$\text{admittance} = \text{Fourier transform of } \langle X(0)Y(t)\rangle_{\text{eq}}/k_{\text{B}}T$$

These are consistent with each other in classical systems.

Are they consistent in quantum systems? $\Rightarrow$ **No**, according to this talk

Some consequences for thermalization

- Phenomenology should be correct on a macroscopic scale, so

$$\begin{aligned}&\text{relaxation (thermalization) time from a nonequilibrium state}\\&= \tau \text{ of an additive observable of slowest relaxation}\\&\geq \tau_{\mathrm{L}} \text{ of such an observable}\\&= \text{determined by admittance}\end{aligned}$$

- After equilibirum is reached,

$$\begin{aligned}\text{relaxation time of fluctuation} &= \text{relaxation time of symTC}\\&\neq \text{relaxation time determined by admittance}\end{aligned}$$

- For both relaxation times,

$$\begin{aligned}\text{relaxation times} &= \text{material-dependent time scales}\\&\neq \text{Boltzmann time } \frac{\hbar}{k_{\mathrm{B}}T}\end{aligned}$$

Probability density of getting outcome $\boldsymbol{a_\bullet}$

$t = 0^-$: equilibrium state $= |\beta\rangle$ (thermal pure quantum state)

$\downarrow$

► $t = 0$: measurement of $\hat{A} = \hat{a}\sqrt{N}$ $\Rightarrow$ outcome $A_\bullet = a_\bullet\sqrt{N}$

Gaussian f

$$\delta a_{\rm err}^2 = w^2 = O(1) \qquad (\text{i.e., } \delta A_{\rm err} = O(\sqrt{N})),$$

$$p(a_\bullet) = \frac{1}{[2\pi(\delta a_{\rm eq}^2 + \delta a_{\rm err}^2)]^{1/2}} \exp\left[-\frac{1}{2(\delta a_{\rm eq}^2 + \delta a_{\rm err}^2)}(\Delta a_\bullet)^2\right],$$

where $\delta a_{\rm eq}^2 \equiv \delta A_{\rm eq}/\sqrt{N}$, and $\Delta a_\bullet \equiv a_\bullet - \langle \hat{a} \rangle_{\rm eq}$.

general f

Similar results, which depend on f. (see K. Fujikura and AS, 2016)

Width of $p(a_\bullet) \sim \delta a_{\rm eq}^2 + \delta a_{\rm err}^2$

Definition of equilibrium states in this talk

AS, *Principles of Thermodynamics*, Univ. Tokyo Press, 2007

(i) **Isolated system**

Consider an isolated macroscopic system. After a sufficiently long time, it evoloves to a state s.t. all macroscopic variable is macroscopically constant;

$$\frac{\text{variation}}{\text{value}} \to 0 \text{ in the thermodynamic limit (t.d.l).}$$

Such a state is called a (thermal) equilibrium state.

(ii) **Non-isolated system** (subsystem)

Consider a macroscopic system that is not isolated from other systems. Suppose that its state is macroscopically identical to an equilibrium state in the above sense, i.e., for all macroscopic variable

$$\frac{\text{its value}}{\text{its value in an equilibrium state (of an isolated system)}} \to 1 \text{ in the t.d.l..}$$

Such a state is also called a (thermal) equilibrium state.

♣ Other definitions $\Rightarrow$ violation of many theorems of thermodynamics