Ch. grand canonical TPQ (gTPQ) state

$$|\beta,\mu\rangle = \sum_\nu z_\nu e^{-\beta(\hat{H}-\mu\hat{N})/2}|\nu\rangle$$

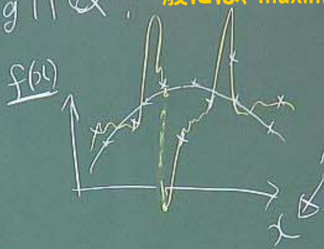
$$\langle\hat{A}\rangle^{TPQ}_{\beta,\mu} \xrightarrow{P} \langle\hat{A}\rangle^{ens}_{\beta,\mu}$$

$$\langle\beta,\mu|\beta,\mu\rangle \xrightarrow{P} \Xi(\beta,\mu) \text{ : grand partition function}$$

exponentially fast!

N<+∞で、N→∞に最も近い結果を与えるのは、gTPQ!

一般には、maximally canonical TPQ



Strategyの例

- phase tr. からはなれたところ → gTPQ
- 〃 の近く → mTPQ

Ch. 「熱ゆらぎ」とは?

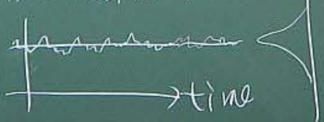
(ア)「アンサンブルゆらぎ」 ← これをギロンする。

(イ) 時間的ゆらぎ

古典系の(ア)

$\frac{1}{Z}e^{-\beta H}$ において、$\langle(M-\langle M\rangle)^2\rangle = \langle(\Delta M)^2\rangle \neq 0$

(イ)との関係は、



だろう。

ここでは、量子系の(ア)にしぼる!

S. Sugiura and A S, Kinki Univ. Series on Quantum Computing 9, 245 (2014)
arXiv: 1312.5145

Gibbs state を用いた、ふつうのギロン

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}} = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n|$$

一般に

$\hat{\rho} = \sum_{\lambda} w_{\lambda} |\lambda\rangle\langle\lambda| \quad (\sum_{\lambda} w_{\lambda} = 1,\ w_{\lambda} \geq 0)$

のとき、

$\langle\lambda|(\hat{A} - \langle\lambda|\hat{A}|\lambda\rangle)^2|\lambda\rangle$: $|\lambda\rangle$における $\hat{A}$の quantum fluctuation (QF).

から、

「$\hat{\rho}$におけるQF」$\equiv \langle(\Delta A)^2\rangle^{ens}_{q}$

$\equiv \sum_{\lambda} w_{\lambda} \langle\lambda|(\hat{A} - \langle\lambda|\hat{A}|\lambda\rangle)^2|\lambda\rangle$

としたくなる。すると、

$\langle(\Delta A)^2\rangle^{ens} = \mathrm{Tr}\left[\hat{\rho}\,(\overset{\hat{A}-\mathrm{Tr}(\hat{\rho}\hat{A})}{\overset{/\!/}{\Delta\hat{A}}})^2\right]$

$= \langle(\Delta A)^2\rangle^{ens}_{q} + \underbrace{\langle(\Delta A)^2\rangle^{ens}_{th}}$ ←「thermal fluctuation」(TF)

のはずなので: (「と考えると」という意味)

$\langle(\Delta\hat{A})^2\rangle^{ens}_{th}$

自分で $\triangleq \sum_{\lambda} w_{\lambda} \langle\lambda|\hat{A}|\lambda\rangle^2 - \left(\sum_{\lambda} w_{\lambda} \langle\lambda|\hat{A}|\lambda\rangle\right)^2$

一方、同じ eq. state を TPQ state $|\psi(\beta)\rangle$で表すと、

$\hat{\rho} = |\psi(\beta)\rangle\langle\psi(\beta)|$

より、

$\langle(\Delta A)^2\rangle^{TPQ}_{q} = \langle(\Delta A)^2\rangle^{TPQ} \overset{\text{exponentially small error}}{\doteq} \langle(\Delta A)^2\rangle^{ens}$

$\langle(\Delta A)^2\rangle^{TPQ}_{th} = 0$

∴ TPQ形式では、(ρ)の1コの

「熱ゆらぎ」も「量子ゆらぎ」

に含まれている!

実は、$\langle(\Delta A)^2\rangle^{ens}_{q}$ と $\langle(\Delta A)^2\rangle^{ens}_{th}$ を

別々に測ることはできない!

なぜなら $\hat{\rho}$ を $\sum_{\lambda} w_{\lambda} |\lambda\rangle\langle\lambda|$ の形に

表わすのは ∞ 種類ある!

(※ $\langle\lambda|\lambda'\rangle \neq 0$ でもよい!)

ex) $\hat{\rho} = \frac{2}{3}|\uparrow\rangle\langle\uparrow| + \frac{1}{3}|\downarrow\rangle\langle\downarrow|$

自分で $\triangleq \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-|$

$\left(|\pm\rangle \equiv \sqrt{\frac{2}{3}}|\uparrow\rangle \pm \sqrt{\frac{1}{3}}|\downarrow\rangle\right)$

$$\hat\rho = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n| \to \langle(\Delta\hat H)^2\rangle_q^{ens} = 0$$

$$= \sum_\lambda w_\lambda |\lambda\rangle\langle\lambda| \to \langle(\Delta\hat H)^2\rangle_q^{ens} > 0$$

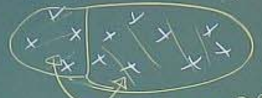
∴ $\langle(\Delta\hat H)^2\rangle_q^{ens}$ は、実験的には測れない！

→ $\langle(\Delta\hat H)^2\rangle_{th}^{ens}$ も、〃 〃 ！

測れるとすると、密度演算子で量子状態が定まることに矛盾する。

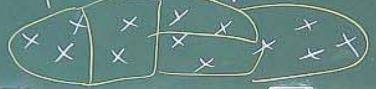
Ch. Entanglement

多くの分野では、bi-partite entanglementのみ！ ← ここでは、これをやる！



2つの parts 間の entanglement ← そのmeasureは∞種類ある
(pure stateについては、実質的に1つ)

multi-partite entanglementは？



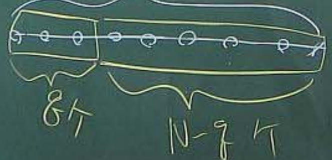
$\hat\rho^{ens}$ と $|\beta\rangle$ は、$\forall \hat A$: mechanical variables については等価！ でも、entanglementは exp. 倍異なる！

ex. Heisenberg chain. (interaction = J)

T≫J なら、$\hat\rho^{ens} \approx \hat 1/\dim\mathcal{H}$ → entanglement ≃ 0

※ vNやRenyi-2は measureになる例！

ところが、$|\beta\rangle$ の entanglementは、T≫J でも almost max.!



reduced density op.

$$\hat\rho_q \equiv \mathrm{Tr}_{N-q}(|\beta\rangle\langle\beta|)$$

→ $S_{vN} = -\mathrm{Tr}[\hat\rho \ln\hat\rho]$

代用 → $S_2 = -\ln \mathrm{Tr}\underbrace{(\hat\rho^2)}_{\text{purity}}$; Renyi-2

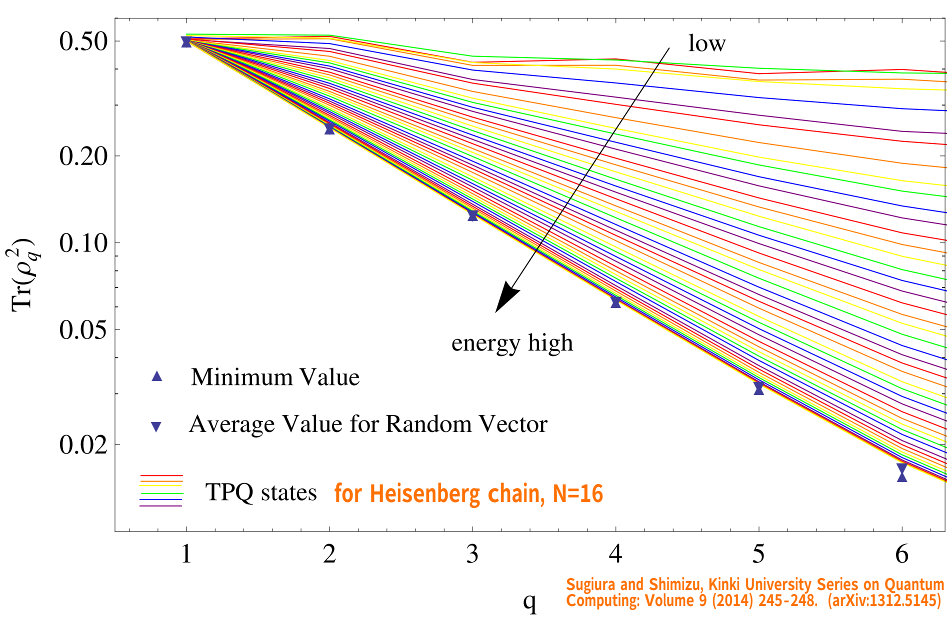
同じeq. stateについて、entanglementが

min. → Gibbs state

max. → TPQ state

中間もある！

∴ entanglementは eq. stateに固有の量ではない！



low
energy high
Minimum Value
Average Value for Random Vector
TPQ states
for Heisenberg chain, N=16
$\mathrm{Tr}(\rho_q^2)$
0.50
0.20
0.10
0.05
0.02
1
2
3
4
5
6
q
Sugiura and Shimizu, Kinki University Series on Quantum Computing: Volume 9 (2014) 245-248. (arXiv:1312.5145)

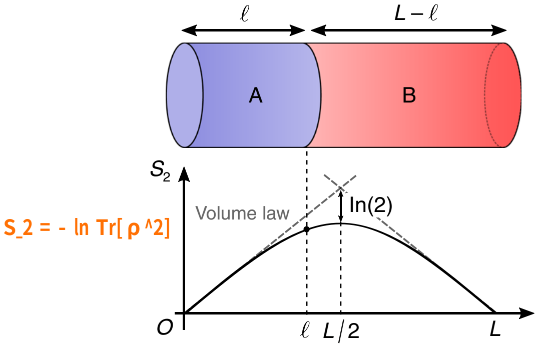


Fig. 1 A schematic picture of our setup. The second Rényi Page curve for pure states, $S_2(\ell)$, follows the volume law when ℓ is small, but gradually deviates from it as ℓ grows. At the middle, $\ell = L/2$, the maximal value is obtained, where the deviation from the volume law is ln 2 (see the Results section). Past the middle $\ell = L/2$, it decreases toward $\ell = L$ and becomes symmetric under $\ell \leftrightarrow L - \ell$

Nakagawa, Watanabe, Fujita, Sugiura, Nature Comm. 1635 (2018).

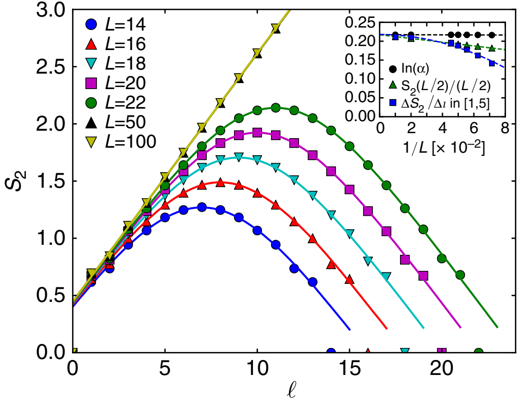


Fig. 2 Second Rényi Page curve in cTPQ states. The dots represent the second Rényi Page curves in the cTPQ states of the spin system (9) at an inverse temperature $\beta = 4$ calculated by Eq. (3) for various system sizes L. The lines are the fits by Eq. (5) for the numerical data. The inset shows the fitted values of ln a, $S_2(L/2)/(L/2)$, and the average slope of the curve between ℓ=1 and ℓ=5. The dotted lines are the extrapolations to $L \to \infty$ by $1/L$ scaling for ln a and $S_2(L/2)/(L/2)$ and by $1/L^2$ scaling for the average slope

Nakagawa, Watanabe, Fujita, Sugiura, Nature Comm. 1635 (2018).

§ TPQ states や Energy eigenstate は 実現するか? 近未来に実験的に!

↑ TPQ formulation ↑ ETH, thermalization

少数自由度 → どっちも実現できる!

多 〃 → 〃 〃 できない!

しかし、実現できる状態の「よいモデル化」になってる!

↑ prepareしやすい intial stateから、free evolutionする、など。

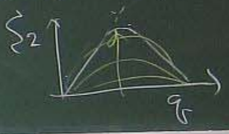
(1) ・TPQ states → mechanical variables の平衡値を与える。

・e. eigenstates $\xrightarrow{\text{ETHが成り立てば}}$ 〃

local ops. の低次多項式

・entanglement についても、これとほとんど同じ結果を与える!

Ref. Nakagawa et al, Nature Commun. 1635 (2018)



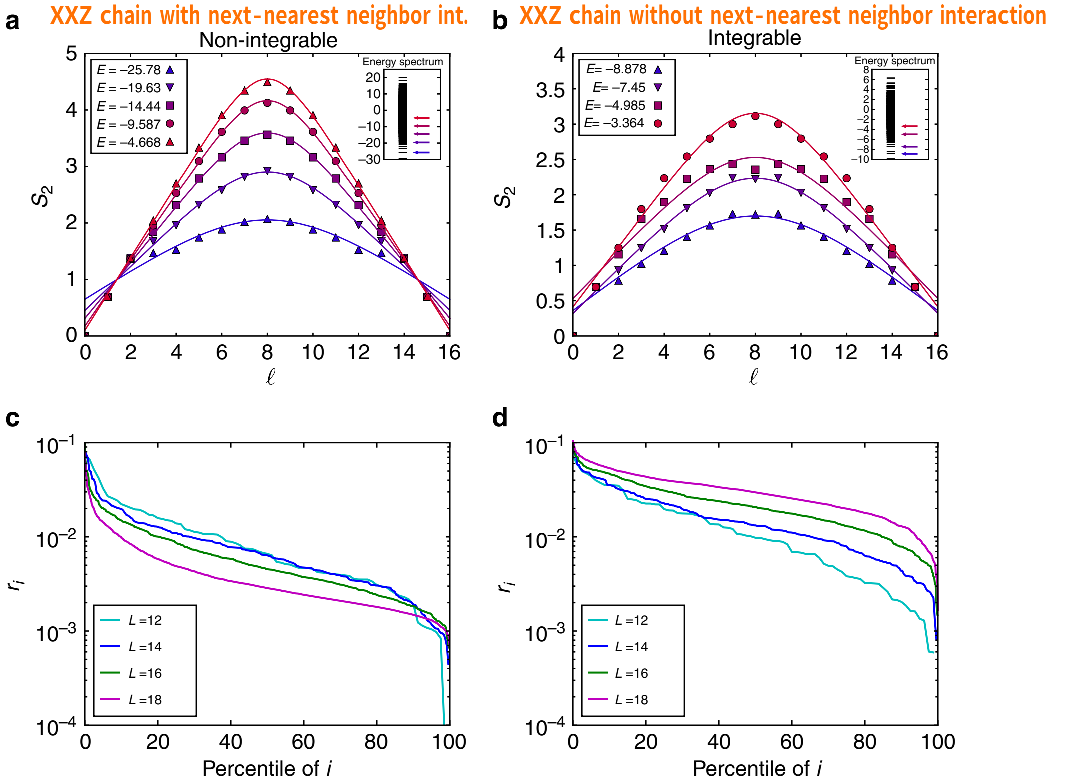


Fig. 3 Second Rényi Page curve for general energy eigenstates. **a** 2RPCs of several energy eigenstates of the non-integrable Hamiltonian, Eq. (9) with $\Delta = 2$ and $J_2 = 4$ (dots), and the fits by our formula (5) (lines). The inset shows the energy spectrum of the Hamiltonian, and the arrows indicate the eigenstates presented in the figure. **b** Same as figure **a** for the integrable Hamiltonian ($\Delta = 2$, $J_2 = 0$). **c** Residuals of fits per site $r_i \equiv L^{-1}\sum_{\ell=0}^{L}(S_2(\ell)_{i,\mathrm{data}} - S_2(\ell)_{i,\mathrm{fit}})^2$, where $S_2(\ell)_{i,\mathrm{data}}$ is the 2REE of the i-th eigenstate and $S_2(\ell)_{i,\mathrm{fit}}$ is a fitted value of it, for all eigenstates of the non-integrable Hamiltonian (10) with $\Delta = 2$ and $J_2 = 4$ (we consider only the sector of a vanishing total momentum and magnetization). The eigenstates are sorted in descending order in terms of the residuals, and the horizontal axis represents their percentiles. The fits become better as the size of the system increases. **d** Same as figure **c** for the integrable Hamiltonian ($\Delta = 2$, $J_2 = 0$). The fits become worse as the size of the system increases

Nakagawa, Watanabe, Fujita, Sugiura, Nature Comm. 1635 (2018)

Ch. 時間発展

§ TPQ states without 外場

同じ eq. state を表わす, 異なる realization の TPQ states の間をへめぐる。

平衡状態はマクロには時間変化しないが、
ミクロには時間変化して構わない！

$$\because\ |\beta\rangle = \sum_n z_n e^{-\beta \hat{H}/2} |n\rangle$$

$$= \sum_n \boxed{z_n} e^{-\beta E_n/2} |n\rangle$$

$$\xrightarrow{\text{evolution}} \sum_n \boxed{z_n e^{-i\omega_n t}} e^{-\beta E_n/2} |n\rangle$$

eq. properties について、exponential に高い精度で一致する！

§ TPQ state に、とつぜん外場をかける。

$$\hat{H} \longrightarrow \hat{H} + \hat{H}_{ext}$$

$t=0$ で"とつぜん"

$$|\beta\rangle \longrightarrow \text{noneq. state}$$

「quench」と呼ぶ。
最近、実験が盛んに。

$$\hat{U}(t) \equiv e^{-i(\hat{H}+\hat{H}_{ext})t/\hbar} \qquad (t \geq 0)$$

キカク化しておく

$$|\psi(\beta)\rangle \longrightarrow \hat{U}(t)\,|\psi(\beta)\rangle$$

興味があるのは、

$$\Delta A(t) = \underbrace{\langle\psi(\beta)|\overbrace{\hat{U}^{\dagger}(t)\,\hat{A}\,\hat{U}(t)}^{=\hat{A}(t)}|\psi(\beta)\rangle}_{\equiv \langle \hat{A}(t)\rangle_\beta} - \underbrace{\langle\psi(\beta)|\hat{A}|\psi(\beta)\rangle}_{\equiv \langle \hat{A}\rangle_\beta}$$

low order poly. ではない!

low order poly.

$$D^2_{\hat{A}(t)} = \overline{\left(\langle \hat{A}(t)\rangle^{TPQ}_\beta - \langle \hat{A}(t)\rangle^{ens}_\beta\right)^2}$$

$$\leq \frac{\langle (\Delta\hat{A}(t))^2\rangle^{ens}_{2\beta} + \left(\langle \hat{A}(t)\rangle^{ens}_{2\beta} - \langle \hat{A}(t)\rangle^{ens}_\beta\right)^2}{\exp\left[2\beta\{F(T/2) - F(T)\}\right]}$$

$$= \frac{\mathrm{Poly}(N)}{\exp[\Theta(N)]} \xrightarrow{\mathrm{TDL}} 0$$

∴ mechanical variables の noneq. evolution も、TPQ state を initial state として正しく求まる!

何がうれしいか?

同じ計算を Gibbs でやったら?

$$\hat{A}(t) = e^{i(\hat{H}+\hat{H}_{ext})t}\,\overset{\text{matrix}}{\hat{A}}\,e^{-i(\quad)t}$$

$2^N \times 2^N$ matrix

…けいさんしんどい!

じゃあ、Schrödinger picture でやろう!

$$\hat{\rho}^{ens}_\beta = \frac{1}{Z}e^{-\beta\hat{H}}$$

$$\downarrow$$

$$\hat{U}(t)\,\hat{\rho}^{ens}_\beta\,\hat{U}^{\dagger}(t)$$

$$= e^{-i(\hat{H}+\hat{H}_{ext})t}\,\overset{\text{matrix}}{\frac{1}{Z}e^{-\beta\hat{H}}}\,e^{+i(\;+\;)t}$$

…もっとしんどい!

TPQなら、

$$|\psi(\beta)\rangle \propto e^{-\frac{\beta}{2}\hat{H}}|0\rangle$$

random vector

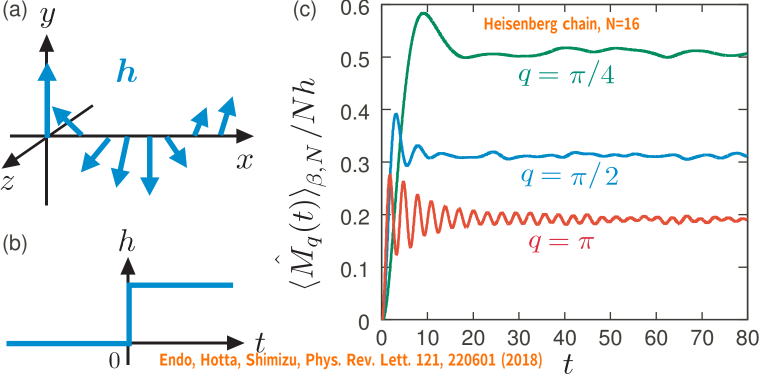
$$\downarrow$$

$$\hat{U}(t)\,|\psi(\beta)\rangle$$

$$\propto e^{-i(\hat{H}+\hat{H}_{ext})t}\,\overbrace{e^{-\frac{\beta}{2}\hat{H}}|0\rangle}^{\text{vector}}$$

← チェビシェフ多項式展開

← けいさんできる using mTPQ states



(a)
y
$\boldsymbol{h}$
x
z
(b)
h
t
0
(c)
Heisenberg chain, N=16
$q=\pi/4$
$q=\pi/2$
$q=\pi$
$\langle \hat{M}_q(t) \rangle_{\beta,N} / Nh$
t
0.6
0.5
0.4
0.3
0.2
0.1
0
0
10
20
30
40
50
60
70
80
Endo, Hotta, Shimizu, Phys. Rev. Lett. 121, 220601 (2018)

Linear and nonlinear susceptibility.—The LR and NLR need to be discussed separately. When h is small enough, the response extrapolates to that obtained from the LR theory [1–4]. In this LR regime, the linear susceptibility (or admittance) $\chi(\omega)$, which is the Fourier transform of the LR function [1–4], does not depend on the profile of $\boldsymbol{h}$ along the time axis. Therefore, it is sufficient to consider the specific time dependent profile Eq. (2), to obtain the general form of $\chi(\omega)$ as a function of frequency ω. Assuming that $\hat{A}$ is an additive observable, we obtain the following formula:

$$\chi(\omega) = \frac{\Delta A(+\infty)}{Nh} - i\omega \int_0^\infty \frac{\Delta' A(t)}{Nh} e^{i\omega t} dt, \qquad (5)$$

where $\Delta' A(t) := \langle \hat{A}(t) \rangle_{\beta,N} - \langle \hat{A}(+\infty) \rangle_{\beta,N}$. According to Kubo [1], $\chi(\omega)$ is explicitly given by the retarded Green function at equilibrium, which contains the information on the elementary excitations, whose nature could thus be examined by evaluating $\langle \hat{A}(t) \rangle_{\beta,N}$ for sufficiently small h. One can further specify the wave number $\boldsymbol{q}$ in $\boldsymbol{h}$, in order to obtain the $\boldsymbol{q}$-dependent susceptibility $\chi(\boldsymbol{q}, \omega)$. These points will be illustrated shortly.

At larger h, the correspondence with the LR theory breaks down. Still, we use Eq. (5) as the definition of the *nonlinear susceptibility* $\chi(\boldsymbol{q}, \omega; h)$ with explicit h dependence, because it is well defined even in this NLR regime and is continuously connected to the linear one.

Here, we do not follow the conventional perturbative definition in nonlinear optics [5]. Our $\chi(\boldsymbol{q}, \omega; h)$ could treat nonperturbative effects such as the nonlinear band deformation, as we see shortly.

遠藤論文の $\chi(\omega)$

一般に、外場 $f(t)$ に対する A の線型応答は、

$$\langle A\rangle_t^f - \langle A\rangle_{eq}^{f=0} =: \text{論文の } \Delta A(t)$$

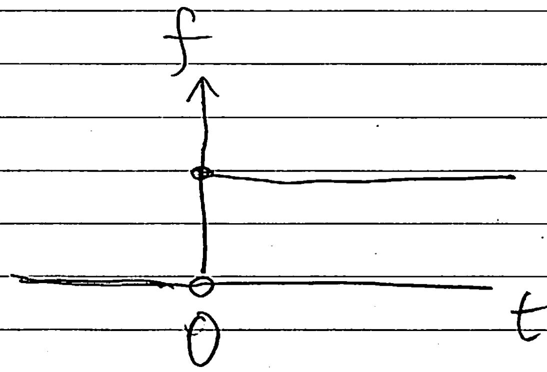
$$= \int_{-\infty}^{t} \Phi(\underbrace{t-t'}_{=\tau}) f(t')\,dt' = \int_0^{\infty} \underbrace{\Phi(\tau)}_{\text{response function}} f(t-\tau)\,d\tau$$

admittanceは、

$$\chi(\omega) = \int_{-\infty}^{\infty} \Phi(\tau) e^{i\omega\tau}\,d\tau$$

特に、

$$f(t) = f\,\theta(t)$$



のときは、

$$\langle A\rangle_t^f - \langle A\rangle_{eq}^{f=0}$$

$$= f\int_0^t \Phi(\underbrace{t-t'}_{=\tau})\,dt' = f\int_0^t \Phi(\tau)\,d\tau$$

Date

特に、$t \to +\infty$ でこの値が収束するとすると、

$$\langle A \rangle^{f}_{\infty} - \langle A \rangle^{f=0}_{eq}$$

$$= f \int_0^\infty \Phi(\tau)\, d\tau$$

辺々引き算して、

$$\langle A \rangle^{f}_{t} - \langle A \rangle^{f}_{\infty} =: \Delta' A(t)$$

$$= -f \int_t^\infty \Phi(\tau)\, d\tau$$

$$= \Delta A(t) - {} + \langle A \rangle^{f=0}_{eq} - \langle A \rangle^{f}_{\infty}$$

両辺を微分する：

$$\frac{d}{dt} \Delta' A(t) = f\, \Phi(t)$$

両辺を $[0, \infty)$ で FT する：

$$\int_0^\infty e^{i\omega t} \frac{d}{dt} \Delta' A(t) = f\, \chi(\omega)$$

$$= \left[e^{i\omega t} \Delta' A(t) \right]_0^\infty - i\omega \int_0^\infty e^{i\omega t} \Delta' A(t)$$

$$= \underbrace{\Delta' A(\infty)}_{=0} - \Delta' A(0) - i\omega \int_0^\infty e^{i\omega t} \Delta' A(t)\, dt$$

$$= \langle A \rangle^f_\infty - \underbrace{\langle A \rangle^f_0}_{= \langle A \rangle^f_{eq}} - i\omega \int_0^\infty e^{i\omega t} \Delta' A(t)\, dt$$

$$= \Delta A(\infty) - i\omega \int_0^\infty e^{i\omega t} \Delta' A(t)\, dt$$

ゆえに、

$$\boxed{\chi(\omega) = \frac{1}{f}\left[\Delta A(\infty) - i\omega \int_0^\infty e^{i\omega t} \Delta' A(t)\, dt\right]}$$

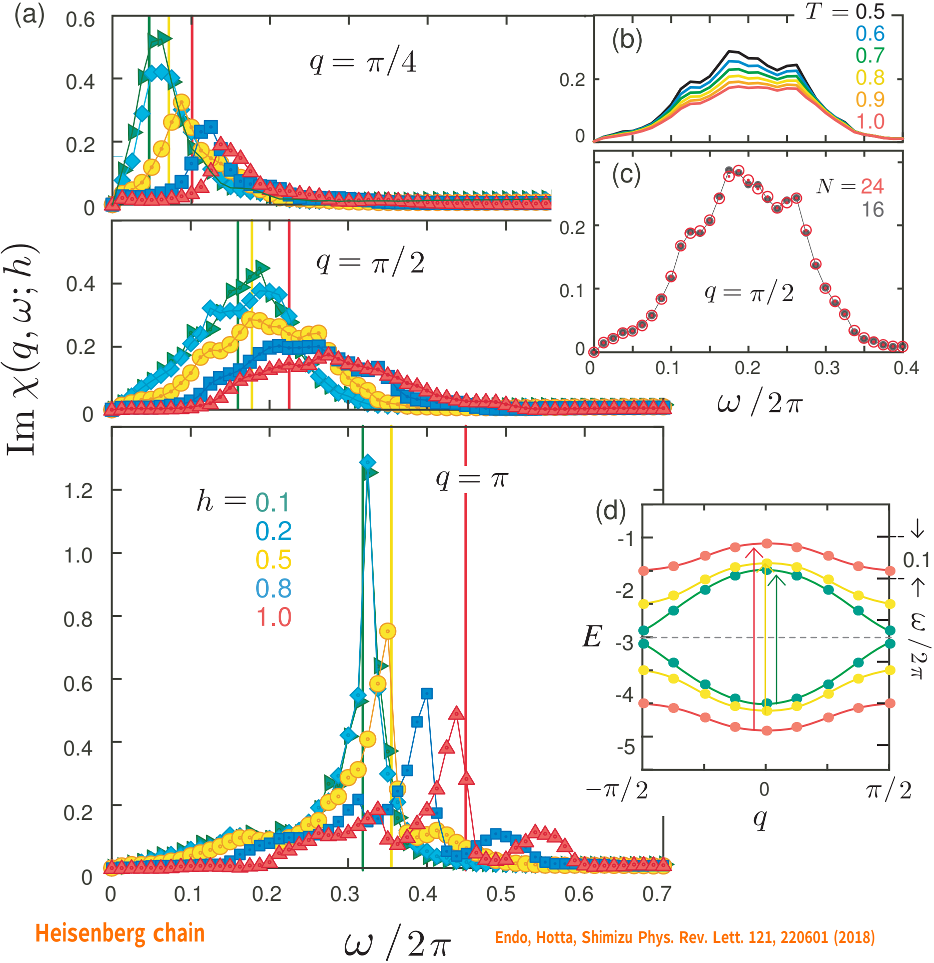
これは、定義により、$t \to +\infty$ で、

$$\Delta' A(t) \to \langle A \rangle^f_\infty - \langle A \rangle^f_\infty = 0$$

となるので、reasonableな公式！

ために収束因子を入れてもよい $(\varepsilon \searrow +0)$：

$$\chi(\omega) = \frac{1}{f}\left[\Delta A(\infty) - i\omega \int_0^\infty e^{i\omega t - \varepsilon t} \Delta' A(t)\, dt\right]$$



Heisenberg chain

Endo, Hotta, Shimizu Phys. Rev. Lett. 121, 220601 (2018)

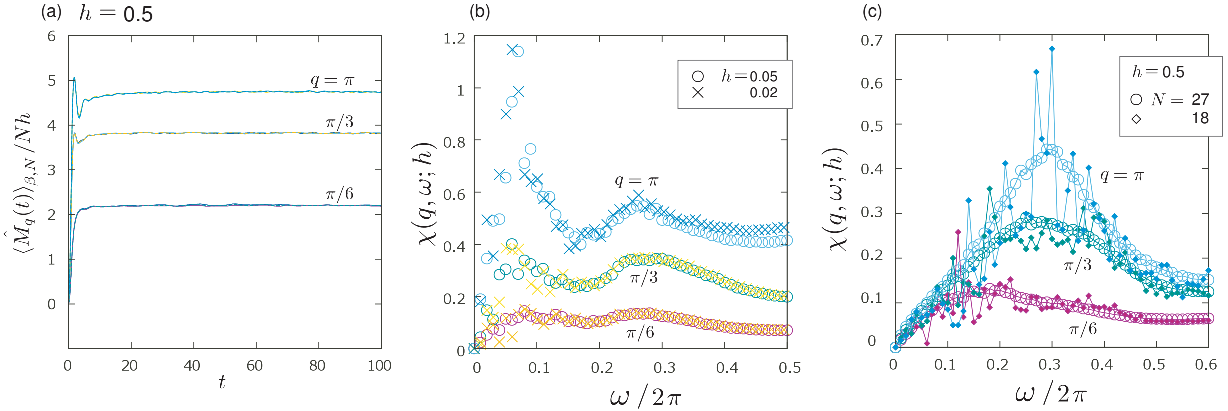
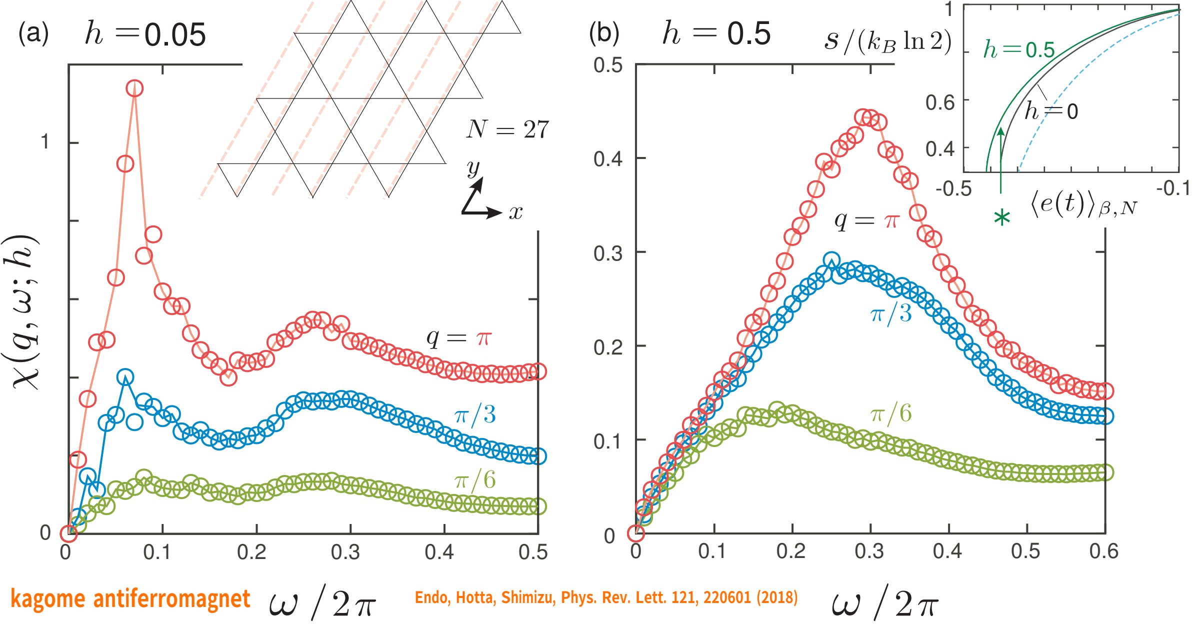


FIG. S2. Supporting results of the spin-1/2 kagome antiferromagnet at $N = 27$. (a) Time evolution of $\langle M_q(t) \rangle$ that yields the nonlinear response (Fig. 3(b)) at $h = 0.5$ and $k_BT = 0.1$. The solid lines give the results starting from different TPQ states, and the broken lines are their averages. (b) Comparison of $\chi(q, \omega; h)$ between $h = 0.02$ and 0.05 at $k_BT = 0.1$. The latter is the same as given in Fig. 3(a). A somewhat oscillating deviation of $h = 0.02$ at small ω dissolves when taking an average of many samples (while here, we take three sample averages for all data in this figure). (c) Comparison of $\chi(q, \omega; h)$ at $h = 0.5$ between $N = 27$ and 18. The spikes found in $N = 18$ data is due to the small system size which is smoothed out already at $N = 27$.

kagome antiferromagnet

Endo, Hotta, Shimizu, Phys. Rev. Lett. 121, 220601 (2018), supplemental material



(a) $h = 0.05$
$N = 27$
y
x
$\chi(q, \omega; h)$
$q = \pi$
$\pi/3$
$\pi/6$
0
1
0 0.1 0.2 0.3 0.4 0.5
$\omega / 2\pi$
(b) $h = 0.5$
$s/(k_B \ln 2)$
1
0.6
0.4
-0.5 -0.1
$h = 0.5$
$h = 0$
$\langle e(t) \rangle_{\beta, N}$
*
0.5
0.4
0.3
0.2
0.1
0
$q = \pi$
$\pi/3$
$\pi/6$
0 0.1 0.2 0.3 0.4 0.5 0.6
$\omega / 2\pi$
kagome antiferromagnet
Endo, Hotta, Shimizu, Phys. Rev. Lett. 121, 220601 (2018)