Statistical Mechanics without Ensembles
— Thermal Pure Quantum Formulation

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References:

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M. Hyuga, K. Sakai, S. Sugiura and AS, in preparation

Equlibrium Statistical Mechanics: Conventional

Ensemble formulation (Boltzmann, Gibbs, von Neumann)

I. Principle of equal weight, giving an equilibirum state

All states in the energy shell $(E-\Delta E, E]$ are found with equal probability:

$$\langle \hat{A} \rangle = \frac{1}{W} {\sum_n}' \langle n | \hat{A} | n \rangle \quad (|n\rangle : \text{energy eigenstate}, W : \#\text{ of } |n\rangle\text{'s in the shell})$$

$$= \mathrm{Tr}\left(\hat{\rho}^{\mathrm{ens}} \hat{A}\right) \quad \text{for every observable } \hat{A}.$$

$\hat{\rho}^{\mathrm{ens}}$: density operator of the (*micro canonical*) *Gibbs state*,

$$\hat{\rho}^{\mathrm{ens}} = \frac{1}{W} {\sum_n}' |n\rangle\langle n| \xrightarrow{\text{classical}} \rho^{\mathrm{ens}}_{\mathrm{cl}}(q,p) = \frac{1}{\text{volume of the shell}}$$

II. Boltzmann formula $(k_{\mathrm{B}} = 1)$, giving thermodynamic entropy

$$S = \ln W$$

$$= -\mathrm{Tr}\left[\hat{\rho}^{\mathrm{ens}} \ln \hat{\rho}^{\mathrm{ens}}\right] \xrightarrow{\text{classical}} -\int dq dp [\hat{\rho}^{\mathrm{ens}}_{\mathrm{cl}}(q,p) \ln \hat{\rho}^{\mathrm{ens}}_{\mathrm{cl}}(q,p)]$$

$\hat{\rho}^{\text{ens}}$ is a mixed state

Any quantum state can be represented by a density operator $\hat{\rho}$, where

$$\langle \hat{A} \rangle = \mathrm{Tr}\,[\hat{\rho}\hat{A}] \quad \text{for every observable } \hat{A}.$$

(A rough) **definition** : pure/mixed

- Every vector state $|\psi\rangle = \sum_n c_n |n\rangle \quad (c_n \in \mathbb{C})$ is a pure state, for which

$$\hat{\rho} = |\psi\rangle\langle\psi| \xrightarrow{\text{classical}} \rho_{\text{cl}}(q,p) = \delta(q - q^0, p - p^0)$$

- Other quantum states are mixed states, whose $\hat{\rho}$ can be decomposed as

$$\hat{\rho} = \sum_j p_j |\psi_j\rangle\langle\psi_j| \xrightarrow{\text{classical}} \rho_{\text{cl}}(q,p) = \sum_j p_j \delta(q - q^j, p - p^j)$$

using some $\{p_j,\ |\psi_j\rangle\}_j$ (not unique) s.t. $0 \le p_j < 1$, $\sum_j p_j = 1$.

$\therefore\ \hat{\rho}^{\text{ens}} = {\sum_n}' \dfrac{1}{W} |n\rangle\langle n|$ is a mixed state. $\left(p_j = 1/W,\ |\psi_j\rangle = |n\rangle \text{ in the shell}\right)$

W is Exponentially Large

From thermodynamics,

$$S(E,V,N) = Ns(u,v) \qquad (u = E/N, v = V/N),$$

entropy density $s(u,v) = O(1)$.

Since $S = \ln W$,

$$W = e^S = e^{Ns} = e^{O(N)}.$$

Therefore,

An exponentially large # of pure states are mixed in $\hat{\rho}^{\mathrm{ens}} = \dfrac{1}{W}\sum_n{}' |n\rangle\langle n|$.

Change of Independent Variables

ex. $E \to \beta$ $(=1/T)$: $S(E,V,N)$ entropy function $\xrightarrow{\text{Legendre tr.}}$ $\mathcal{F}(\beta,V,N)$ Mathieu function $= -\beta F(T,V,N)$ Free energy

Ensemble formulation (canonical)

I. An equilibirum state is given by the *canonical Gibbs state*

$$\hat{\rho}_{\mathrm{c}}^{\mathrm{ens}} = \frac{1}{Z} e^{-\beta \hat{H}} = \frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle\langle n| \qquad \left(Z \equiv \mathrm{Tr}\, e^{-\beta \hat{H}} \right),$$

in which an exponentially large # of pure states are mixed.

II. Mathieu function is given by

$$\mathcal{F} = \ln Z = -\mathrm{Tr}\,[\hat{\rho}_{\mathrm{c}}^{\mathrm{ens}} \ln \hat{\rho}_{\mathrm{c}}^{\mathrm{ens}}]$$

Similarly for other ensembles (e.g., grand canonical).

Theorem: Equivalence of ensembles

All ensembles give the equivalent results in the thermodynamic limit, $E \propto V \propto N \to \infty$. $\Leftarrow$ abbreviated as $V \to \infty$ or $N \to \infty$.

Summary of the Ensemble Formulation, and Questions

Ensemble formulation

I. An equilibirum state is given by

$$\hat{\rho}^{\text{ens}} = \frac{1}{W}\sum_n{}' |n\rangle\langle n| \quad \text{or} \quad \hat{\rho}_{\text{c}}^{\text{ens}} = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n|$$

II. Thermodynamic function $(S, \mathcal{F}, \cdots)$ is given by

$$S = -\text{Tr}\left[\hat{\rho}^{\text{ens}} \ln \hat{\rho}^{\text{ens}}\right] \quad \text{or} \quad \mathcal{F} = -\text{Tr}\left[\hat{\rho}_{\text{c}}^{\text{ens}} \ln \hat{\rho}_{\text{c}}^{\text{ens}}\right]$$

QI. Are the Gibbs states the only representations of an equilibirum state?

AI. No. *Many* other states are possible!

Even a *single* pure state $|\psi\rangle$ can represent the same equilibirum state.

$\to$ Thermal Pure Quantum (TPQ) state

QII. $\text{Tr}\left[\hat{\rho} \ln \hat{\rho}\right] = 0$ if $\hat{\rho} = |\psi\rangle\langle\psi|$. How to obtain $S, \mathcal{F}, \cdots$ from $|\psi\rangle$?

AII. An *appropriate* TPQ state gives S.

$\to$ TPQ formulation of statistical mechanics

Almost all states in the energy shell are an equilibrium state

— a rough argument —

For $\hat{M}_z = \sum_{\boldsymbol{r}} \hat{s}_z(\boldsymbol{r})$ (total magnetization), $\hat{\rho}^{\text{ens}}$ gives

$$\langle \hat{M}_z \rangle = O(V) \quad : \text{extensive}$$
$$\sqrt{\langle (\Delta \hat{M}_z)^2 \rangle} = O(\sqrt{V})$$

Relative deviation

$$\sqrt{\langle (\Delta \hat{M}_z)^2 \rangle} \Big/ \langle \hat{M}_z \rangle = O(1/\sqrt{V}) \to 0 \text{ as } V \to \infty$$

Similarly for all extensive (additive) variables.

For extensive variables, almost all states $|n\rangle$ in $\hat{\rho}^{\text{ens}} = \dfrac{1}{W}\sum_n{}' |n\rangle\langle n|$ have the same expectation values, in the sense that relative deviations $= O(V^{-\alpha}) \to 0$.

Well known among some physisists. (lecture by AS; books by T. Tasaki, Y. Oono,...)

But, the points in red are very unsatisfactory.

Almost all states in the energy shell are an equilibrium state

— a rigorous argument —

A. Sugita, RIMS Kokyuroku (Kyoto) **1507**, 147 (2006).

(more limited results by Popescu et al. (2006), Goldstein et al. (2006), P. Reimann (2007))

- Hilbert space: $\mathcal{H}_N$ $\quad (N$: number of spins of particles)
- Energy shell: $\mathcal{E}_{uN}$: subspace of $\mathcal{H}_N$ in $(E - \Delta E, E]$. $\quad (u \equiv E/N)$

$$\dim \mathcal{E}_{uN} = W = e^{Ns} \quad (s \equiv S/N = O(1))$$

- Probability measure: a random vector in $\mathcal{E}_{uN}$,

$$|\psi_{\mathrm{rnd}}\rangle = \sum_i{}' c_i |i\rangle$$

c_i : random complex numbers drawn uniformly from the sphere $\sum_i{}' |c_i|^2 = 1$.

$|i\rangle$: aribitrary basis of $\mathcal{E}_{uN}$.

This measure is invariant under choice of the basis. $\rightarrow$ natural measure!

- Physical quantities to define an equilibrium state: mechanical variables

— Two types of macroscopic variables in equilibirum statistical mechanics —

Mechanical Variables and Genuine Thermodynamic Variables

Mechanical variables

- Low-degree polynomials (i.e., their degree $= o(N)$) of local operators:

$$\hat{H},\ \hat{M}_z = \sum_{\boldsymbol{r}} \hat{s}_z(\boldsymbol{r}),\ (\hat{H})^2,\ \hat{s}_x(\boldsymbol{r})\hat{s}_y(\boldsymbol{r'}), \cdots$$

- To exclude foolish operators (such as $N^N \hat{H}$), we assume

$$|\langle \hat{A} \rangle| \leq K N^m \quad (\langle \cdot \rangle : \text{equilibrium value}),$$

where $K = O(1)$ and $m = o(N)$ are constants independent of $\hat{A}$.

Genuine thermodynamic variables

- Thermodynamic variables that cannot be represented as such operators:

$$T, \mu, \cdots, S, F, \cdots$$

$\notin$ quantum-mechanical observables in the standard sense.

- All genuine thermodynamic variables can be derived from one of thermodynamic functions, $S(E, N, V), F(T, V, N), \cdots$. ($\Leftrightarrow$ second law!)

Almost all states in the energy shell are an equilibrium state

— a rigorous argument —

Theorem (Sugita, 2006) : For a random vector in the energy shell, $|\psi_{\rm rnd}\rangle = \sum_i{}' c_i |i\rangle$,

$$\langle \psi_{\rm rnd} | \hat{A} | \psi_{\rm rnd} \rangle \xrightarrow{P} \langle \hat{A} \rangle^{\rm ens} \quad \left(= {\rm Tr}\, [\hat{\rho}^{\rm ens} \hat{A}] \right)$$

for every mechanical variable $\hat{A}$ uniformly, and exponentially fast, as $N \to \infty$.

That is (slightly improving Sugita's one), for ${}^\forall \epsilon > 0$

$$\mathrm{P}\left(\left| \langle \psi_{\rm rnd} | \hat{A} | \psi_{\rm rnd} \rangle - \langle \hat{A} \rangle^{\rm ens} \right| \geq \epsilon \right) \leq \frac{1}{\epsilon^2} \cdot \frac{O(|\langle \hat{A} \rangle^{\rm ens}|^2)}{\dim \mathcal{E}_{uN}} \leq \frac{1}{\epsilon^2} \cdot \frac{O(N^{2m})}{e^{Ns}} \to 0$$

for every mechanical variable $\hat{A}$, as $N \to \infty$.

- rough: only extensive variables $\to$ all mechanical variables.
- rough: only expectation values $\to$ also fluctuations and correlations.
- rough: relative deviation $\to$ deviation itself, even if value $= O(N^m)$.
- rough: slow convergence $O(V^{-\alpha})$ $\to$ exponentially fast convergence $e^{-O(N)}$.

It's not purification

An example of purification:

$$\hat{\rho} = (2/3)\,|1\rangle\langle 1| + (1/3)\,|2\rangle\langle 2| \quad : \text{ a mixed state on } \mathcal{H}_N.$$

By attaching an auxiliary system, enlarge $\mathcal{H}_N$ to $\mathcal{H}_N \otimes \mathcal{H}_{\text{aux}}$, and consider

$$|\Psi\rangle = \sqrt{2/3}\,|1\rangle \otimes |1'\rangle + \sqrt{1/3}\,|2\rangle \otimes |2'\rangle \quad : \text{ a pure state in } \mathcal{H}_N \otimes \mathcal{H}_{\text{aux}}.$$

Then,

$$\langle \Psi|(\hat{a} \otimes \hat{1})|\Psi\rangle = \text{Tr}\,[\hat{\rho}\hat{a}] \quad \text{for all observables } \hat{a} \text{ on } \mathcal{H}_N.$$

Purification

It is *always* possible to represent a mixed state $\hat{\rho}$ on $\mathcal{H}_N$ as a pure state $|\Psi\rangle$ in an enlarged space $\mathcal{H}_N \otimes \mathcal{H}_{\text{aux}}$. They are the same state on $\mathcal{H}_N$.

ex. Thermo Field Dynamics (TFD) utilizes purification.

By contrast, in Sugita's theory

- $|\psi_{\text{rnd}}\rangle$ is a pure state in $\mathcal{H}_N$.
- $|\psi_{\text{rnd}}\rangle\langle\psi_{\text{rnd}}| \neq \hat{\rho}^{\text{ens}}$ on $\mathcal{H}_N$ (manifest by entanglement $\leftarrow$ discuss later)
- But, $|\psi_{\text{rnd}}\rangle$ and $\hat{\rho}^{\text{ens}}$ are statistical-mechanically identical!

Answer to Question I, and further questions

QI. Are the Gibbs states $\hat{\rho}^{\mathrm{ens}}$ the only representations of an equilibirum state?

AI. No. A pure state $|\psi_{\mathrm{rnd}}\rangle$ represents the same equilibirum state.

Problems and further questions:

1. For $\hat{\rho} = |\psi_{\mathrm{rnd}}\rangle\langle\psi_{\mathrm{rnd}}|$, the conventional formula gives a wrong result, $S = \mathrm{Tr}\,[\hat{\rho}\ln\hat{\rho}] = 0$.

   → Impossible to obtain genuine thermodynamic variables from $|\psi_{\mathrm{rnd}}\rangle$.

   → **QII.** How to obtain $S, \mathcal{F}, \cdots$ from (another) $|\psi\rangle$?

2. Generally, the canonical Gibbs state (specified by T, V, N) is much more convenient than the microcanonical Gibbs state (specified by E, V, N).

   $|\psi_{\mathrm{rnd}}\rangle$ (specified by E, V, N) corresponds to the microcanonical one.

   → **QIII.** Another $|\psi\rangle$ specified by T, V, N?

3. Practically, $|\psi_{\mathrm{rnd}}\rangle$ is harder to obtain than $\hat{\rho}^{\mathrm{ens}}$.

   → **QIV.** Another $|\psi\rangle$ easier to obtain?

Our Solutions — TPQ formulation of statistical mechanics

S. Sugiura and AS, Phys. Rev. Lett. **108** (2012) 240401.
S. Sugiura and AS, Phys. Rev. Lett. **111** (2013) 010401.
S. Sugiura and AS, arXiv:1312.5145.
M. Hyuga, K. Sakai, S. Sugiura and AS, in preparation

1. *Generally* define **Thermal Pure Quantum (TPQ) state** as a pure state that represents an equilibirum state. **ex.** $|\psi_{\rm rnd}\rangle$ is one of TPQ states.
2. *New types* of TPQ states $|\beta, V, N\rangle$, $|\beta, V, \mu\rangle$, ...
   $\to$ **Yes** to **QIII.** Another $|\psi\rangle$ specified by T, V, N?
3. *Formulas for getting thermodynamic functions* from $|\beta, V, N\rangle, |\beta, V, \mu\rangle$, ...
   $\to$ **Solutions** to **QII.** How to obtain $S, \mathcal{F}, \cdots$ from (another) $|\psi\rangle$?
4. $|\beta, V, N\rangle, |\beta, V, \mu\rangle$, ... are *much easier* to obtain than $\hat{\rho}^{\rm ens}$ and $|\psi_{\rm rnd}\rangle$.
   $\to$ **Yes** to **QIV.** Another $|\psi\rangle$ easier to obtain?
5. Practical formulas.

Setup

Quantum system

- composed of N sites or particles, confined in a box of volume V.
- (irreducible) Hilbert space is $\mathcal{H}_N$. dim $\mathcal{H}_N$ can be ∞.
- each equilibrium state is specified by $E, V, N, \ldots \rightarrow$ abbreviated as E, V, N.

Assumptions : Ensemble formulation gives correct results, which are *consistent with thermodynamics* in the t.d.l ($E \propto V \propto N \to \infty$).

- $S(E, V, N)/N \to s(u, v)$: entropy density, $u \equiv E/N$, $v \equiv V/N$.
- $s(u, v)$ is a concave function, continuously differentiable even at phase transitions. see, e.g., 清水「熱力学の基礎」(東大出版会, 2007)
- For every mechanical variable $\hat{A}$,

$$|\langle \hat{A} \rangle^{\mathrm{ens}}| \leq K N^m$$

where $K = O(1)$ and $m = o(N)$ are constants independent of $\hat{A}$.

Thermal Pure Quantum (TPQ) state

A state $|\psi\rangle$ $(\in \mathcal{H}_N)$, which has a random variable, is called a TPQ state if

$$\langle \hat{A} \rangle_N^{\psi} \equiv \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle} \overset{P}{\to} \langle \hat{A} \rangle_N^{\text{ens}} \equiv \text{Tr}\,[\hat{\rho}^{\text{ens}} \hat{A}]$$

for every mechanical variable $\hat{A}$ uniformly, as $N \to \infty$.

That is, $\forall \epsilon > 0$ there exists a function $\eta_\epsilon(N)$ that vanishes as $N \to \infty$ and

$$\text{P}\left(\left| \langle \hat{A} \rangle_N^{\psi} - \langle \hat{A} \rangle_N^{\text{ens}} \right| \geq \epsilon \right) \leq \eta_\epsilon(N)$$

for every mechanical variable $\hat{A}$.

Remark: cannot be obtained by purifying $\hat{\rho}^{\text{ens}}$ because $|\psi\rangle \in \mathcal{H}_N$.

Independent variables

- β, V, N : canonical TPQ state $|\beta, V, N\rangle$.
- β, V, μ : grand-canonical TPQ state $|\beta, V, \mu\rangle$.

Canonical TPQ state : $|\beta, V, N\rangle$ abbreviated as $|\beta, N\rangle$

★ PRL version (2013) assumed $\dim \mathcal{H}_N < +\infty$.

Here, slightly generalized s.t. applicable to $\dim \mathcal{H}_N = \infty$.

Let

- $\{|\nu\rangle\}_\nu$: an aribitrary basis of $\mathcal{H}_N$ (c.f. Sugita's $\{|i\rangle\}_i$: a basis of $\mathcal{E}_{uN}$)
- x_ν, y_ν : real random variables, obeying the standard normal distribution
- $c_\nu \equiv (x_\nu + i y_\nu)/\sqrt{2}$. (c.f. PRL version imposed $\sum_\nu |c_\nu|^2 = 1$)

Then,

$$|\beta, N\rangle \equiv \sum_\nu c_\nu \exp[-\beta \hat{H}/2] |\nu\rangle \quad \text{(well-defined even when } \dim \mathcal{H}_N = \infty)$$

is the canonical TPQ (cTPQ) state, specified by β, N;

$$\langle \hat{A} \rangle^{\text{TPQ}}_{\beta,N} \equiv \frac{\langle \beta, N | \hat{A} | \beta, N \rangle}{\langle \beta, N | \beta, N \rangle} \xrightarrow{P} \langle \hat{A} \rangle^{\text{ens}}_{\beta,N} \equiv \frac{1}{Z} \text{Tr}\,[e^{-\beta \hat{H}} \hat{A}]$$

for every mechanical variable $\hat{A}$ uniformly, in the t.d.l.

Outline of Proof

We use a Markov-type inequality:

$$\text{For } \forall\epsilon > 0,\ \ \mathrm{P}\left(|x-y| \geq \epsilon\right) \leq \overline{(x-y)^2}/\epsilon^2.$$

Taking $x = \langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,N}$, $y = \langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N}$, $\overline{(x-y)^2} = \overline{(\langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,N} - \langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N})^2} \equiv D_N(A)^2$,

$$\mathrm{P}\left(\left|\langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,N} - \langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N}\right| \geq \epsilon\right) \leq D_N(A)^2/\epsilon^2.$$

Using $\overline{c^*_\nu c_\xi} = \delta_{\nu,\xi}$, $\overline{c^*_\nu c_\xi c^*_\eta c_\zeta} = \delta_{\nu,\xi}\delta_{\eta,\zeta} + \delta_{\nu,\zeta}\delta_{\eta,\xi}$, etc, and dropping smaller-order terms, we find

$$D_N(A)^2 \leq \frac{\langle(\Delta\hat{A})^2\rangle^{\mathrm{ens}}_{2\beta,N} + (\langle A\rangle^{\mathrm{ens}}_{2\beta,N} - \langle A\rangle^{\mathrm{ens}}_{\beta,N})^2}{\exp[2N\beta\{f(1/2\beta;N) - f(1/\beta;N)\}]} \leq \frac{N^{2m}}{e^{O(N)}}$$

where

$\langle(\Delta\hat{A})^2\rangle^{\mathrm{ens}}_{\beta,N} \equiv \langle(\hat{A} - \langle A\rangle^{\mathrm{ens}}_{\beta,N})^2\rangle^{\mathrm{ens}}_{\beta,N}$,

$f(T;N) \equiv F/N$ (free energy density) $\to f(T)$ as $N \to \infty$,

$f(1/2\beta;N) - f(1/\beta;N) = O(1) > 0$ because $s = -\partial f/\partial T = O(1) > 0$.

Probability of Error

Therefore, for $\forall \epsilon > 0$,

$$\mathrm{P}\left(\left|\langle \hat{A} \rangle^{\mathrm{TPQ}}_{\beta,N} - \langle \hat{A} \rangle^{\mathrm{ens}}_{\beta,N}\right| \geq \epsilon\right)$$

$$\leq \frac{1}{\epsilon^2} \cdot \frac{\langle (\Delta \hat{A})^2 \rangle^{\mathrm{ens}}_{2\beta,N} + (\langle A \rangle^{\mathrm{ens}}_{2\beta,N} - \langle A \rangle^{\mathrm{ens}}_{\beta,N})^2}{\exp[2N\beta\{f(1/2\beta; N) - f(1/\beta; N)\}]} \leq \frac{1}{\epsilon^2} \cdot \frac{N^{2m}}{e^{O(N)}} \to 0.$$

This shows that

$$\langle \hat{A} \rangle^{\mathrm{TPQ}}_{\beta,N} \xrightarrow{P} \langle \hat{A} \rangle^{\mathrm{ens}}_{\beta,N} \text{ for every mechanical variable } \hat{A} \text{ unifromly.}$$

Therefore,

- $|\beta, N\rangle$ is the canonical TPQ (cTPQ) state.
- Its single realization gives the equilibrium values of mechanical variables, with exponentially small probability of error, as $\langle \hat{A} \rangle^{\mathrm{TPQ}}_{\beta,N}$.

■

Formula for Thermodynamic Function

Let $Z(\beta, N) \equiv \mathrm{Tr}\, e^{-\beta \hat{H}}$ (partition function). We can show

$$\mathrm{P}\left(\left| \frac{\langle \beta, N | \beta, N \rangle}{Z(\beta, N)} - 1 \right| \geq \epsilon \right) \leq \frac{1}{\epsilon^2} \cdot \frac{1}{\exp[2N\beta\{f(1/2\beta; N) - f(1/\beta; N)\}]} \leq \frac{1}{\epsilon^2} \cdot \frac{1}{e^{O(N)}}.$$

This shows

$$\langle \beta, N | \beta, N \rangle \xrightarrow{P} Z(\beta, N).$$

A single realization of $|\beta, N\rangle$ gives $f = F/N$, with exponentially small probability of error, by

$$-\beta f(1/\beta; N) = \frac{1}{N} \ln \langle \beta, N | \beta, N \rangle.$$

All genuine thermodynamic variables can be calculated from f.

Only a single realization of the TPQ state gives all variables of statistical-mechanical interest.

Self-Validation

Using f obtained from this formula, one can estimate the upper bounds of errors of f itself and $\langle \hat{A} \rangle^{\mathrm{TPQ}}_{\beta,N}$.

- Our formulas are almost self-validating.
- This is particularly useful in practical applications!

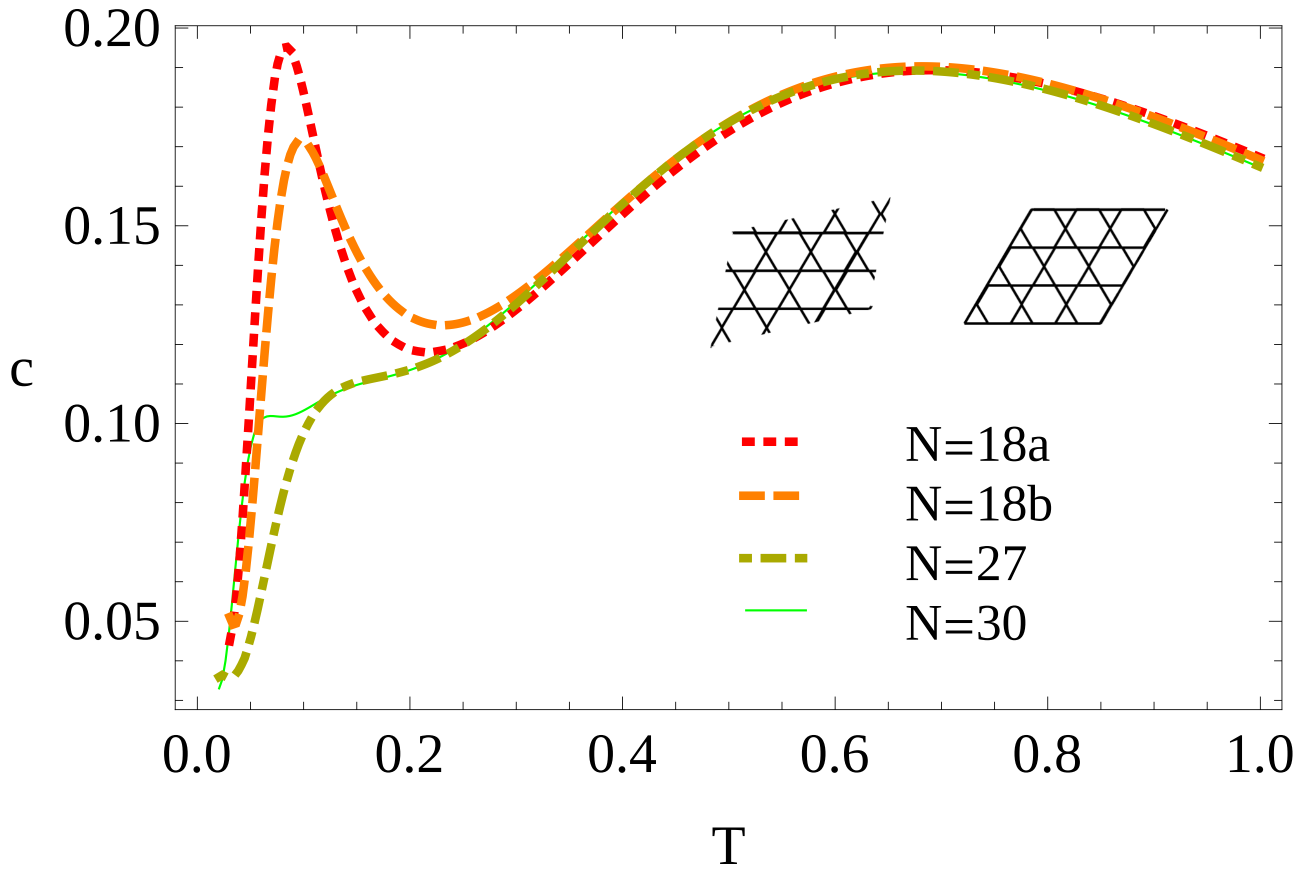
Application to the spin-1/2 kagome Heisenberg antiferromagnet

A frustrated two-dimensional quantum spin system

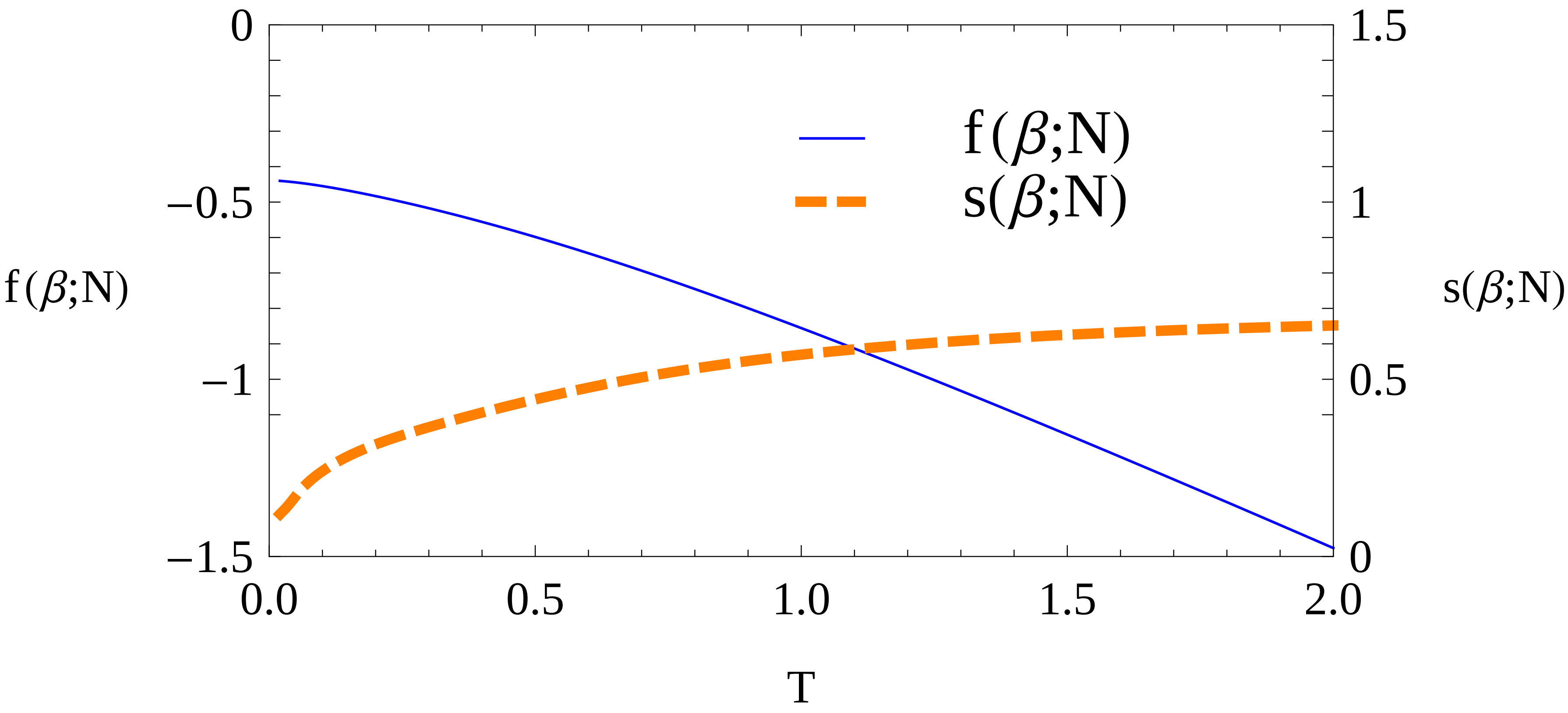
$\rightarrow$ Sign problem is fatal to quantum Monte Carlo method.

Numerical diagonalization : $N \lesssim 18 \rightarrow$ double peaks in the specific heat?

cTPQ : $N = 27 - 30 \rightarrow$ disapperance of the lower peak!



Thermodynamic functions f and s of KHA



45% of the total entropy $(= N \ln 2)$ remains at $T = 0.2J$.

$\rightarrow$ typical to frustration systems.

$\rightarrow$ hard with most other methods.

$\rightarrow$ But, favorable to TPQ formulation because error $\sim 1/e^{Ns}$.

From our formulas for errors, errors $\leq 1\%$ for $T \geq 0.1J$.

Practical Formulas using microcanonical TPQ (mTPQ) states

In practical computations, one introduces a cutoff to make $\dim \mathcal{H}_N$ finite.
Since $\dim \mathcal{H}_N < +\infty$,

- Using an arbitrary basis $\{|\nu\rangle\}$, such as a trivial one, one can easily generate a random vector $\in \mathcal{H}_N$ as

$$|0\rangle \equiv \sum_{\nu} c_\nu |\nu\rangle \quad (\neq \text{Sugita's } |\psi_{\mathrm{rnd}}\rangle \in \mathcal{E}_{uN})$$

- $\hat{h} \equiv \hat{H}/N$ has the maximum eigenvalue $e_{\max}$.

  $\Rightarrow$ One can take an aribitray number l such that $l \geq e_{\max}$.

Using these, compute

$$|k\rangle \equiv (l - \hat{h})^k |0\rangle$$

iteratively for $k = 0, 1, 2, \ldots$.

We can show: $u \equiv E/N$ has a sharp peak around $u \simeq \langle k|\hat{h}|k\rangle / \langle k|k\rangle$

$\Rightarrow$ a mTPQ state $(\neq$ Sugita's $|\psi_{\mathrm{rnd}}\rangle)$

In terms of *normalized* mTPQ states,

$$|\psi_k\rangle \equiv (1/\sqrt{Q_k})|k\rangle \quad (Q_k \equiv \langle k|k\rangle),$$

the cTPQ state $|\beta, N\rangle$ can be expanded as

$$e^{N\beta l/2}|\beta, N\rangle = \sum_{k=0}^{\infty} \frac{(N\beta/2)^k}{k!}|k\rangle = \sum_{k=0}^{\infty} R_k|\psi_k\rangle \quad \left(R_k \equiv \frac{(N\beta/2)^k}{k!}\sqrt{Q_k} \right).$$

- this sum is uniformly convergent on any finite interval of β.
- R_k takes significant values only for k s.t. $\langle\psi_k|\hat{h}|\psi_k\rangle = \langle\hat{h}\rangle^{\mathrm{TPQ}}_{\beta,N} + O(1/V)$.
- As k moves away from such values, R_k vanishes exponentially fast.

$|\beta, N\rangle$ is superpositon of $|\psi_k\rangle$'s which represent the same equilibirum state.

- One can terminate the sum at a finite number k_{term}, which depends on the largest β of interest, β_{max}.
- For any $\beta_{\mathrm{max}} = O(1)$, we can show that $k_{\mathrm{term}} = O(N)$.
- $|1\rangle, |2\rangle, \cdots, |k_{\mathrm{term}}\rangle$ can be obtained iteratively by simply multiplying $(l - \hat{h})$ with a random vector k_{term} times.

One can obtain $|\beta, N\rangle$ by multiplying $(l - \hat{h})$ with a random vector $|0\rangle \in \mathcal{H}_N$, repeatedly $O(N)$ times.

- Larger $l \;\Rightarrow\;$ better results but larger $k_{\rm term}$.

Advantages when Applied to Numericl Computations

- Free from the sign problem

  $\Rightarrow$ frustrated systems, fermion systems

- Applicable to any spatial dimensions
- Effective over a wide range of T
- Self-validating
- Only matrix multiplications of $O(N)$ times.
- Only two vectors (i.e., computer memory)

Entanglement

TPQ state vs. Gibbs state

- Identical concerning mechanical variables.
- But, maximally different with respect to entanglement.

Example: $T \gg J$

$\hat{\rho}^{\text{ens}} \simeq \hat{1} \;\Rightarrow\;$ no entanglement.

$|k\rangle, |\beta, N\rangle, \ldots$ have almost maximum (exponentially large) entanglement.

> An equilibrium state can be represented either by a TPQ state with exponentially large entanglement or by a mixed state with much less entanglement.

Their difference can be detected only by high-order correlations of local operators, which are not of statistical-mechanical interest.

- A. Sugita and AS, J. Phys. Soc. Jpn. **74** (2005) 1883.
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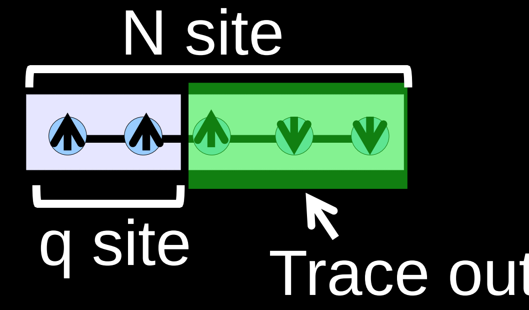
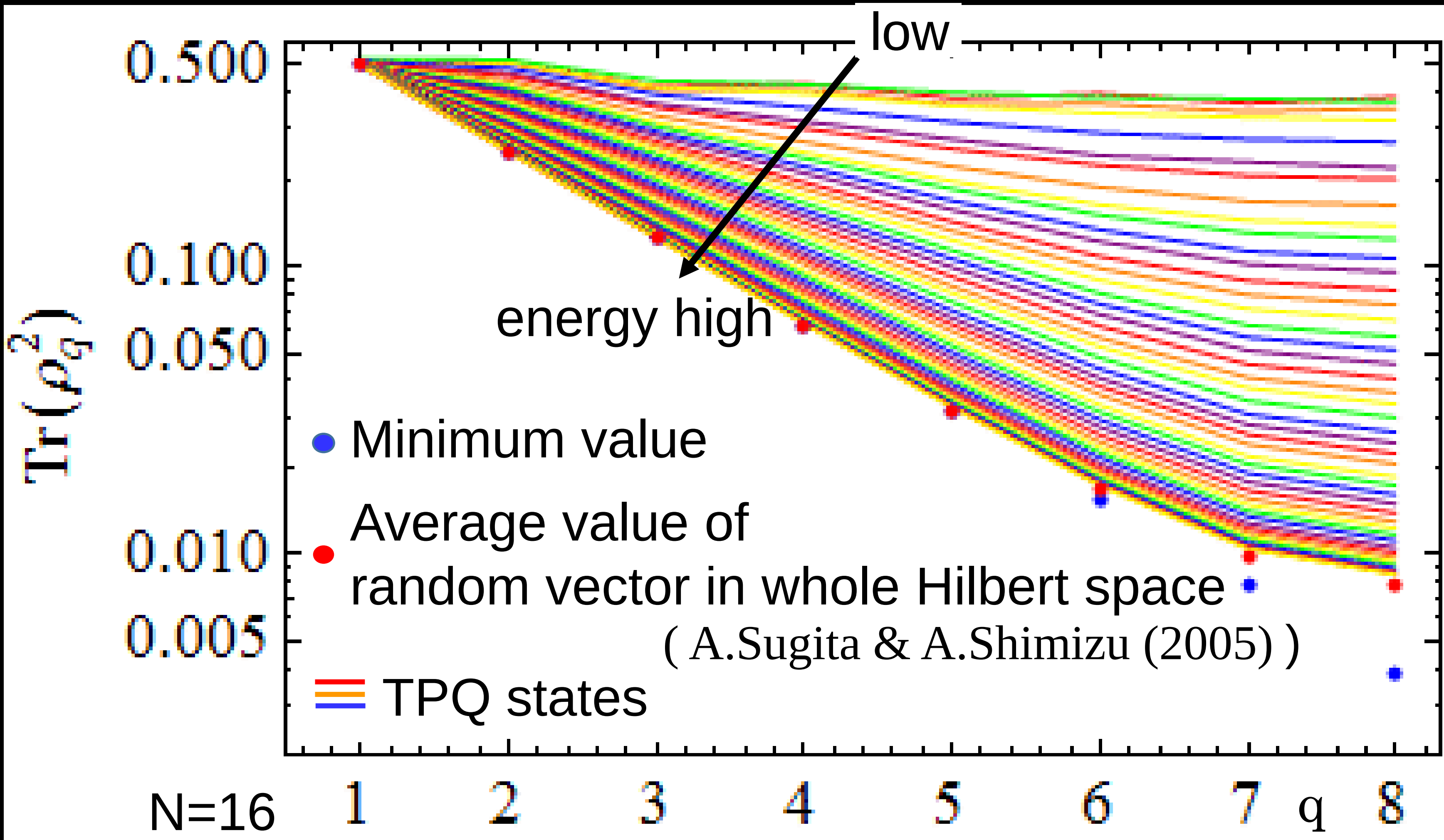
- S. Sugiura and AS, 物理学会2013春

Entanglement -Purity





TPQ states are almost maximally entangled

More Practical Formulas # 1

Let

$$\{\hat{A}\}'_{\beta,N} \equiv \sum_{k=0}^{\infty} \frac{(N\beta)^{2k}}{(2k)!} \langle k|\hat{A}|k\rangle + \sum_{k=0}^{\infty} \frac{(N\beta)^{2k+1}}{(2k+1)!} \langle k|\hat{A}|k+1\rangle,$$

$$\{\hat{A}\}^{\mathrm{TPQ}}_{\beta,N} \equiv \{\hat{A}\}'_{\beta,N} / \{\hat{1}\}'_{\beta,N}.$$

We can show that

$$\{\hat{1}\}'_{\beta,N} \xrightarrow{P} Z(\beta,N),$$

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

exponentially fast and uniformly.

Useful because one needs only to calculate $\langle k|\hat{A}|k\rangle$ and $\langle k|\hat{A}|k+1\rangle$ for all $k \leq k_{\mathrm{term}}$ to obtain the results for *all* $\beta \leq \beta_{\mathrm{max}}$.

More Practical Formulas # 2

When computer resources are not sufficient to treat large enough N
$\Rightarrow$ e^{Ns} is not large enough.
$\Rightarrow$ One can reduce errors by averaging over many realizations of the cTPQ states because

$$\frac{1}{V}\ln\overline{\langle\beta,N|\beta,N\rangle} = \frac{1}{V}\ln\overline{\{\hat{1}\}'_{\beta,N}} = -\beta f(1/\beta;N).$$

$$\frac{\overline{\langle\beta,N|\hat{A}|\beta,N\rangle}}{\overline{\langle\beta,N|\beta,N\rangle}} = \frac{\overline{\{\hat{A}\}'_{\beta,N}}}{\overline{\{\hat{1}\}'_{\beta,N}}} = \langle\hat{A}\rangle^{\text{ens}}_{\beta,N},$$

Averaging over M realiztions reduces the error, as measured by the standard deviation, by the factor of $1/\sqrt{M}$.

Summary — TPQ formulation of statistical mechanics

1. *Generally* define Thermal Pure Quantum (TPQ) state as a pure state that represents an equilibirum state.

2. *New types* of TPQ states $|\beta, V, N\rangle$, $|\beta, V, \mu\rangle$, ...

3. *Formulas for getting thermodynamic functions* from $|\beta, V, N\rangle, |\beta, V, \mu\rangle,$ ....

4. $|\beta, V, N\rangle, |\beta, V, \mu\rangle,$ .... are *much easier* to obtain than $\hat{\rho}^{\text{ens}}$ and $|\psi_{\text{rnd}}\rangle$.

5. Practical formulas.

6. Many advantages when applied to numerical computations.