Statistical Mechanics without Ensembles

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Reference:

S. Sugiura and AS, arXiv:1112.0740.

CONTENTS

Ergodic hypothesis is not neccessary for statistical mechanics

See, e.g., Y. Oono, H. Tasaki, A. Sugita, ...

Is ‘equal a priori probability postulate’ (等重率の原理) necessary?

Lecture by AS at Univ. Tokyo, Komaba (since > 10 years ago)

熱力学： 清水「熱力学の基礎」（東大出版会）

要請 II-(ii), (iv)

単純系のSは，エネルギーEを含むいくつかの相加変数の組$E, X_1, ..., X_t$（エントロピーの自然な変数）のC^1級関数である：$S = S(E, X_1, \cdots, X_t)$.
平衡状態は，$E, X_1, ..., X_t$で一意的に指定される.

統計力学：清水「統計力学の基礎」（清水研 HP にて公開中）

定義：ミクロカノニカル集団

$E, X_1, \cdots, X_t$の値が（相対的に無視できるゆらぎの範囲内で）等しいようなミクロ状態を全て集めた集合を$\mathrm{ens}(E, X_1, \cdots, X_t)$と記す.

要請 $\mathbf{A_0}$

孤立した単純系では，$\mathrm{ens}(E, X_1, \cdots, X_t)$の中から任意にひとつミクロ状態を選び出したとき，それはほとんど確実に，その$E, X_1, \cdots, X_t$で指定される平衡状態（に対応するミクロ状態のひとつ）である.

That is,

$$\begin{tikzcd}
\text{equilibrium state} \arrow[r, Longrightarrow] \arrow[d, shift right] & \text{many microstates} \\
E, X_1, \cdots, X_t \arrow[u, shift right] \arrow[d] & \\
\text{ens}(E, X_1, \cdots, X_t) \arrow[r, Longrightarrow] & \text{many microstates} \arrow[uu, "\text{almost all}"']
\end{tikzcd}$$

Therefore, for macrovariables (which can be represented as observables)

$$\text{equilibrium value} = \begin{cases} \text{its value in a state in } \text{ens}(E, X_1, \cdots, X_t), \\ \qquad \text{or} \\ \text{its average in } \text{ens}(E, X_1, \cdots, X_t). \end{cases}$$

For most practical purposes, the latter is more convenient.

- Can avoid the risk of taking exceptional states.
- Can avoid troubles specific to integrable systems.

Replace A_0 with a practical hypothesis A

定義：ミクロカノニカル分布

$\mathrm{ens}(E, X_1, \cdots, X_t)$に属する全てのミクロ状態に等しい確率を与えた確率分布.

要請A：等重率の原理（と本書では呼ぶ）

孤立した単純系の，エントロピーの自然な変数$E, X_1, \cdots, X_t$で指定される平衡状態は，ミクロカノニカル分布と，熱力学的に同じ状態になる.

Remarks:

- Postulte $\mathrm{A}_0 \;\Rightarrow\;$ Postulte A
- One can employ Postulte A for most practical purposes.
- For deeper understanding, however, Postulate A_0 should be taken.
- Boltzmann formula is also necessary (Postulate B).

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1. Introduction: Principles of statistical mechanics revisited.
2. Thermal Pure Quantum states (TPQs)
3. Formulation of statistical mechanics with TPQs
    (a) Construction of a new class of TPQs
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    (c) Application to numerical computaion
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Partial proof of postulate A$_0$

Notation:

- Abbreviate $E, X_1, \cdots, X_t$ to E, N.
- $\mathcal{E}_{E,N}$: 'Energy shell' ($\equiv$ Hilbert subspace corresponding to ens(E, N))
- $\hat{\rho}^{eq}$: Gibbs state (e.g., $\hat{\rho}^{eq} = e^{-\beta \hat{H}}/Z$)

The following have been shown (roughly speaking):

(Popescu et al. (2006), Goldstein et al. (2006), A. Sugita (2006), P. Reimann (2007))

1. Almost all $|\psi\rangle$'s in $\mathcal{E}_{E,N}$ are macrosopically identical; $\langle\psi|\hat{A}|\psi\rangle \simeq \langle\psi'|\hat{A}|\psi'\rangle$.
2. Almost all $|\psi\rangle$'s in $\mathcal{E}_{E,N}$ satisfy $\langle\psi|\hat{A}|\psi\rangle \simeq \mathrm{Tr}\left(\hat{\rho}^{eq}\hat{A}\right)$.

Remark: Postulate A$_0$ (or A) is not fully proved.

$$\langle\psi|\hat{A}|\psi\rangle \simeq \mathrm{Tr}\left(\hat{\rho}^{eq}\hat{A}\right) = ?$$

To *derive thermodynamics*, one needs to derive the complete set of axioms of thermodynamics (such as those given in 清水「熱力学の基礎」).

‘Almost all’ states in $\mathcal{E}_{E,N}$?

A random vector in $\mathcal{E}_{E,N}$

$$|\psi\rangle = \sum_{\nu}{}' c_\nu |\nu\rangle.$$

$\{|\nu\rangle\}_\nu$: an arbitrary orthonormal basis set of $\mathcal{E}_{E,N}$

$\displaystyle\sum_{\nu}{}'$: sum over this basis

$\{c_\nu\}_\nu$: a set of random complex numbers, drawn uniformly from the unit sphere $\sum_\nu' |c_\nu|^2 = 1$ in the complex space of dimension $\dim \mathcal{E}_{E,N}$.

Subsystem

S. Popescu, A.J. Short, and A. Winter, Nature Phys. **2**, 758 (2006).
S. Goldstein *et al*, Phys. Rev. Lett. **96**, 050403 (2006).

Look at a small subsystem.

Let β be the (unknown) value of $1/T$ at the energy density E/N.

Theorem: For almost all $|\psi\rangle$ in $\mathcal{E}_{E,N}$, the subsytem is in the canonical Gibbs state. That is, as $N \to \infty$ (while E/N is fixed),

$$\langle\psi|\hat{A}_{\text{sub}}|\psi\rangle \sim \mathrm{Tr}\left(\frac{1}{Z_{\text{sub}}}e^{-\beta\hat{H}_{\text{sub}}}\hat{A}_{\text{sub}}\right)$$

for every observables of the subsystem.

Total system

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

P. Reimann, Phys. Rev. Lett. **99**, 160404 (2007).

Let $\hat{\rho}_{E,N}$ be the microcanonical Gibbs state corresponding to ens(E, N).
It is clear that

$$\langle\psi|\hat{A}|\psi\rangle \sim \mathrm{Tr}\left(\hat{\rho}_{E,N}\hat{A}\right)$$

does not hold for every observables of the total system.
However, it holds for every observables of statistical mechanical interest!

Let $\hat{A}$ be a low-degree polynomial (i.e., degree $\ll N$) of local operators.
We call such an observable mechanical variable.

Theorem: For an arbitrary positive number ϵ

$$\mathrm{Prob}\left(\left|\langle\psi|\hat{A}|\psi\rangle - \mathrm{Tr}\left(\hat{\rho}_{E,N}\hat{A}\right)\right| \geq \epsilon\right) \leq \frac{\|\hat{A}\|^2}{\epsilon^2 \dim \mathcal{E}_{E,N}} \to 0$$

as $N \to \infty$ (while E/N is fixed), for every mechanical variable $\hat{A}$.

Important for deeper understanding of statistical mechanics.
But, we want to go further.

For conceptual clarity ...

We call generally a set of pure quantum states *thermal pure quantum states* (TPQs) for the microcanonical ensemble if for an arbitrary positive number ϵ

$$\mathrm{Prob}\left(\left|\langle\psi|\hat{A}|\psi\rangle - \mathrm{Tr}\left(\hat{\rho}_{E,N}\hat{A}\right)\right| \geq \epsilon\right) \leq \eta_\epsilon(N)$$

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

$\eta_\epsilon(N)$: a function which vanishes as $N \to \infty$.

Furthermore ...

- We call each state of TPQs a TPQ.
- TPQs for other ensembles are similarly defined.

Getting a single TPQ is sufficient, with high probability, for evaluating equilibrium values of mechanical variables.

Example: ${\sum_\nu}' c_\nu |\nu\rangle$ of the previous works.

Problems:

1. Genuine thermodynamic variables (such as T, S) ?

   Cannot be calculated as $\langle \psi | \hat{A} | \psi \rangle$.

2. Hard to construct.

   Needs to prepare a basis $\{|\nu\rangle\}_\nu$ of the energy shell.

Our solution

S. Sugiura and AS, arXiv:1112.0740.

- A new class of TPQs.
- A simple method for constructing them.
- Formulas giving genuine thermodynamic variables.

From a single TPQ, one can calculate all variables of statistical-mechanical interest, including genuine thermodynamic variables, at finite temperature.

What does it imply?

Formulation of Statistical Mechanics

Conventional : ensembles and $S = \ln W$ or $F = -T \ln Z$ (and ergodicity)

$$\downarrow$$

New : TPQ and our formula for genuine thermodynamic variables

Statistical mechanics based on TPQs

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Systems under consideration (and notation)

- A discrete quantum system composed of N sites.
- Hilbert space $\mathcal{H}_N$ of dimension $D = \lambda^N$, where λ is a constant of $O(1)$.

Primary purpose

Obtain results in the thermodynamic limit: $N \to \infty$ while E/N is fixed.

- Quantities per site:
  - $\hat{h} \equiv \hat{H}/N$
  - $u \equiv E/N$
  - $(u; N)$ instead of (E, N).
- Do not write explicitly variables other than u and N, such as a magnetic field.

Assumptions: Statistical mechanics is applicable

- Boltzmann formula is applicable (although we do not use it):

$$S(E,N) = \ln\left[g(u;N)\Delta E\right] + o(N),$$

where $g(u;N)$ is the density of states.

- It gives the correct thermodynamic entropy:

$$\lim_{N\to\infty} \frac{S(E,N)}{N} = s(u;\infty).$$

That is,

$$\boxed{g(u;N) = \exp[N s(u;N)], \qquad \lim_{N\to\infty} s(u;N) = s(u;\infty).}$$

- The system is thermodynamically stable:

$$\boxed{\beta' \equiv \frac{\partial \beta}{\partial u} \le 0.}$$

Here, $\beta(u;N) \equiv \dfrac{\partial s(u;N)}{\partial u}$ is the inverse temperature.

Remarks

- spin models, Hubburd models, ...
- Since D $(= \dim \mathcal{H}_N)$ is finite, $\beta < 0$ in a high-energy region.

  → We construct TPQs in a low-energy region, where $\beta > 0$.

Construction of a new class of TPQs

1. Take a random vector from the whole Hilbert space $\mathcal{H}_N$;

$$|\psi_0\rangle \equiv \sum_i c_i|i\rangle.$$

- $\{|i\rangle\}_i$: an arbitrary orthonormal basis of $\mathcal{H}_N$
- $\{c_i\}_i$: a set of random complex numbers drawn uniformly from the unit sphere $\sum |c_i|^2 = 1$ of the D-dimensional complex space.

This construction is independent of the choice of $\{|i\rangle\}_i$.
→ Can use a trivial basis (such as a set of product states).
→ $|\psi_0\rangle$ can be generated easily (unlike $\sum_\nu' c_\nu|\nu\rangle$).

Amplitude is almost equally distributed over *all* the energy eigenstates.

$$\therefore \ [\text{distribution of energy in } |\psi_0\rangle] \propto g(u;N).$$

2. Take a constant l of $O(1)$ such that $l \geq e_{\rm max}$.
Here, $e_{\rm min} \leq$ [eigenvalue of $\hat{h}$] $\leq e_{\rm max}$.

3. Starting from $|\psi_0\rangle$, calculate

$$\begin{aligned} u_k &\equiv \langle \psi_k | \hat{h} | \psi_k \rangle, \\ |\psi_{k+1}\rangle &\equiv (l - \hat{h}) |\psi_k\rangle / \| (l - \hat{h}) |\psi_k\rangle \| \end{aligned}$$

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

Note: Multiplying $\hat{h}$ is much easier than diagonalizing it.

4. Terminate the iteration when u_k gets low enough for one's purpose (k at this point is denoted by $k_{\rm term}$).

We will show

- u_0 corresponds to $\beta = 0$, i.e., $g(u; N)$ takes the maximum at $u = u_0$.
- $u_0 > u_1 > u_2 > \cdots \geq e_{\mathrm{min}}$.
- $k_{\mathrm{term}} = O(N)$ at finite temperature,
- $|\psi_0\rangle, |\psi_1\rangle, \cdots$ become a series of TPQs corresponding to various energy densities, $u_0, u_1, \cdots$.
- Can calculate the equilibrium value of an arbitrary mechanical variable $\hat{A}$ as $\langle\psi_k|\hat{A}|\psi_k\rangle$, as a function of u_k.
- Dependence of $\langle\psi_k|\hat{A}|\psi_k\rangle$ on $\{c_i\}_i$ is exponentially small in size N.

  → Only a single TPQ suffices for getting a fairly accurate value.

Proof of $|\psi_{\boldsymbol{k}}\rangle$ = TPQ

$|\psi_0\rangle = \sum_i c_i|i\rangle$: independent of the choice of the basis

→ Take the energy eigenstates $\{|n\rangle\}_n$ as $\{|i\rangle\}_i$

(although we never use such a basis in practical calculations)

$$|\psi_0\rangle = \sum_n c_n|n\rangle$$

After k-times multiplication of $l - \hat{h}$,

$$|\psi_k\rangle \propto (l - \hat{h})^k|\psi_0\rangle = \sum_n c_n(l - e_n)^k|n\rangle \quad (\hat{h}|n\rangle = e_n|n\rangle)$$

The distribution function of u is

$$r_k(u;N) \propto \frac{1}{\delta_r} \sum_{n \text{ s.t.} e_n \in [u-\delta_r/2, u+\delta_r/2)} |c_n|^2(l - e_n)^{2k} \qquad (\delta_r = o(1))$$

$$= \frac{1}{D}\frac{1}{\delta_r}\int_{u-\delta_r/2}^{u+\delta_r/2} (l - u)^{2k} g(u;N)du \qquad (D = \dim \mathcal{H}_N)$$

Recalling that

$$g(u;N) = \exp[Ns(u;N)]$$

we have

$$\begin{aligned} r_k(u;N) &\propto D^{-1}\exp[Ns(u;N) + 2k\ln(l-u)] \\ &= D^{-1}\exp[N\xi(u;N)], \end{aligned}$$

where

$$\begin{aligned} \xi(u;N) &\equiv s(u;N) + 2\kappa\ln(l-u), \\ \kappa &\equiv k/N. \end{aligned}$$

See PDF.

We define

$$\hat{\rho}_k \equiv \frac{1}{\sum_n (l - e_n)^{2k}} \sum_n (l - e_n)^k |n\rangle\langle n| (l - e_n)^k.$$

Its energy distributes according to $r_k(u; N)$.

→ It represents an equilibrium state specified by $(u_\kappa^*; N)$.

→ We call the corresponding ensemble the smooth microcanonical ensemble.

By generalizing the proof for $\sum_\nu' c_\nu |\nu\rangle$ by A. Sugita (2006), we can show

For an arbitrary positive number ϵ

$$\mathrm{Prob}\left(\left| \langle \psi_k | \hat{A} | \psi_k \rangle - \mathrm{Tr}[\hat{\rho}_k \hat{A}] \right| \geq \epsilon \right) \leq \frac{\|\hat{A}\|^2 r_k(e_{\min}; N)}{\epsilon^2 r_k(u_\kappa^*; N)},$$

$$\overline{\langle \psi_k | \hat{A} | \psi_k \rangle} = \mathrm{Tr}[\rho_k \hat{A}]$$

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

- $\|\hat{A}\|^2$ grows at most as a low-degree polynomial of N.
- $\dfrac{r_k(e_{\min}; N)}{r_k(u_\kappa^*; N)}$ decreases exponentially at finite temperature (i.e., $u_\kappa^* > e_{\min}$).

Therefore,

- $|\psi_k\rangle$'s are TPQs for the smooth microcanonical ensemble.
- $\langle \psi_k | \hat{A} | \psi_k \rangle$ is insensitive to the choice of $\{c_i\}_i$.
- Random average gives even better results.

Remarks

1. When $\hat{A}$ is unbounded, $\|\hat{A}\|$ should be replaced with
$$\max_{|\phi\rangle \in \mathcal{H}_N^{\subset}} |\langle \phi | \hat{A} | \phi \rangle|,$$
where $\mathcal{H}_N^{\subset}$ denotes a Hilbert subspace in which the values of macroscopic variables (such as u and m_z) are limited to certain finite ranges.

2. $|\psi_k\rangle$ remains to be a TPQ after time evolution.
$$\begin{aligned} e^{\hat{H}t/i\hbar}|\psi_k\rangle &\propto \sum_n e^{-ie_n t/\hbar} c_n (l - e_n)^k |n\rangle \\ &\propto |\psi_k\rangle \text{ with another } \{c_n\}_n. \end{aligned}$$
c.f. Erroneous statement: "$\hat{\rho}$ of an equilibrium state should be invariant under time evolution, hence should be a function of $\hat{H}$."

Genuine thermodynamic variables

- $T, S, \cdots \neq$ mechanical variables

  $\rightarrow$ Cannot be calculated as $\langle\psi|\hat{A}|\psi\rangle$.

- Ensemble formalism

  - equal a priori probability postulate $\rightarrow$ mehcanical variables (and fluctuation)
  - Boltzmann formula $\rightarrow$ genuine thermodynamc variables (and mehcanical variables)

- Impossible to obtain $T, S, \cdots$ from TPQs?

Possible because information about them is encoded in $r_k(u; N)$.

Formula for $\beta(u;N)$

$r_k(u;N)$ takes the peak at $u = u^*_\kappa$ that satisfies

$$\underset{\substack{\uparrow \\ \text{unknown function}}}{\beta(u^*_\kappa;N)} = 2\kappa/(l - \underset{\substack{\uparrow \\ \text{unknown value}}}{u^*_\kappa}).$$

Substituting u_κ for u^*_κ, we get

simple formula for $\beta(u;N)$

$$\boxed{\beta(u_\kappa;N) = 2\kappa/(l - u_\kappa) + O(1/N).}$$

→ $\beta(u_\kappa;N)$ as a function of u_κ.

→ error $= O(1/N)$

→ sufficient for analytic calculations, but rather large for numerical computaions.

Better formula for $\beta(u; N)$

Let

$$u_\kappa^\bullet \equiv u_\kappa - \xi_\kappa'''/2N\xi_\kappa''^2.$$

One can evaluate ξ_κ'' and ξ_κ''' easily by

$$\begin{aligned}\langle\psi_k|(\hat{h} - u_\kappa)^2|\psi_k\rangle &= 1/N|\xi_\kappa''| + O(1/N^2),\\ \langle\psi_k|(\hat{h} - u_\kappa)^3|\psi_k\rangle &= \xi_\kappa'''/N^2|\xi_\kappa''|^3 + O(1/N^3).\end{aligned}$$

We can show

$$u_\kappa^* = u_\kappa^\bullet + O(1/N^2).$$

Substituting $u_\kappa^\bullet$ for u_κ^*, we get

better formula for $\beta(u; N)$

$$\beta(u_\kappa^\bullet; N) = 2\kappa/(l - u_\kappa^\bullet) + O(1/N^2).$$

→ $\beta(u_\kappa; N)$ as a function of u_κ, with an error of $O(1/N^2)$

→ sufficient for both analytic and numerical calculations.

However,

- $\beta(u;N)$ is the inverse temperature of a *finite* system.

$$|\beta_{\text{our formula}}(u;N) - \beta(u;N)| = O(1/N^2). \quad \text{very good}$$

- One is most interested in its thermodynamic limit $\beta(u;\infty)$.
- In general,

$$|\beta(u;N) - \beta(u;\infty)| \gg O(1/N^2). \quad \text{exact, but finite-size effect}$$

- Therefore,

$$|\beta_{\text{our formula}}(u;N) - \beta(u;\infty)| \gg O(1/N^2). \quad \text{rather poor}$$

Even better formula for $\beta(u;\infty)$

Consider C identical copies of the N-site system.

We denote quantities of this CN-site system by tilde;

$$\begin{aligned} |\tilde{\psi}_0\rangle &\equiv |\psi_0\rangle^{\otimes C}, \\ |\tilde{\psi}_k\rangle &\propto (l-\tilde{h})^{Ck}|\tilde{\psi}_0\rangle, \\ \tilde{h} &\equiv (\hat{H}\otimes\hat{1}^{\otimes(C-1)}+\hat{1}\otimes\hat{H}\otimes\hat{1}^{\otimes(C-2)}+\cdots+\hat{1}^{\otimes(C-1)}\otimes\hat{H})/CN. \end{aligned}$$

Taking the limit of $C \to \infty$, we have

$$\begin{aligned} \tilde{u}^*_\kappa &= \tilde{u}^\bullet_\kappa + O(1/N^2), \\ \tilde{u}^\bullet_\kappa &\equiv u^\bullet_\kappa + \frac{\xi'''_\kappa + \kappa/(l-u_\kappa)^3}{2N[\xi''_\kappa + \kappa/(l-u_\kappa)^2]^2}. \end{aligned}$$

Substituting $\tilde{u}^\bullet_\kappa$ for u^*_κ, we get

even better formula for $\beta(u;\infty)$

$$\tilde{\beta}(\tilde{u}^\bullet_\kappa;\infty) = 2\kappa/(l-\tilde{u}^\bullet_\kappa) + O(1/N^2).$$

Entropy density

Since $\beta = \dfrac{\partial s}{\partial u}$, integration of $\beta(u;N), \beta(u;\infty)$ gives $s(u;N), s(u;\infty)$.

By generalizing Simpson's rule, we have

formula for entropy density

$$s(u_{2p}) - s(u_{2q}) = \sum_{\ell=p}^{q-1} v(u^{\bullet}_{2\ell}, u^{\bullet}_{2\ell+1}, u^{\bullet}_{2\ell+2}) + O(\frac{1}{N^2}).$$

Here,

$$\begin{aligned}
u^{\bullet} &= (u;N) \text{ or } (u;\infty), \\
p, q &= \text{integers} \\
v(x,y,z) &\equiv \frac{(x-z)\{\beta(x)+\beta(z)\}}{2} \\
&\quad - \frac{(x-z)^2[x\{\beta(z)-\beta(y)\} + y\{\beta(x)-\beta(z)\} + z\{\beta(y)-\beta(x)\}]}{6(x-y)(y-z)}.
\end{aligned}$$

Remark

We have also developed another method of calculating s, in which $g(u; N)$ is directly evaluated from the inner products of different series of TPQs.

(S. Sugiura and A. Shimizu, Proc. Meeting of Phys. Soc. Jpn. 2011, paper number 23aGA-6.)

Summary of our formulation

Take an arbitrary basis set of the whole Hilberet space.

Superpose the basis vectors with random complex numbers.

→ a random vector in the whole Hilberet space.

Multiply $(l - \hat{h})$ iteratively.

→ a new class of TPQs

→ values of all variables of statistical-mechanical interest.

Application to numerical computation

Purpose: demonstrate that our formalism does work well.

To give evidences, we need to apply our method to models such that

- rigorous results are known at finite temperature.
- results should be known for many quantities

  (magnetization as a function of the magnetic field, correlation functions, temperature as a function of the energy density, ...)

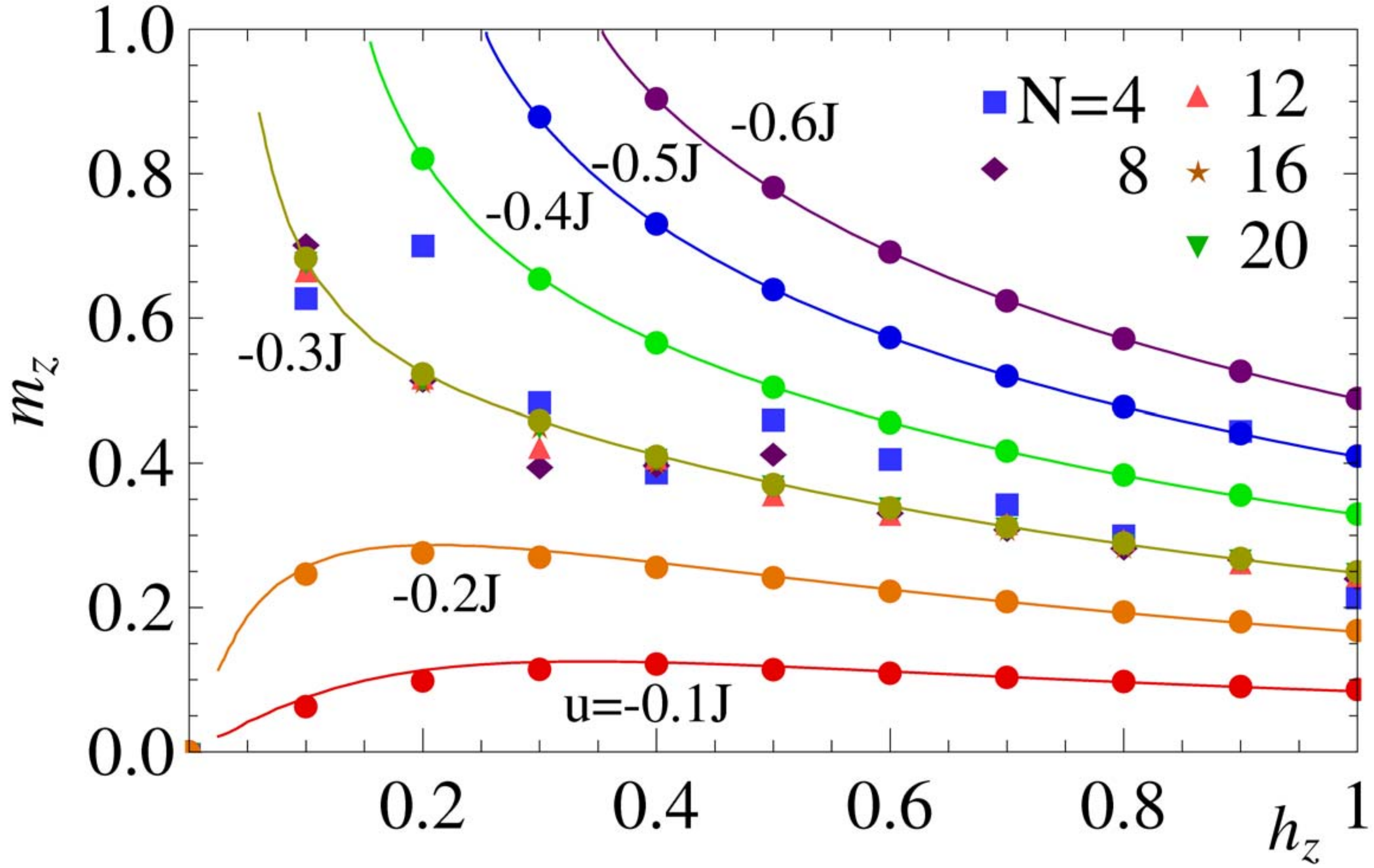
There are only a few models that meet this purpose!

The Heisenberg chain is one of such a few models.

$$\hat{H} = \frac{J}{4} \sum_{i=1}^{N} \left[\hat{\boldsymbol{\sigma}}(i) \cdot \hat{\boldsymbol{\sigma}}(i+1) - h_z \hat{\sigma}_z(i) \right]$$

Here, $J = -1$ (ferromagnetic) or $J = 1$ (antiferromagnetic).

Magnetization vs. magnetic field $(J = -1)$

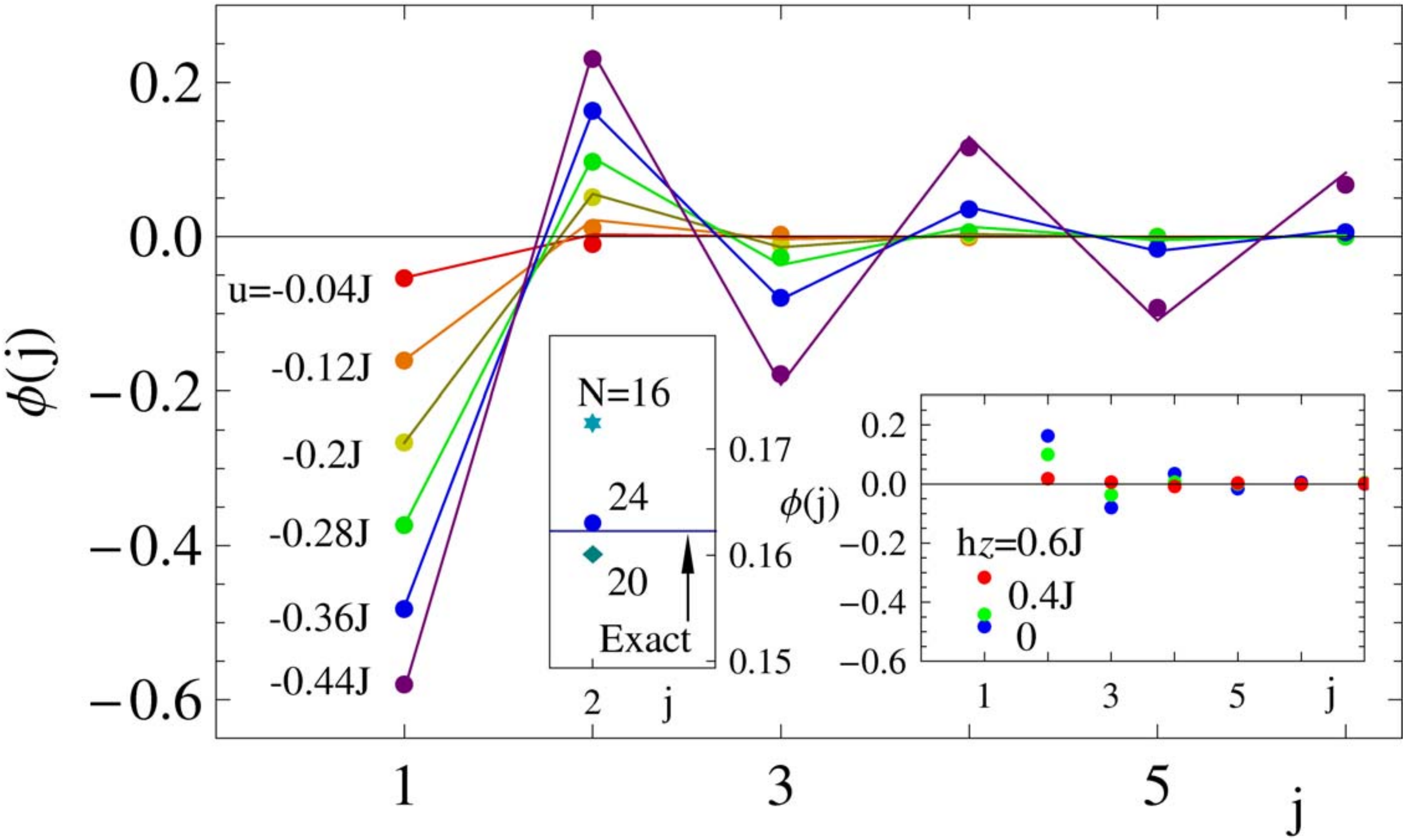


Solid lines: exact results for $N \to \infty$ for various values of the energy density u.

(H. Nakamura and M. Takahashi, JPSJ **63**, 2563 (1994)).

Circles: our method for $N = 24$ (those for $N = 4$-20 are also shown for $u = -0.3J$).

Correlation function vs. distance $(J = +1 \text{ and } h_z = 0)$



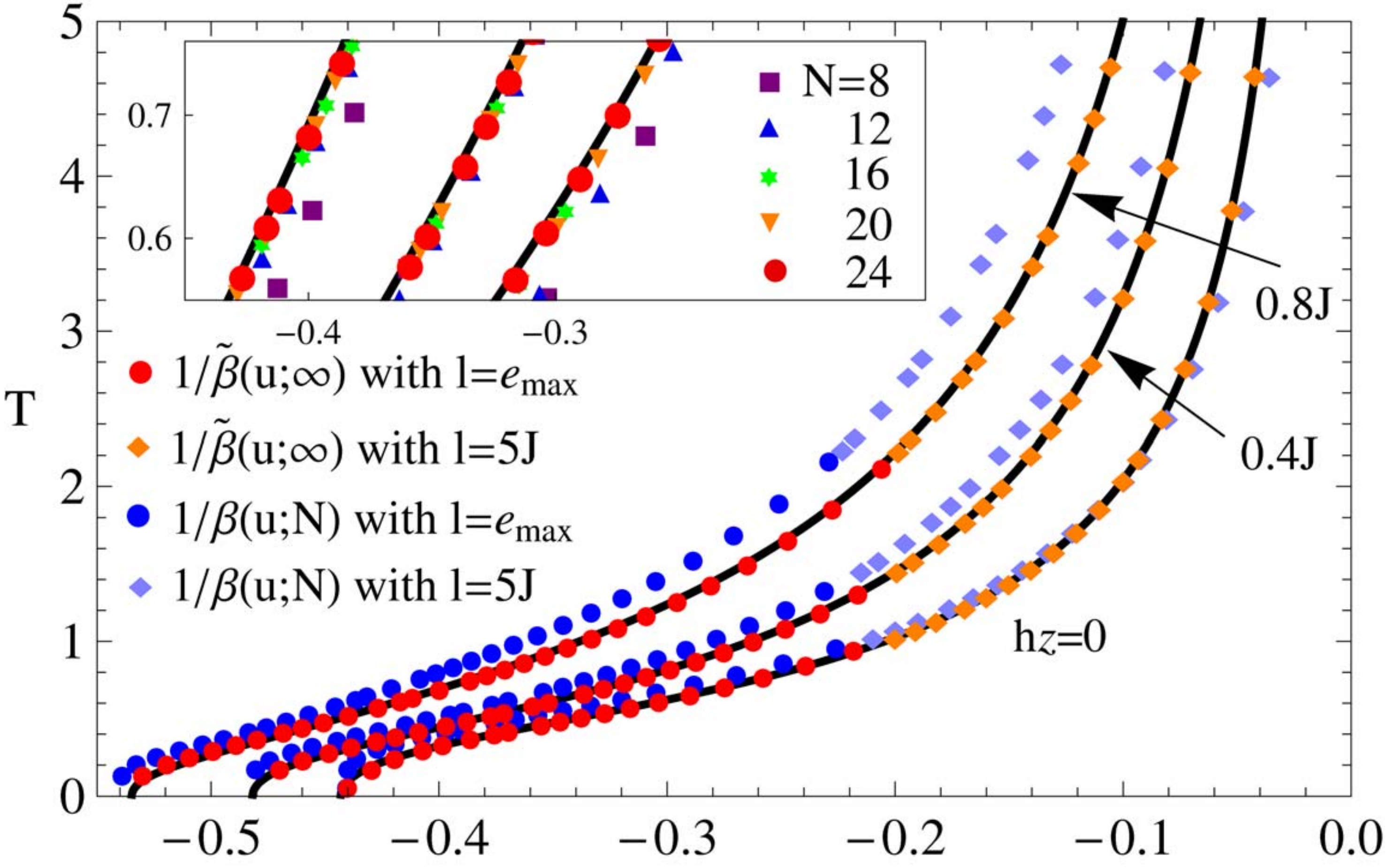
Solid lines: exact results for $N \to \infty$ for various values of the energy density u.

(J. Sato *et al*, Phys. Rev. Lett **106**, 257201 (2011)).

Circles: our method for $N = 24$. **Left inset:** $N =$ 16-24 at $j = 2$ for $u = -0.36J$.

Right inset: $\phi(j)$ at finite h at $T \simeq 0.45J$.

Temperature vs. energy density $(J = +1)$



Solid lines: exact results for $N \to \infty$ for various values of a magnetic field h_z.

(K. Sakai, private communication).

Circles and diamonds: our method for $N = 24$.

Inset: $1/\tilde{\beta}(u;\infty)$ for $N =$ 8-24.

Our method is effective over a wide range of T

Good results over a wide range of T, from $T \ll J$ to $T \gg J$.

Reason:

$$\mathrm{P}\left(\left|\langle\psi_k|\hat{A}|\psi_k\rangle - \mathrm{Tr}[\hat{\rho}_k\hat{A}]\right| \geq \epsilon\right) \leq \frac{\|\hat{A}\|^2 r_k(e_{\mathrm{min}}; N)}{\epsilon^2 r_k(u^*_\kappa; N)}$$

is exponentially small as long as s (and hence T) is finite of $O(1)$.

Practical computations with finite N:

T $(= 1/\tilde{\beta}(u^\bullet_\kappa; \infty))$ can be lowered as long as $\dfrac{r_k(e_{\mathrm{min}}; N)}{r_k(u^*_\kappa; N)} \ll 1.$

Comparizon with other numerical methods

Finite T

→ exponentially large number of states in $\mathcal{E}_{E,N}$.

→ computation of eigenstates in $\mathcal{E}_{E,N}$ is pretty hard.

→ our method takes full advantage of such a large number of states!

→ just a single TPQ gives all quantities of statistical-mechanical interest.

Applicable to

- systems of any spatial dimensions
- frustrated systems
- fermion systems

Computational resources $\ll$ those of the **diagonalization**.

# of non-vanishing elements of $\hat{H} = O(N2^N)$ for the Heisenberg model.

→ Since $k = O(N)$, the computational time $= O(N^2 2^N)$.

→ Only two hours on a WS to compute all data in the above figures.

→ Even faster by parallelizing the algorithm, which is quite easy in our method.

Quantum Monte Carlo method

Much faster.

But, negative sign problem in

- frustrated systems
- fermion systems.

Density-matrix renormalization group method (S. R. White, 1992)

Successful for $1d$ systems.

Extended to finite temperature.

But, its effectiveness in two- or more-dimensional systems is not clear yet.

Microcanonical Lanczos method (M. W. Long *et al*, PRB **68**, 235106 (2003))

Tried to obtain not TPQs but eigenstates.

Costs more computational time than ours.

Computing genuine thermodynamic variables seems more difficult than ours.

$\therefore$ Our method will make it possible to analyze systems which could not be analyzed with other methods.

Summary of Application to numerical computation

- Application to the Heisenberg chain, for which rigorous results are known for
  - magnetization vs. magnetic field
  - correlation function
  - temperature vs. energy density
- Our results agree well with the rigorous results for all these quantities.
- Over a wide temperature range: from $T \ll J$ to $T \gg J$.
- Extremely fast: only two hours on a WS.
- Applicable to
  - systems of any spatial dimensions
  - frustrated systems
  - fermion systems
- Possible to analyze systems which could not be analyzed with other methods.

CONTENTS

Treatment of phase transitions

ex. a first-order transition

Thermodynamics:

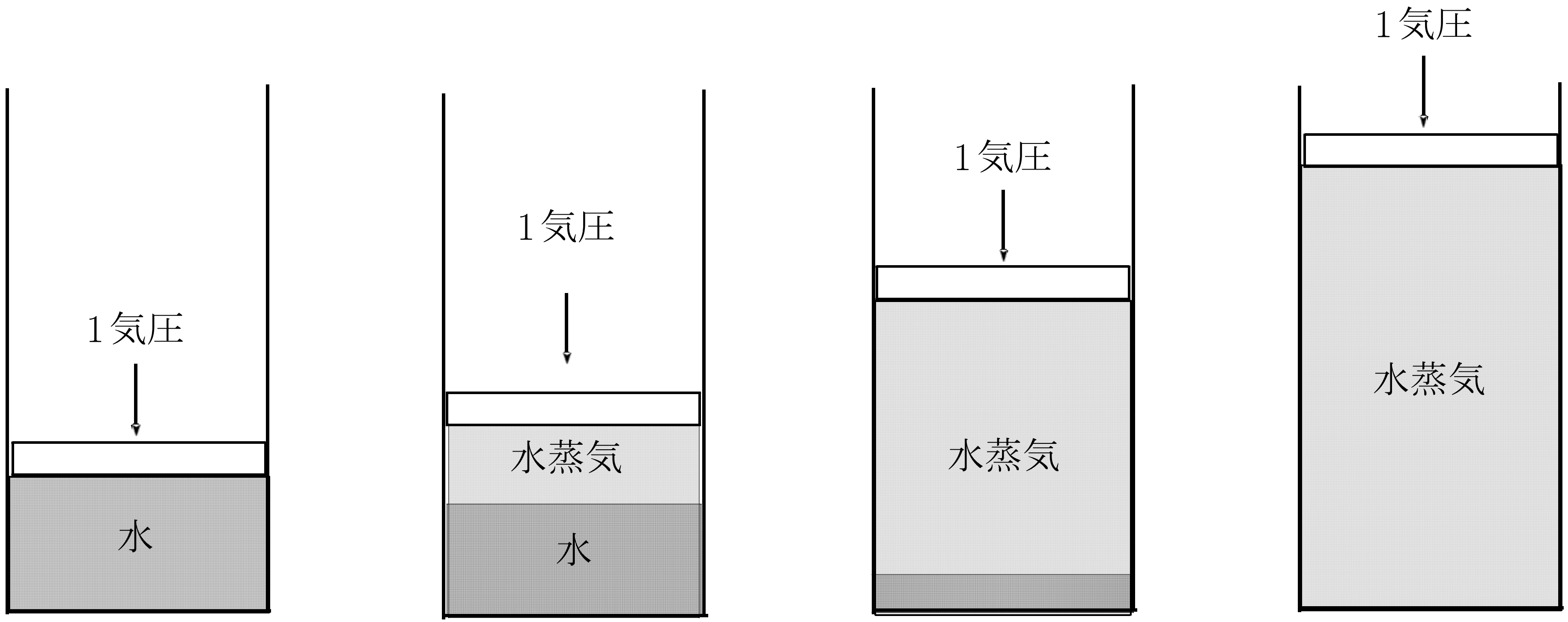
$s(T;\infty)$ is discontinuous at $T = T_{\rm tr}$.
→ $u(T;\infty)$ is discontinuous at $T = T_{\rm tr}$.
→ $c = T\partial s/\partial T = \partial u/\partial T$ diverges at $T = T_{\rm tr}$.

In contrast, $\beta(u;\infty)$ is continuous even at $T = T_{\rm tr}$.
→ $c = -\beta^2/(\partial\beta/\partial u)_N = \infty$ corresponds to $\beta =$ constant.

Phase transition viewed in the entropy representation

Ref. 清水明「熱力学の基礎」(東大出版会, 2007)

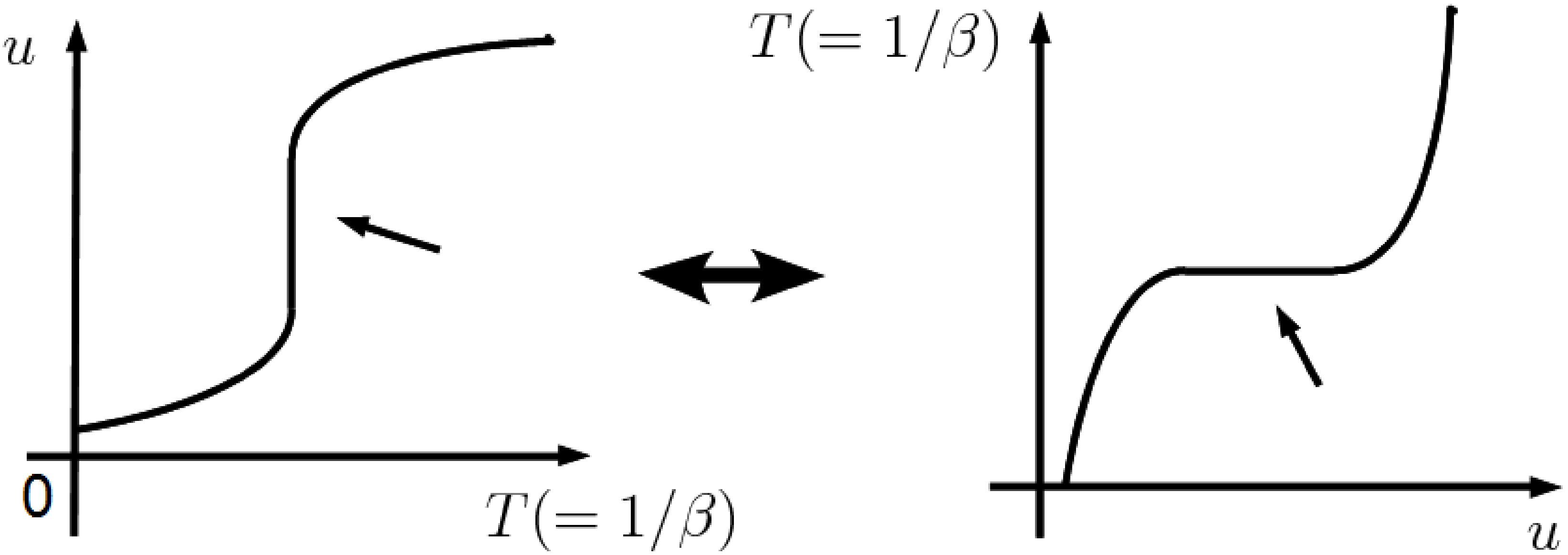
- $G(T, P, N)$: $T, P, N \not\to$ equilibrium state
- $S(U, V, N)$: $U, V, N \to$ equilibrium state



(i) (ii) (iii) (iv)

水を1気圧に保ったまま温める

$u(T, P)$ is discontinuous　　　$T(u, P)$ has a plateau



Spin systems

$V \ \rightarrow \ M_z$, $P \ \rightarrow \ h_z$

$u(T, P) \ \rightarrow \ u(T, h_z)$: canonical formalism

$T(u, P) \ \rightarrow \ T(u, h_z)$: our formalism

Canonical formalism

T is an independent variable

→ calculate a discontinuous function $u(T;\infty)$.

→ calculation is hard around $T = T_{\text{tr}}$.

Our formalism

u is taken as an independent variable

→ calculate $\beta(u;\infty)$, which is continuous even at $T = T_{\text{tr}}$.

→ calculation is easy (e.g., interpolation is effecive)

→ calculate c from $c = -\beta^2/(\partial\beta/\partial u)_N$.

→ $c = \infty$ corresponds to $\beta =$ constant; easily identified!

Our formalism is advantageous to finding phase transitions.

Entanglement

TPQ $|\psi_k\rangle$ and the mixed state $\hat{\rho}_k$ of the corresponding ensemble

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

Example: $T \gg J$

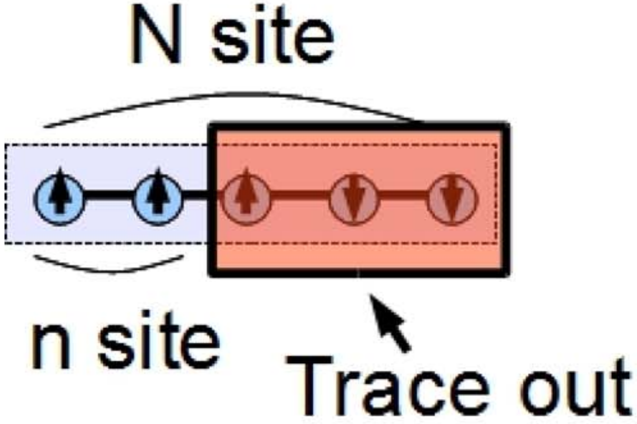
$\hat{\rho}_k \simeq (1/D)\hat{1} \ \leftarrow$ no entanglement.

$|\psi_k\rangle$ has exponentially large entanglement.

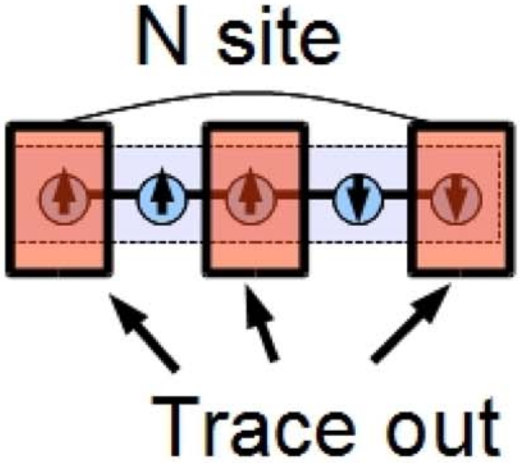
(A. Sugita and AS, JPSJ **74** (2005) 1883).

Bipartite entanglement measured by von Neumann entropy

ρ_n



ρ_n'

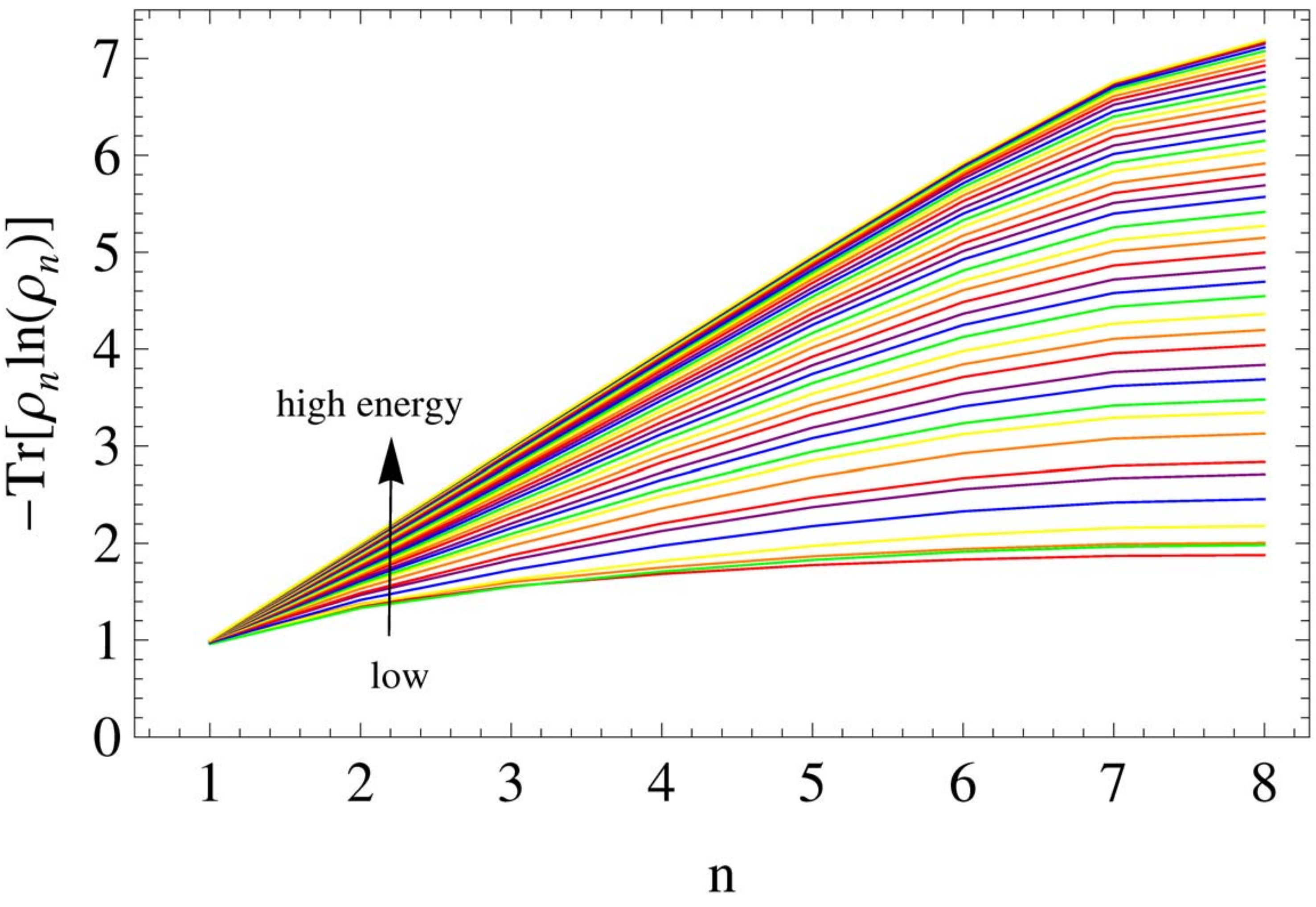


The von Neumann entropy of the subsystem,

$$S_{\mathrm{vN}} \equiv -\mathrm{Tr}(\hat{\rho}_n \log_2 \hat{\rho}_n),$$

is a good measure of bipartite entanglement for pure states.

S_{vN} **vs.** n $(J = +1, N = 16, h_z = 0)$



Solid lines: results for different energy densities, $-0.44J \leq u \leq -0.01J$.

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

Their difference can be detected only by high-order polynomials of local operators, which are not of statistical-mechanical interest. (A. Sugita, 2006)

c.f. Related arguments:

- A. Sugita and AS, J. Phys. Soc. Jpn. **74** (2005) 1883.
- AS and T. Morimae, Phys. Rev. Lett. **95** (2005) 090401.

Other new classes of TPQs

$$|\psi_k\rangle \propto (l-\hat{h})^k|\psi_0\rangle \quad \longrightarrow \quad |\psi\rangle \propto Q(\hat{h})|\psi_0\rangle$$

Here, $Q(u)$ is any differentiable real function such that

- $Q(u)^2 g(u;N)$ has a sharp peak.
- Its width vanishes as $N \to \infty$.
- $Q(u)^2 g(u;N)$ outside the peak decays quickly.

One can calculate various quantities as we have done using $|\psi_k\rangle$, e.g.,

$$\beta(u_\kappa^*;N) = \frac{2\kappa}{(l-u_\kappa^*)} \quad \longrightarrow \quad \beta(u^*;N) = -\frac{2Q'(u^*)}{NQ(u^*)}.$$

What is thermal fluctuation?

See PDF.

Summary

- A new class of TPQs.
- A simple method for constructing them.
- Formulas giving genuine thermodynamic variables.

From a single TPQ, one can calculate all variables of statistical-mechanical interest, including genuine thermodynamic variables, at finite temperature.

What does it imply?

Formulation of Statistical Mechanics

Conventional : ensembles and $S = \ln W$ or $F = -T \ln Z$ (and ergodicity)

$$\downarrow$$

New : TPQ and our formula for genuine thermodynamic variables

Statistical mechanics based on TPQs