

熱的な量子純粋状態を用いた 統計力学の定式化

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SS and A. Shimizu, PRL 108, 240401 (2012)



SS and A. Shimizu, PRL 111, 010401 (2013)



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2. Canonical TPQ State

3. Microcanonical TPQ State
and Its Relation to Canonical TPQ State

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Principle of
Equal Weight

Boltzmann
formula

Microscopic View

All the microstates that have energy E



There are huge number
of states

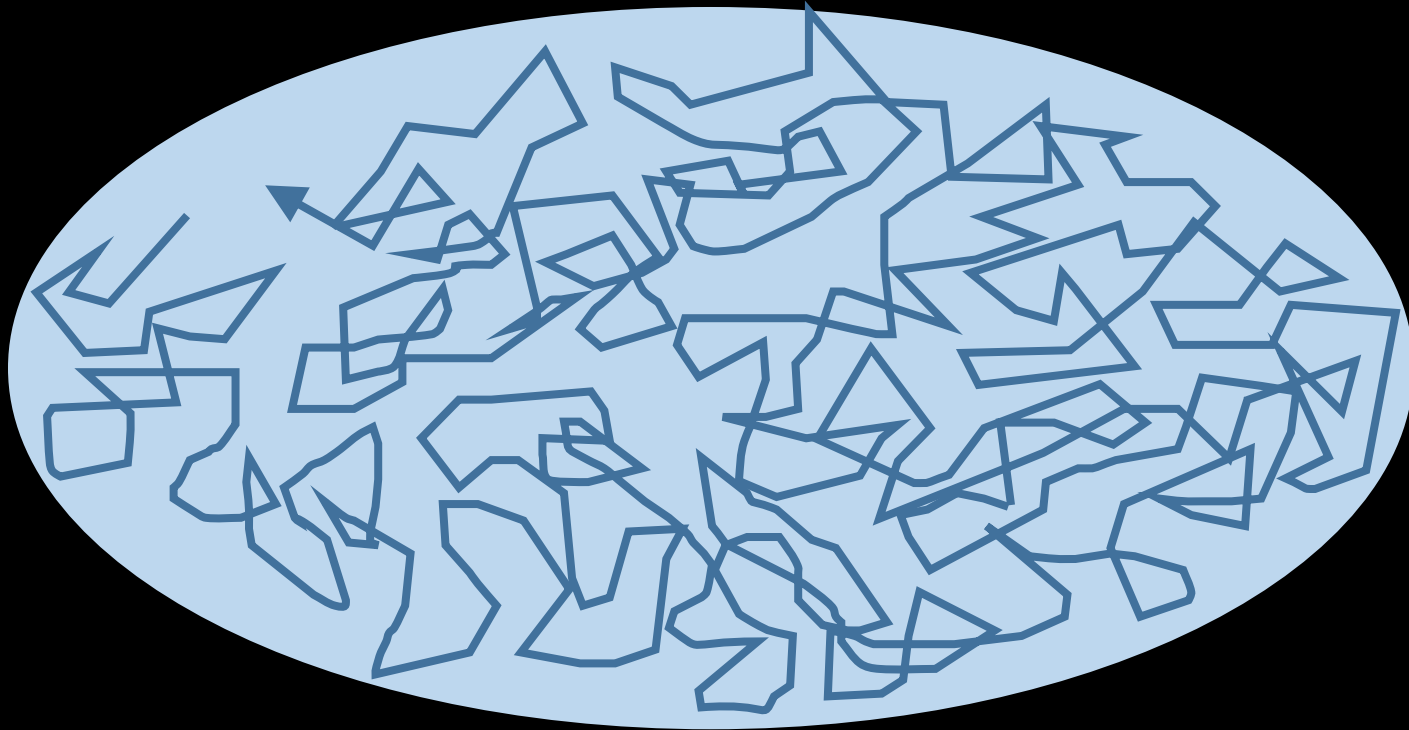
Principle of **Equal Weight**:

When all the microstates emerge in the same probability, the average value give the equilibrium value.

How can we justify this principle?

Explanation using the **Ergodic Hypothesis**

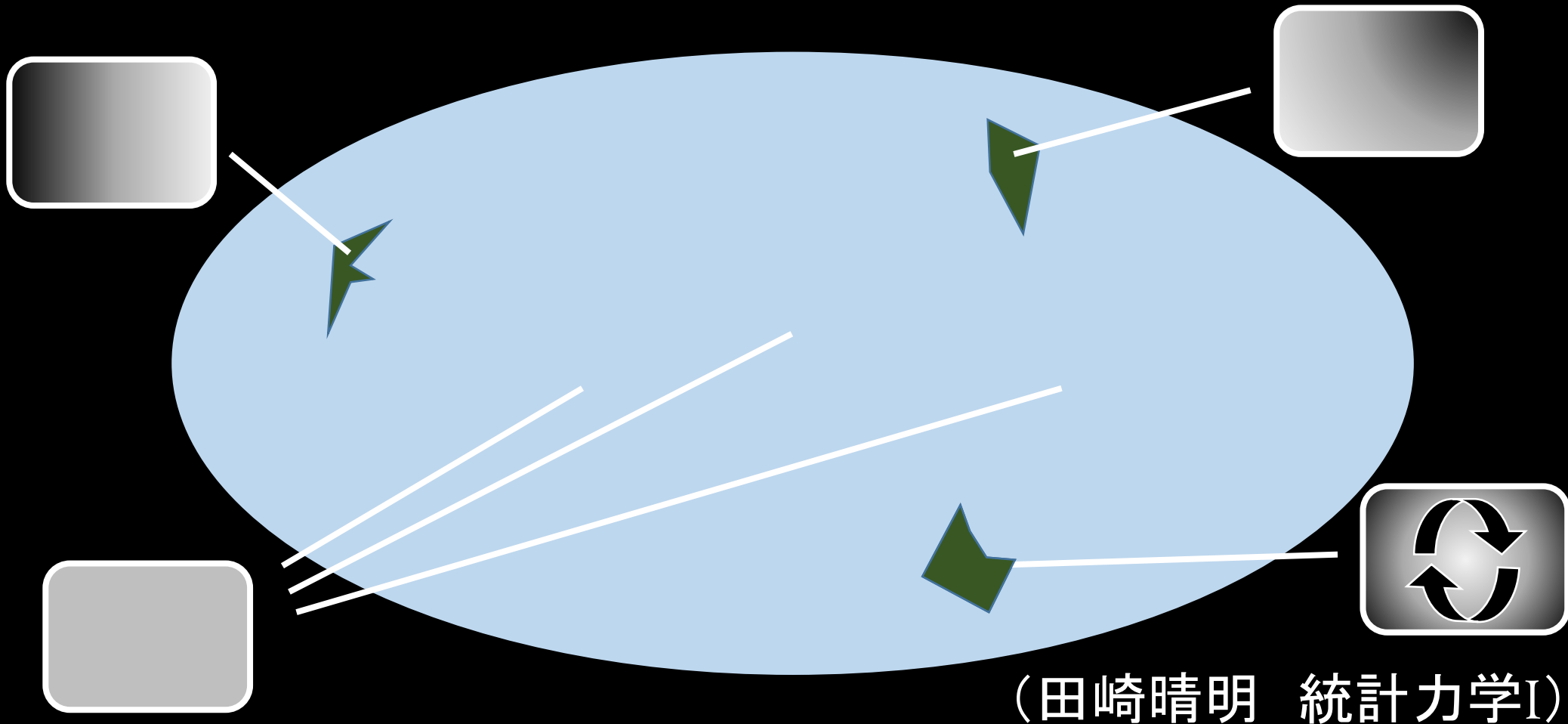
All the microstates that have energy E



Ergodic theory gives the fruitful mathematics
But...

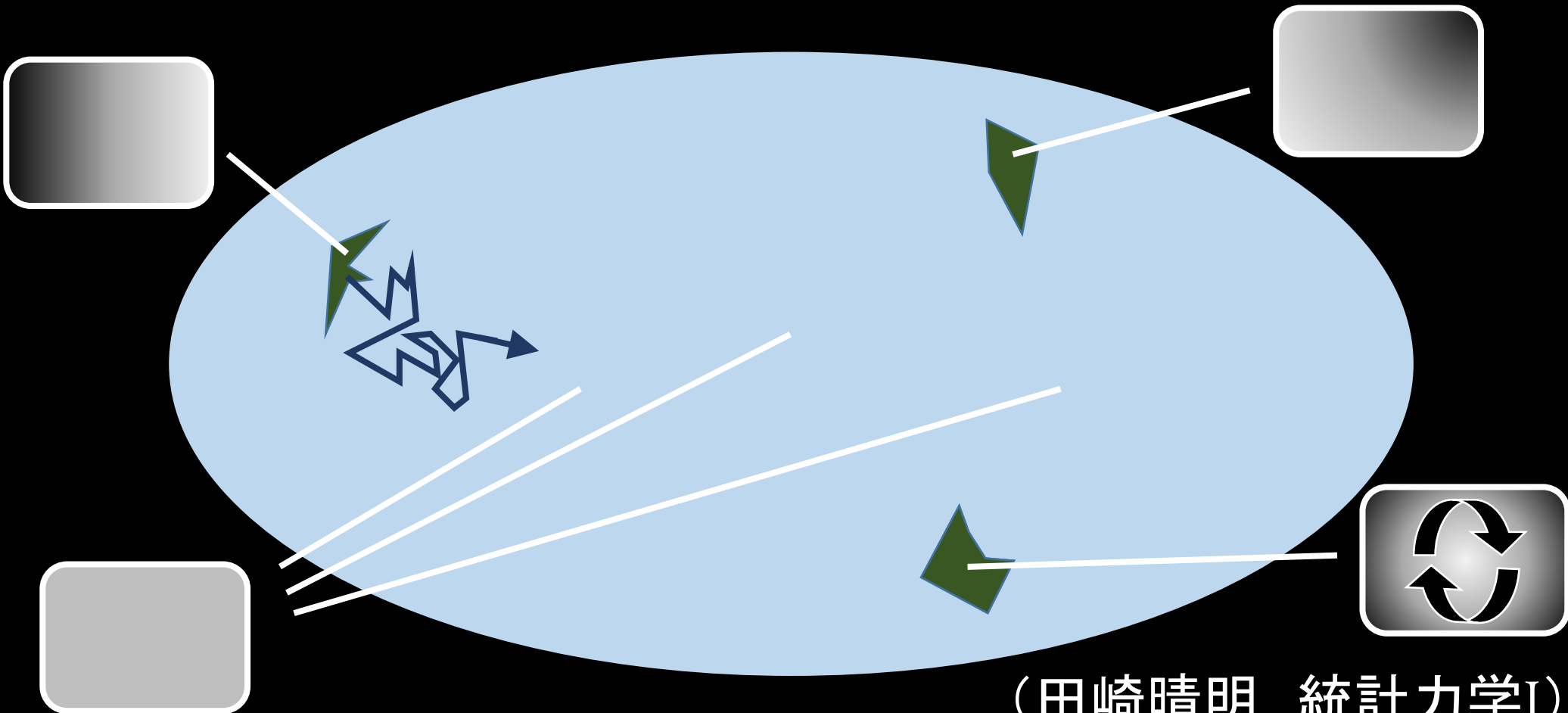
It takes **too much time** (physically nonsense)
It gets harder as the system size increases

Explanation using the **Typicality**



Almost all the microstate at energy E are
macroscopically indistinguishable!

Explanation of the **approach** to equilibrium



(田崎晴明 統計力学I)

Previous Works

	Total System	Sub System
Ensemble Formulation	<p>Mixed</p> $\frac{1}{W(E)} \sum n\rangle \langle n $	<p>Mixed</p> $\exp(-\beta \hat{H}) / Z$
Previous Works	<p>Pure</p> $ \psi\rangle = \sum_n c_n n\rangle$ $\langle \psi \hat{M}_z \psi \rangle = \langle \hat{M}_z \rangle_{E,N}^{\text{ens}}$ <p>+ (exponentially small error)</p> <p>A.Sugita (2007), P.Rieman (2008)</p>	<p>Mixed</p> <p>“Canonical Typicality”</p> $\simeq \exp(-\beta \hat{H}) / Z$ <p>S.Popescu et al. (2006) S.Goldstein et al. (2006)</p>

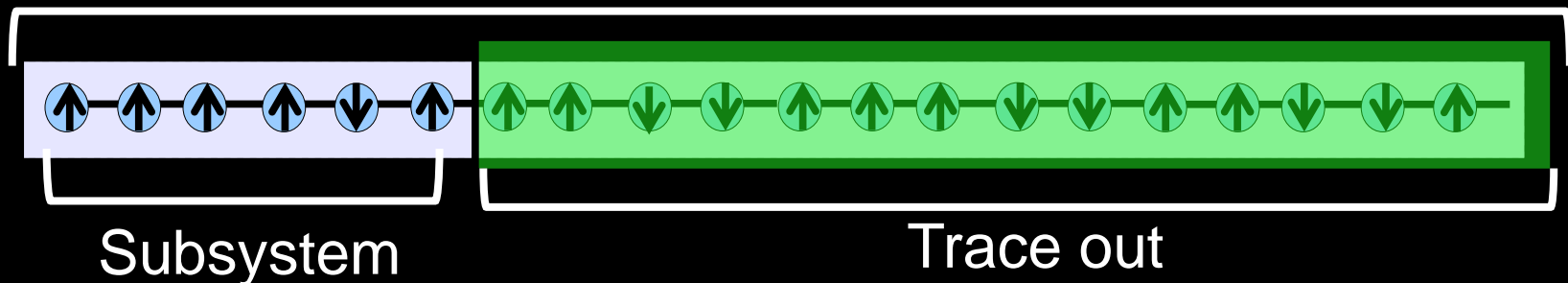
Take a random vector $|\psi_E\rangle \equiv \sum_i c_i |E_n\rangle$

i.e. the random vector in the specified energy shell

$\left(\begin{array}{l} \{|E_n\rangle\}_n : \text{an arbitrary orthonormal basis spanning} \\ \text{the energy shell } [E, E + \Delta E) \\ \{c_i\}_i : \text{a set of random complex numbers} \\ \text{with } \sum_i |c_i|^2 = 1 . \end{array} \right)$

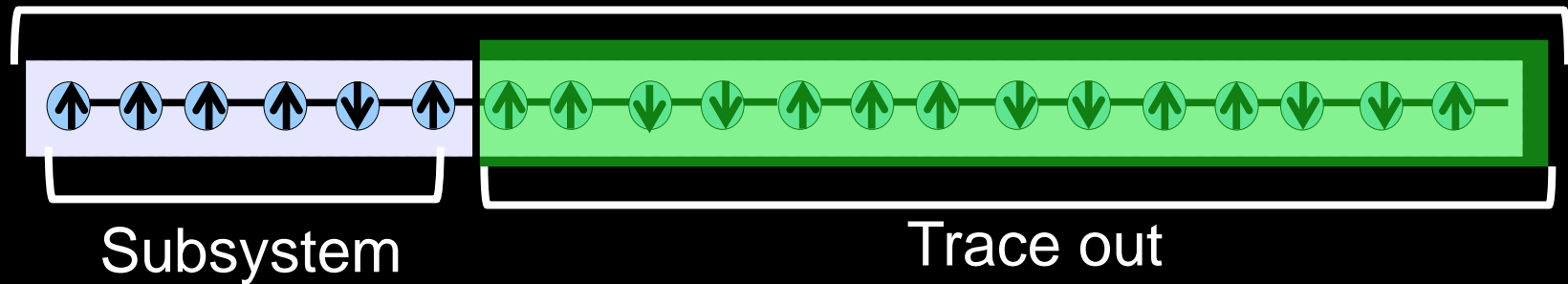
When we see the subsystem of $|\psi_E\rangle$,
the **expectation value** is very close to
the canonical ensemble average

$$\equiv |\psi_E\rangle$$



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the **expectation value** is very close to
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$\equiv |\psi_E\rangle$



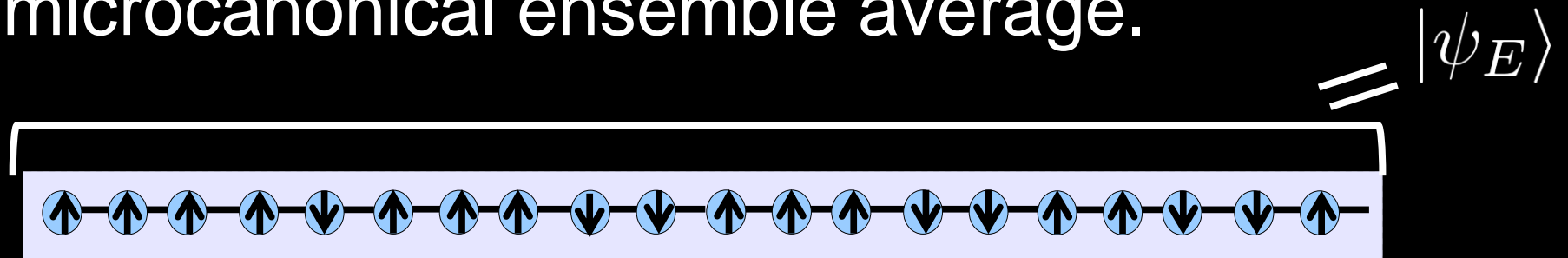
That is, the deviation ratio satisfies

$$P \left(\left| \langle \psi_E | \hat{A} | \psi_E \rangle - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \right| \geq \epsilon \right) \leq \frac{\|\hat{A}\|}{d}$$

$\left[\hat{A} : \text{mechanical variable on the subsystem} \right]$

\longrightarrow Condition for \hat{A} can be weakened

When we see the observables which are **low-degree polynomials of local operators**, the expectation value is very close to the microcanonical ensemble average.



That is,

$$P \left(\left| \langle \psi_E | \hat{A} | \psi_E \rangle - \langle \hat{A} \rangle_{E,N}^{\text{ens}} \right| \geq \epsilon \right) \leq \frac{\|\hat{A}\|}{d}$$

$\left[\hat{A} : \text{mechanical variable on the subsystem} \right]$

(Condition for \hat{A} can be weaken even more)

Previous Works

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Previous Works	<p>Pure</p> $ \psi\rangle = \sum_n c_n n\rangle$ $\langle \psi \hat{M}_z \psi \rangle = \langle \hat{M}_z \rangle_{E,N}^{\text{ens}}$ <p>+ (exponentially small error)</p> <p>A.Sugita (2007), P.Rieman (2008)</p> <p>$S = ? \quad T = ?$</p>	<p>Mixed</p> <p>“Canonical Typicality”</p> $\simeq \exp(-\beta \hat{H}) / Z$ <p>S.Popescu et al. (2006) S.Goldstein et al. (2006)</p> <p>$\psi\rangle = ?$</p>



Purpose of Our Work

Establish the formulation of statistical mechanics using a **single** pure quantum state.

Macroscopic Variables

Mechanical Variables

- Low-degree polynomials of local operators
(i.e. their degree $\leq m = o(N)$)

Ex) Magnetization, Spin-spin correlation function

Genuine Thermodynamic Variables

Ex) Temperature T , Entropy S

- Cannot be represented as mechanical variables
- All genuine thermodynamic variables can be derived from entropy S .

Thermal Pure Quantum (TPQ) State

When $|\Psi\rangle$ is generated from some probability measure, we call $|\Psi\rangle$ a TPQ state if

$$\langle \hat{A} \rangle_N^\Psi \equiv \frac{\langle \Psi | \hat{A} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \xrightarrow{P} \langle \hat{A} \rangle_N^{\text{ens}}$$

uniformly for **every** mechanical variable \hat{A} as $N \rightarrow \infty$

$$\left(\begin{array}{l} \langle \hat{A} \rangle_N^{\text{ens}} : \text{ensemble average of } \hat{A} \\ \xrightarrow{P} : \text{convergence in probability} \end{array} \right)$$

Independent variables

$$u, N : \langle \hat{A} \rangle_{u, N}^\Psi \xrightarrow{P} \langle \hat{A} \rangle_{u, N}^{\text{ens}} \quad \text{Microcanonical TPQ state}$$

↑ energy density E/N

$$\beta, N : \langle \hat{A} \rangle_{\beta, N}^\Psi \xrightarrow{P} \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \quad \text{Canonical TPQ state}$$

New Formulation

	Total System	Sub System
Ensemble	Mixed	Mixed
Previous Works	Pure $ \psi\rangle = \sum_n c_n n\rangle$ $S = ? \quad T = ?$	Mixed “Canonical Typicality” $ \psi\rangle = ?$

New Formulation

	Total System	Sub System
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Previous Works	<p>Pure</p> $ \psi\rangle = \sum_n c_n n\rangle$ <p>$S = ? \quad T = ?$</p>	<p>Mixed</p> <p>“Canonical Typicality”</p> <p>$\psi\rangle = ?$</p>

New Formulation

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Microcanonical TPQ state	Pure $ k\rangle = (l - \hat{h})^k \psi_0\rangle$ $S = ? \quad T = ?$	Mixed
Canonical TPQ state		$ \beta, N\rangle$ $\equiv e^{-N\beta\hat{h}/2} \psi_0\rangle$

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Canonical TPQ state		$ \beta, N\rangle$ $\equiv e^{-N\beta\hat{h}/2} \psi_0\rangle$ $F = ?$

New Formulation

	Total System	Sub System
Ensemble	Mixed	Mixed
Previous Works	Pure $ \psi\rangle = \sum_n c_n n\rangle$	Mixed “Canonical Typicality”
Microcanonical TPQ state	Pure $ k\rangle = (l - \hat{h})^k \psi_0\rangle$ $\langle k k\rangle \leftrightarrow S$	Mixed
Canonical TPQ state		$ \beta, N\rangle \equiv e^{-N\beta\hat{h}/2} \psi_0\rangle$ $\langle \beta, N \beta, N\rangle \leftrightarrow F$

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Setup

System:

- **Discrete** quantum system composed of N sites,
- The dimension of the Hilbert space is D .
- The ensemble formulation gives correct results, which are **consistent with thermodynamics** in $N \rightarrow \infty$
- Assume every mechanical variable \hat{A} is normalized as $\|\hat{A}\| \leq K N^m$ $\left(\begin{array}{l} \text{To exclude foolish operators (ex. } N^N \hat{H} \text{)} \\ K : \text{Constant independent of } \hat{A} \text{ and } N. \end{array} \right)$
- We use quantities per site, $u \equiv E/N$ and $\hat{h} \equiv \hat{H}/N$
- The spectrum of \hat{h} is $e_{\min} \leq u \leq e_{\max}$

Canonical TPQ State

PRL 111, 010401
(2013)

Firstly, take a random vector $|\psi_0\rangle \equiv \sum_i c_i |i\rangle$
from the **whole** Hilbert space.

$\left(\begin{array}{l} \{|i\rangle\}_i : \text{an arbitrary orthonormal basis of} \\ \text{the } \mathbf{whole} \text{ Hilbert space} \\ \{c_i\}_i : \text{a set of random complex numbers} \\ \text{with } \sum_i |c_i|^2 = D. \end{array} \right)$

Notice:

This random vector $|\psi_0\rangle$ is independent of the choice of the basis set $\{|i\rangle\}_i$.

→ Preparation of $|\psi_0\rangle$ is easy.

Canonical TPQ State

PRL 111, 010401
(2013)

Firstly, take a random vector $|\psi_0\rangle \equiv \sum_i c_i |i\rangle$
from the **whole** Hilbert space.

$\left(\begin{array}{l} \{|i\rangle\}_i : \text{an arbitrary orthonormal basis of} \\ \text{the } \mathbf{whole} \text{ Hilbert space} \\ \{c_i\}_i : \text{a set of random complex numbers} \\ \text{with } \sum_i |c_i|^2 = D. \end{array} \right)$

Then, calculate

$$|\beta, N\rangle \equiv \exp[-N\beta\hat{h}/2]|\psi_0\rangle \quad (\hat{h} \equiv \hat{H}/N)$$

$|\beta, N\rangle$ is the **canonical** TPQ state
at temperature $1/\beta$

Mechanical Variables

$$\langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}} \equiv \frac{\langle \beta, N | \hat{A} | \beta, N \rangle}{\langle \beta, N | \beta, N \rangle} \xrightarrow{P} \langle \hat{A} \rangle_{\beta, N}^{\text{ens}}$$

$$\left[|\beta, N\rangle \equiv \exp[-N\beta\hat{h}/2] |\psi_0\rangle \right]$$

Genuine Thermodynamic Variables

Free energy

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

$\left[\lambda^N : \text{Dimension of total Hilbert space} \right]$

Error Probabilisty of Canonical TPQ State

$$\overline{\langle \beta, N | \beta, N \rangle} = Z(\beta, N)$$

$$\left(\begin{array}{l} \overline{\cdot \cdot \cdot} : \text{Random average over } \{c_i\}_i \\ Z(\beta, N) \equiv \text{Tr}[\exp(-N\beta\hat{h})] \\ \lambda^N : \text{Dimension of total Hilbert space} \end{array} \right)$$

$$\begin{aligned} & \text{P} \left(\left| \langle \beta, N | \beta, N \rangle / \overline{\langle \beta, N | \beta, N \rangle} - 1 \right| \geq \epsilon \right) \\ & \leq \frac{1}{\epsilon^2} \frac{1}{\exp[2N\beta\{f(1/2\beta; N) - f(1/\beta; N)\}]} \\ & \leq \frac{1}{\epsilon^2} \frac{1}{\exp[\Theta(N)]} \quad \left[f(\beta; N) : \text{free energy density} \right] \end{aligned}$$

Error Probability of Canonical TPQ State

$$\begin{aligned}\overline{\langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}}} &\equiv \overline{\langle \beta, N | \hat{A} | \beta, N \rangle} / \overline{\langle \beta, N | \beta, N \rangle} \\ &= \langle \hat{A} \rangle_{\beta, N}^{\text{ens}}\end{aligned}$$

$\left[\overline{\quad} : \text{Random average over } \{c_i\}_i \right]$

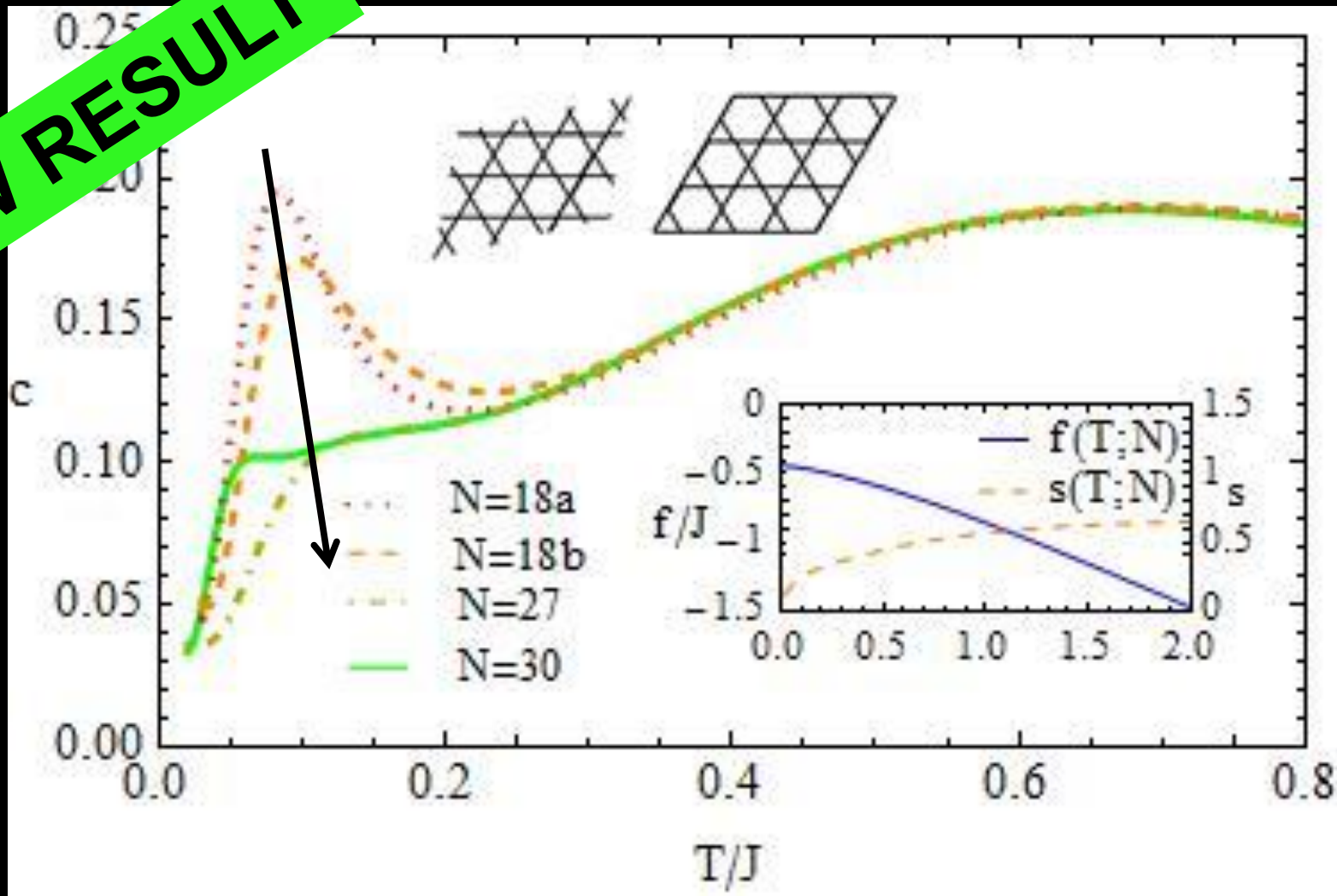
Error Probability of Canonical TPQ State

$$\begin{aligned}\overline{\langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}}} &\equiv \overline{\langle \beta, N | \hat{A} | \beta, N \rangle} / \overline{\langle \beta, N | \beta, N \rangle} \\ &= \langle \hat{A} \rangle_{\beta, N}^{\text{ens}}\end{aligned}$$

$$\begin{aligned}P \left(\left| \langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \right| \geq \epsilon \right) \\ \leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{ f(1/2\beta; N) - f(1/\beta; N) \}]} \\ \leq \frac{1}{\epsilon^2} \frac{N^{2m}}{\exp[\Theta(N)]} \left[\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}} : \text{Variance of } \hat{A} \right]\end{aligned}$$

A single realization of a TPQ state gives the equilibrium values of **all mechanical variables**.

$S=1/2$ kagome-lattice Heisenberg antiferromagnet



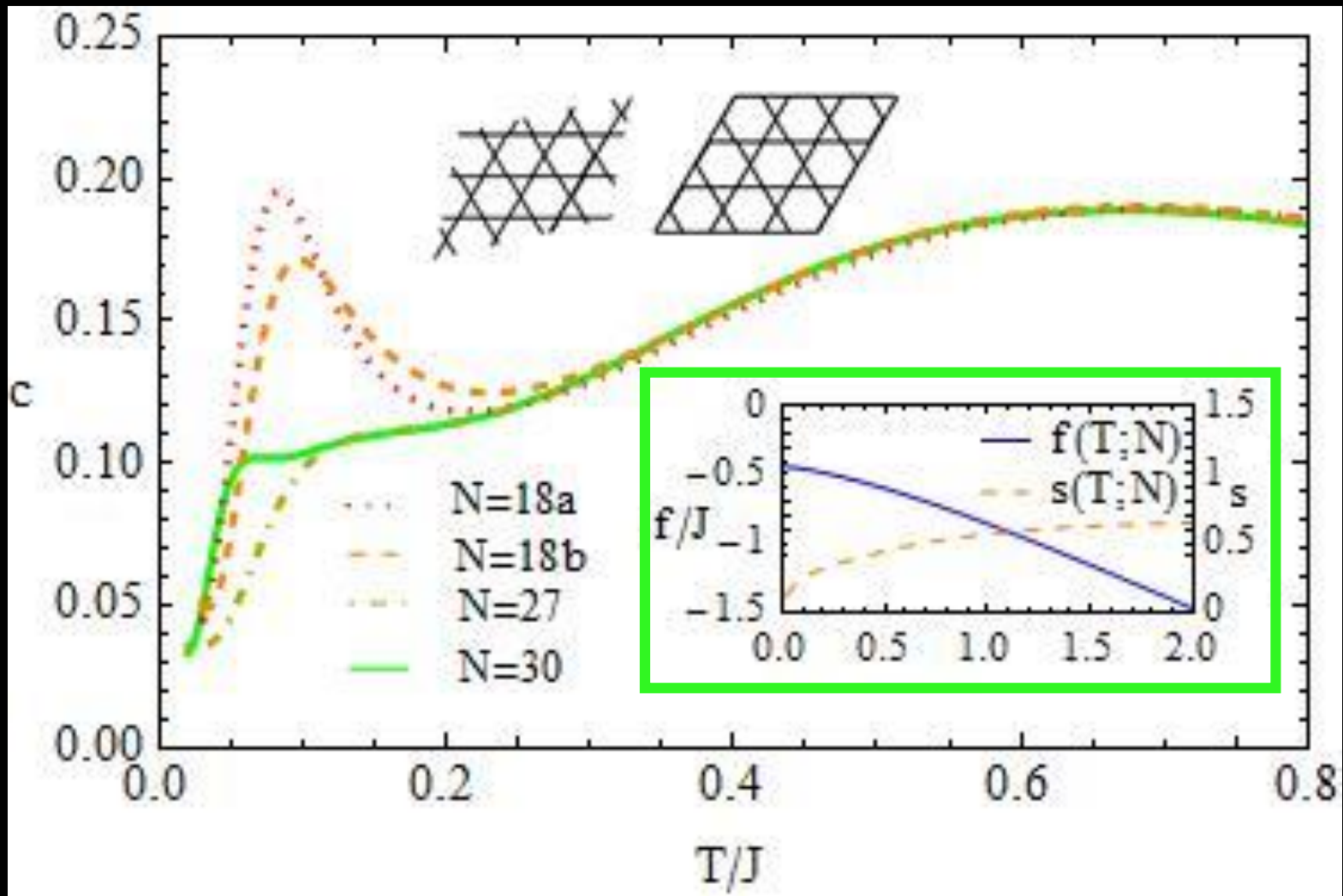
Second peak vanishes as $N \rightarrow \infty$?

Error Probability of Canonical TPQ State

$$\begin{aligned} & \mathbb{P} \left(\left| \langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \right| \geq \epsilon \right) \\ & \leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{f(1/2\beta; N) - f(1/\beta; N)\}]} \end{aligned}$$

Almost self-validating!

$S=1/2$ kagome-lattice Heisenberg antiferromagnet



Error Probability of Canonical TPQ State

$$\begin{aligned} & \mathbb{P} \left(\left| \langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \right| \geq \epsilon \right) \\ & \leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{f(1/2\beta; N) - f(1/\beta; N)\}]} \\ & \left[\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}} \equiv \langle (\hat{A} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}})^2 \rangle_{\beta, N}^{\text{ens}} \right] \end{aligned}$$

Error Probability of Canonical TPQ State

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

$$\left[\leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{f(1/2\beta; N) - f(1/\beta; N)\}]} \right]$$

$$\leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}}}{\exp[N\beta \{f(0; N) - f(1/\beta; N)\}]}$$

$$\left[\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}} \equiv \langle (\hat{A} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}})^2 \rangle_{\beta, N}^{\text{ens}} \right]$$

Error Probability of Canonical TPQ State

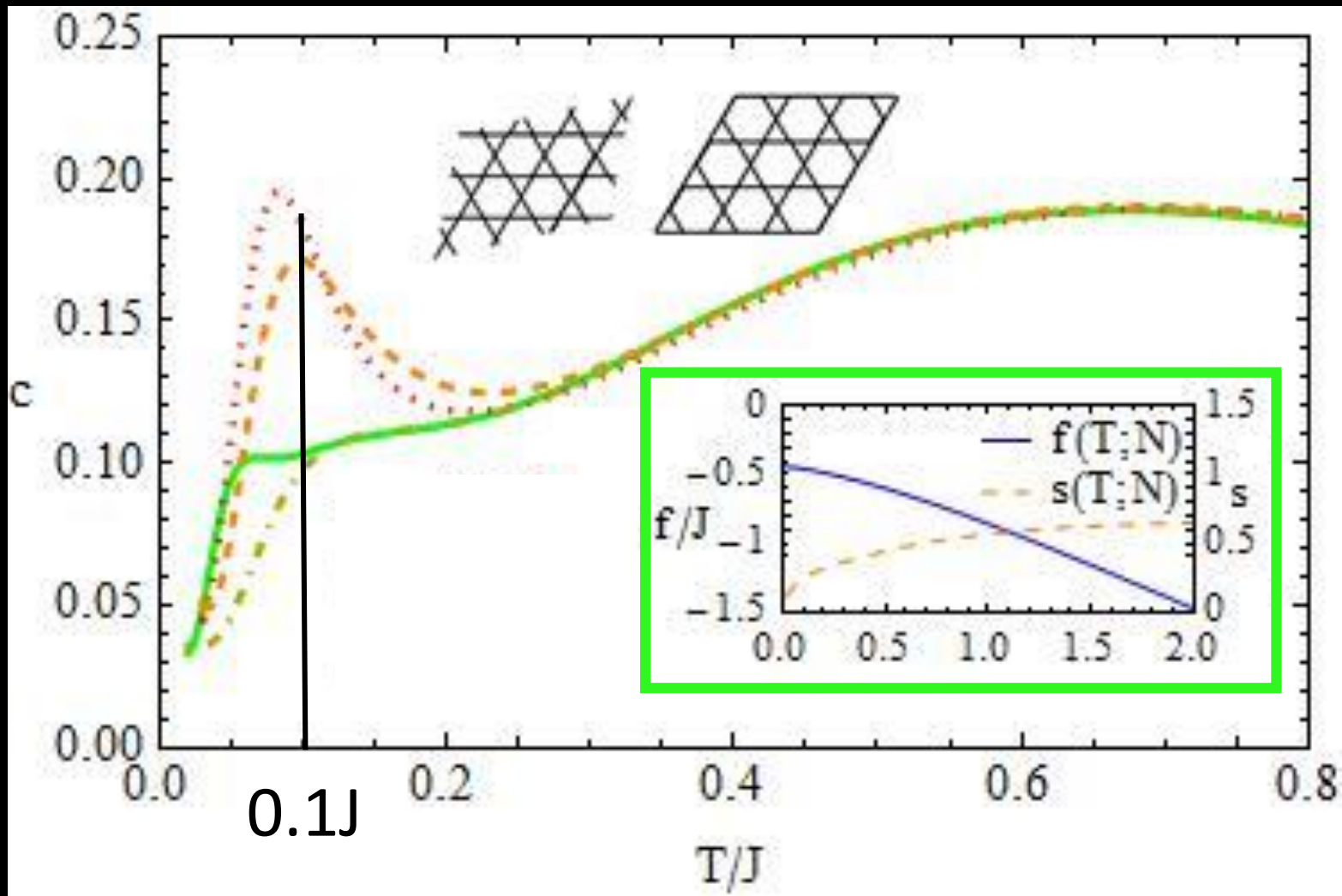
$$P \left(\left| \langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \right| \geq \epsilon \right)$$

$$\left[\leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{f(1/2\beta; N) - f(1/\beta; N)\}]} \right]$$

$$\leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}}}{\exp[N\beta \{f(0; N) - f(1/\beta; N)\}]}$$

$$\left[\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}} \equiv \langle (\hat{A} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}})^2 \rangle_{\beta, N}^{\text{ens}} \right]$$

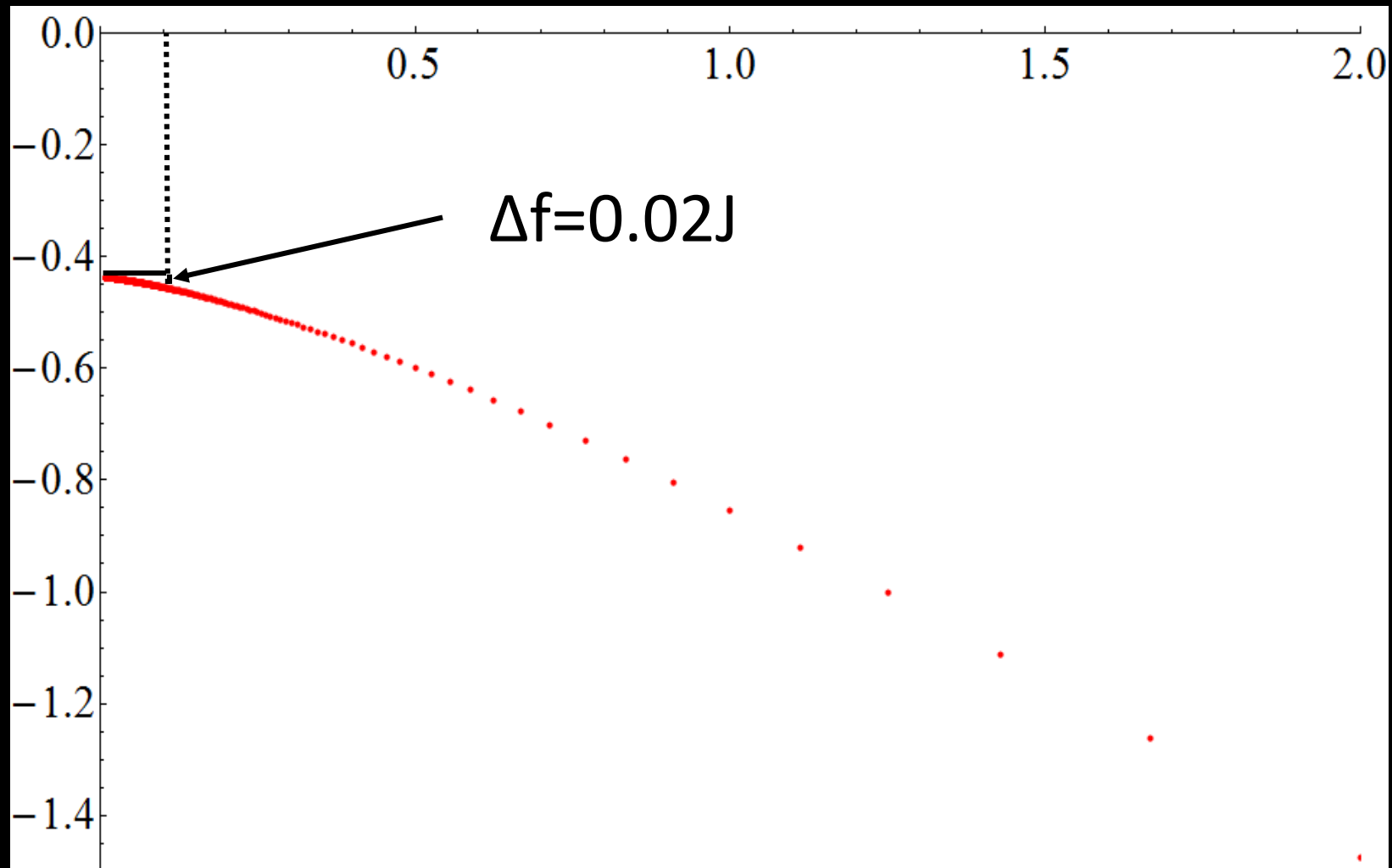
$S=1/2$ kagome-lattice Heisenberg antiferromagnet



Free energy density

Temperature T

Free energy density
f



Error Probability of Canonical TPQ State

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

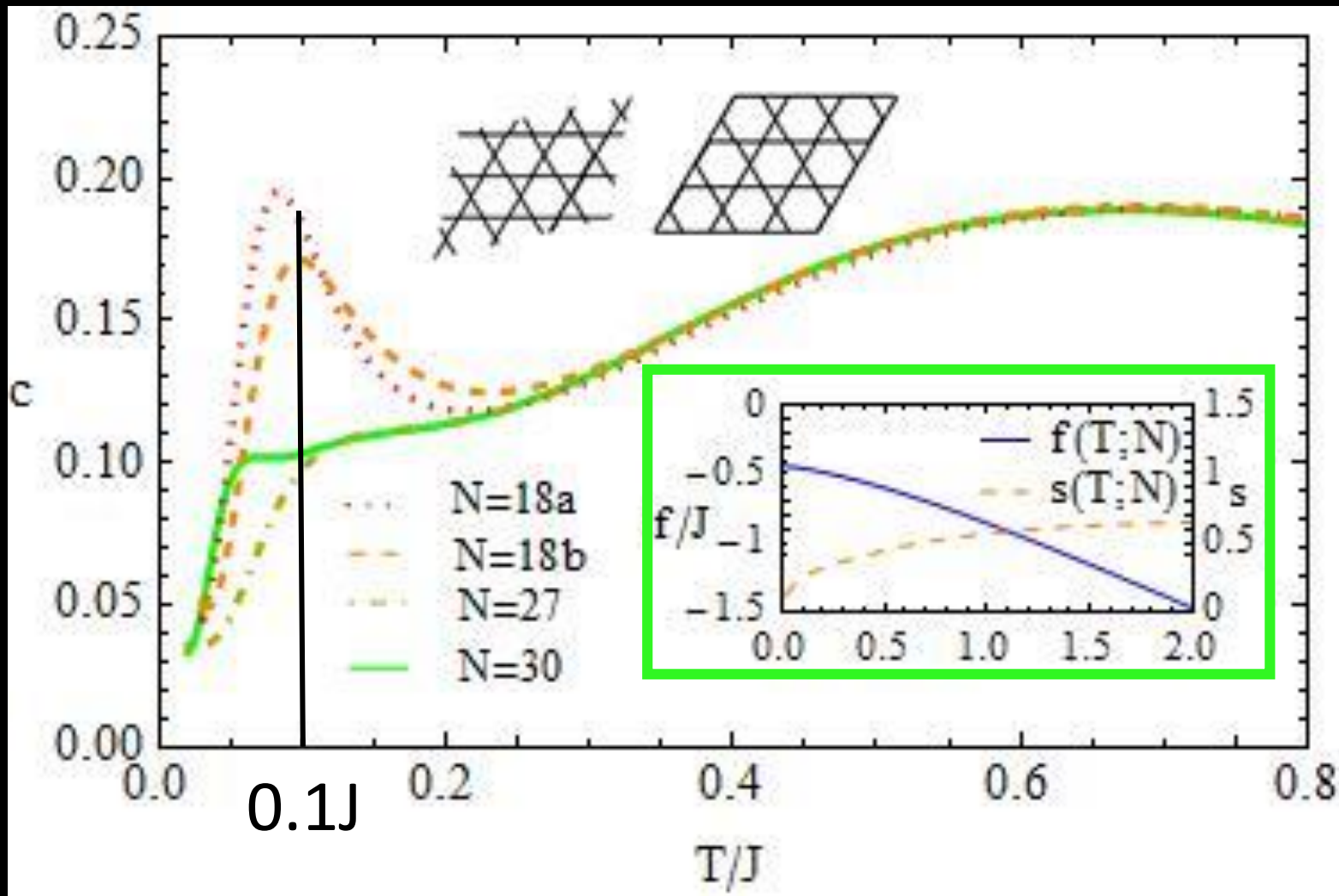
$$\left[\leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{f(1/2\beta; N) - f(1/\beta; N)\}]} \right]$$

$$\leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{\beta, N}^{\text{ens}}}{\exp[N\beta \{f(0; N) - f(1/\beta; N)\}]}$$

$\doteq 1800$

$$\left(\begin{array}{l} \Delta f \doteq 0.02 \\ \beta = 10\text{J} \\ N = 30 \end{array} \right)$$

$S=1/2$ kagome-lattice Heisenberg antiferromagnet



Error is less than 1% down to $T=0.1J$!

Error Probability of Canonical TPQ State

$$\begin{aligned} & \mathbb{P} \left(\left| \langle \hat{A} \rangle_{\beta, N}^{\text{TPQ}} - \langle \hat{A} \rangle_{\beta, N}^{\text{ens}} \right| \geq \epsilon \right) \\ & \leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta, N}^{\text{ens}} + (\langle A \rangle_{2\beta, N}^{\text{ens}} - \langle A \rangle_{\beta, N}^{\text{ens}})^2}{\exp[2N\beta \{f(1/2\beta; N) - f(1/\beta; N)\}]} \\ & \leq \frac{1}{\epsilon^2} \frac{N^{2m}}{\exp[\Theta(N)]} \end{aligned}$$

Even when we replace \hat{A} by the dynamical quantities e.g. $\hat{A}e^{-i\hat{H}t}\hat{B}$, the error is still exponentially small, because $\|\hat{A}e^{-i\hat{H}t}\hat{B}\| = \|\hat{A}\| \|e^{-i\hat{H}t}\| \|\hat{B}\| \leq O(N^4m)$

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Microcanonical TPQ State PRL 108.240401 (2012)

Start from the same state $|\psi_0\rangle \equiv \sum_i c_i |i\rangle$, which is the random vector in the **whole** Hilbert space

Then, calculate

$$\begin{aligned} |k\rangle &\equiv (l - \hat{h})^k |\psi_0\rangle \\ u_k &\equiv \langle k | \hat{h} | k \rangle / \langle k | k \rangle \end{aligned} \quad \left(\begin{array}{l} \hat{h} \equiv \hat{H} / N \\ l : \text{arbitrary constant} \\ \text{of } O(1) \text{ s.t. } l > e_{\max} \end{array} \right)$$

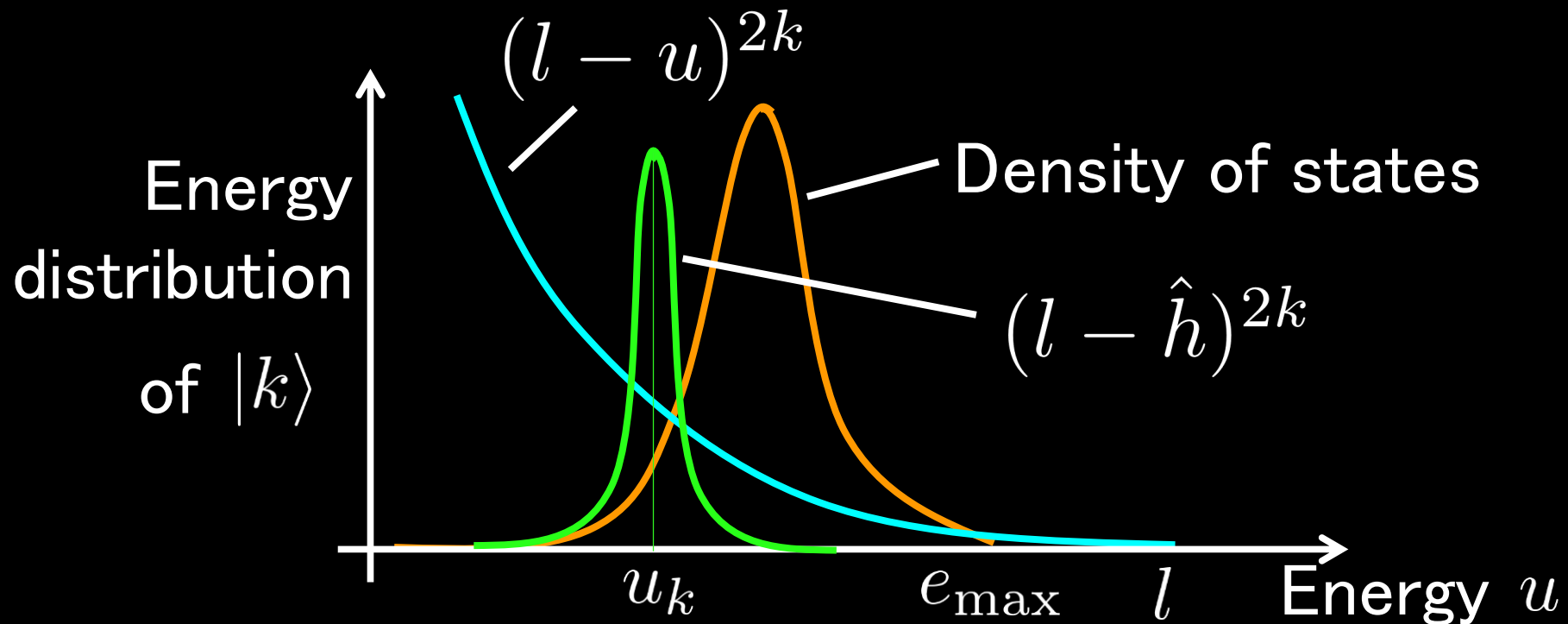
for $k=1,2,\dots$

$|k\rangle$ is the **microcanonical TPQ state**
at energy u_k

Microcanonical TPQ State PRL 108.240401 (2012)

$$\begin{aligned}
 |k\rangle &\equiv (l - \hat{h})^k |\psi_0\rangle \\
 u_k &\equiv \langle k | \hat{h} | k \rangle / \langle k | k \rangle
 \end{aligned}
 \left(\begin{array}{l}
 \hat{h} \equiv \hat{H} / N \\
 l : \text{arbitrary constant} \\
 \text{of } O(1) \text{ s.t. } l > e_{\max}
 \end{array} \right)$$

for $k=1,2,\dots$



Microcanonical TPQ State PRL 108.240401 (2012)

Mechanical Variables

$$\frac{\langle k | \hat{A} | k \rangle}{\langle k | k \rangle} \xrightarrow{P} \frac{\text{Tr}[\hat{A} \rho_{\text{mc}}]}{\text{Tr}[\rho_{\text{mc}}]}$$
$$\left[\rho_{\text{mc}} \equiv (l - \hat{h})^{2k} \right]$$

Genuine Thermodynamic Variables

Entropy

$$s(u_k; N) = \frac{1}{N} \ln \langle k | k \rangle - \frac{2k}{N} \ln(l - u_k) + O(N)$$

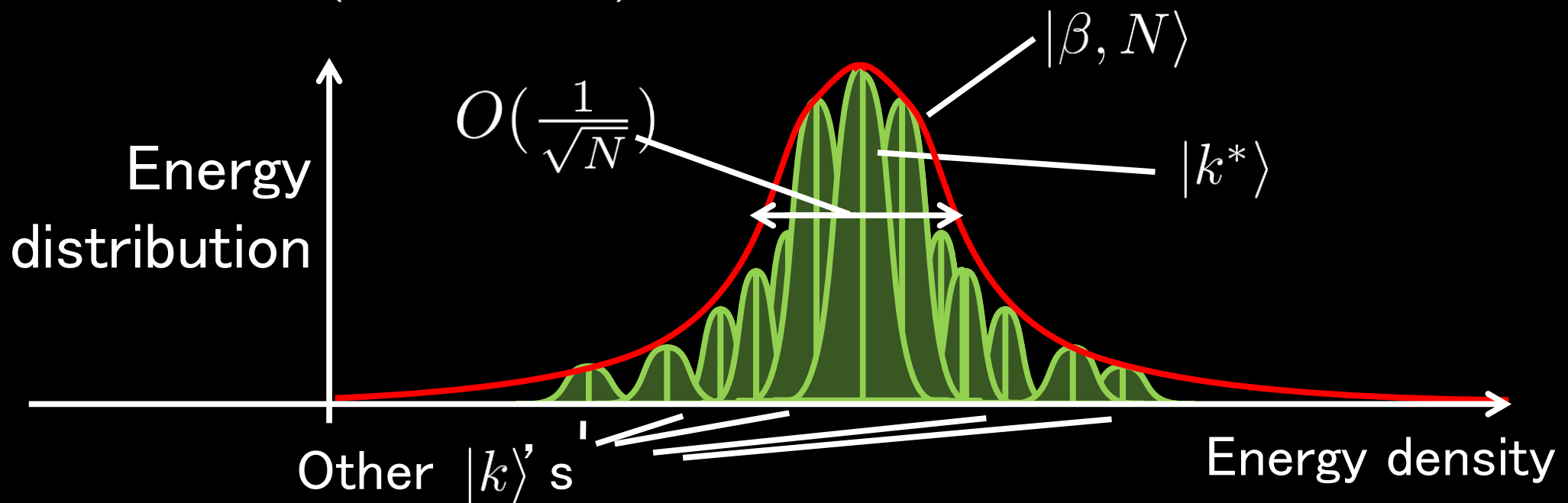
$$\left[|k\rangle \equiv (l - \hat{h})^k |\psi_0\rangle : \text{Unnormalized microcanonical TPQ state at energy } u_k \right]$$

Analytic Relations

Canonical and microcanonical TPQ states are related by simple analytic transformations.

$$\begin{aligned} \exp[-N\beta\hat{h}/2]|\psi_0\rangle &= e^{-N\beta l/2} \sum_{k=0}^{\infty} \frac{(N\beta/2)^k}{k!} |k\rangle \\ &= e^{-N\beta l/2} \sum_{k=0}^{\infty} R_k |\psi_k\rangle. \end{aligned}$$

$$\left[|\psi_k\rangle \equiv \left(1/\sqrt{\langle k|k\rangle}\right) |k\rangle, \quad R_k \equiv (N\beta/2)^k \sqrt{\langle k|k\rangle}/k! \right]$$



Advantages for Numerical Method

$$\exp(-\beta\hat{H})/Z \longrightarrow |\beta, N\rangle \equiv \exp[-N\beta\hat{h}/2]|\psi_0\rangle$$

Many Advantages :

- Free from dimension and structure of Hamiltonian.

Free From Negative Sign Problem
Applicable to Higher Dimensional Systems

- Finite temperature.
- Less amount of calculation than a diagonalization of Hamiltonian.
- Only 2 vectors (i.e. Computer Memory) are needed

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Different Representations of the Same Equilibrium State

Conventional Formulation

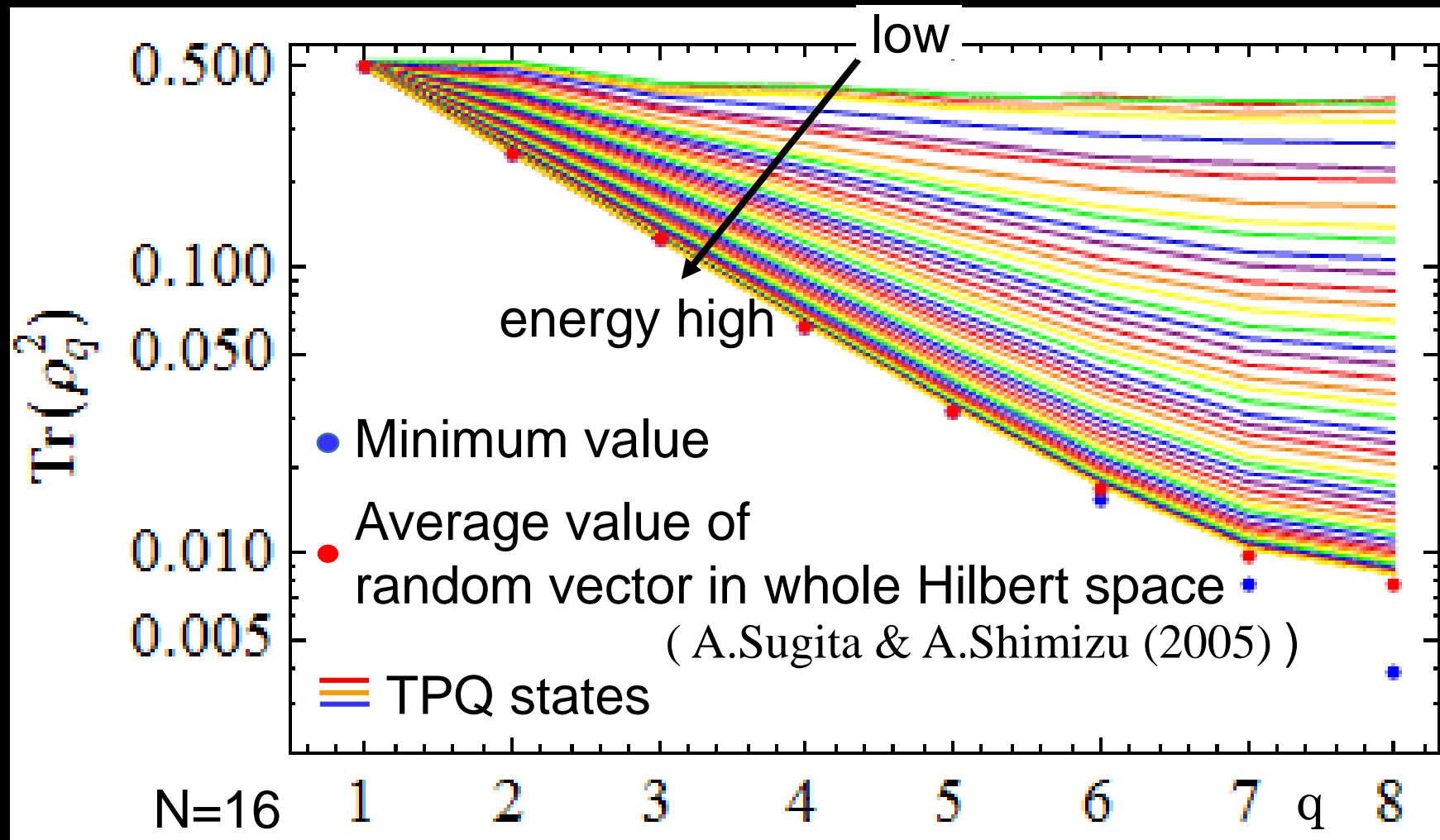
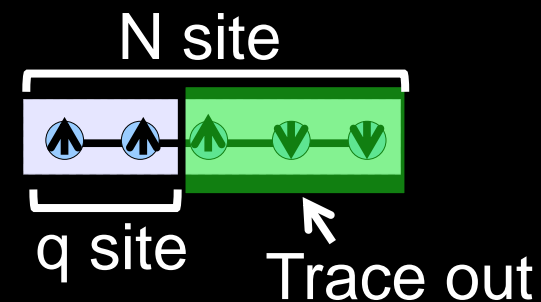
$$\sum_{n \in \text{energy shell}} |n\rangle \langle n|, \exp(-\beta \hat{H})$$

TPQ States Formulation

$$|k\rangle, |\beta, N\rangle$$

As far as we see macroscopic quantities,
we cannot distinguish them.

Entanglement - Purity



TPQ states are almost maximally entangled

Different Representations of the Same Equilibrium State

Conventional Formulation

$$\sum_{n \in \text{energy shell}} |n\rangle \langle n|, \exp(-\beta \hat{H})$$

→ At high temperature, they have little entanglement.

TPQ States Formulation

$$|k\rangle, |\beta, N\rangle$$

→ TPQ states have almost maximum entanglement.

Microscopically completely **different** states represent the **same** equilibrium state.

TPQ State

$$\langle k|k\rangle, \langle \beta, N|\beta, N\rangle$$

Thank You!