Thermal pure quantum state

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SS and A.Shimizu, PRL 108, 240401 (2012)
SS and A.Shimizu, PRL 111, 010401 (2013)
SS and A.Shimizu, arXiv:1312.5145
M.Hyuga, SS, K.Sakai,and A.Shimizu, PRB 90, 121110(R) (2014)

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

4. Equilibrium State and Entanglement

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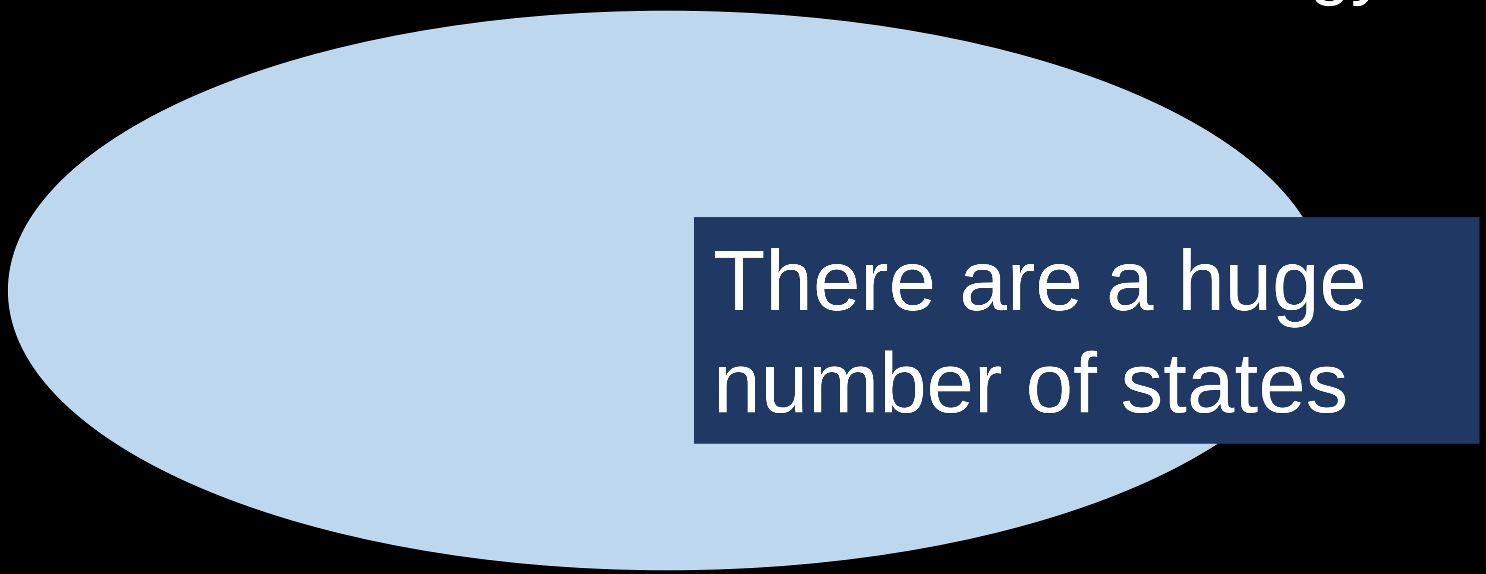
Foundation of Statistical mechanics

Principle of **Equal Weight**:

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

Microscopic View

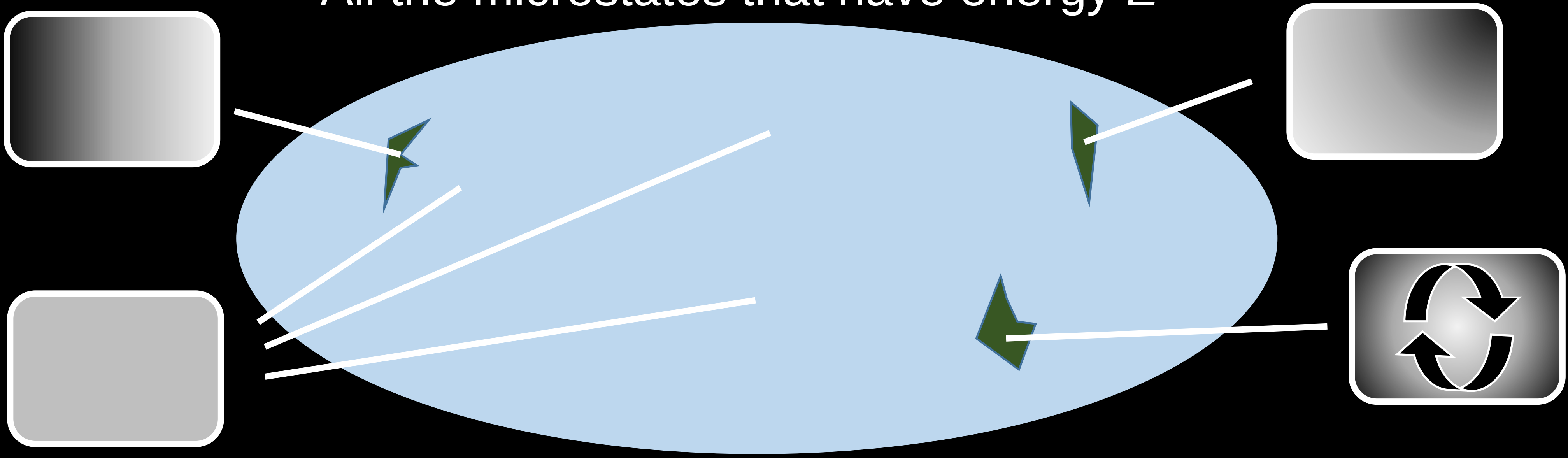
All the microstates that have energy *E*



How can we justify the principle of equal weight?

Explanation using the **Typicality**

All the microstates that have energy *E*



Almost all the microstate at energy E are
macroscopically indistinguishable!

The typicality seems to be more fundamental than the principle of equal weight.

But… does the typicality really hold?

Setup (1) -System

System:

- Isolated quantum system with finite volume V.
- Energy spectrum is discrete.
- The dimension of the Hilbert space can be ∞.

Hamiltonian $\hat{H}$

Energy Eigenstates $\hat{H}|n\rangle = E_n|n\rangle$

- The ensemble formulation gives correct results, which are consistent with thermodynamics in $V \to \infty$

  (We don't consider some exceptional models, e.g., system which have long range interactions.)

Setup (2) -Macroscopic Variables

In statistical mechanics, we have two types of macroscopic variables, mechanical variables and genuine thermodynamic variables.

Mechanical Variables

Ex) Magnetization, Spin-spin correlation function

・Low−degree polynomials of local operators

(i.e. their degree $\leq m = O(1)$)

→ The number of independent mechanical variables is $O(V^m)$!!

Much fewer than the degree of freedom

・Assume every mechanical variable $\hat{A}$ is normalized as $\langle \hat{A}^2 \rangle^{\text{ens}}_{\beta,V} \leq KV^{2m}$

(To exclude foolish operators (ex. $V^V \hat{H}$)
K : Constant independent of $\hat{A}$ and V.)

Setup (2) -Macroscopic Variables

In statistical mechanics, we have two types of macroscopic variables, mechanical variables and genuine thermodynamic variables.

Genuine Thermodynamic Variables

Ex) Temperature T, Entropy S

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

Typicality on Pure Quantum State

P. Bocchieri and A. Loinger (1959), A.Sugita (2007), P.Reiman (2007)

Take a random vector in the specified energy shell :

$$|\psi_E\rangle \equiv \sum_n c_n |n\rangle$$

$\{|n\rangle\}_n$: an arbitrary orthonormal basis spanning enegy shell $[E-\Delta, E]$

$\{c_n\}_n$: a set of random complex numbers with $\sum_n |c_n|^2 = 1$

As far as we look at the mechanical variables, all of their expectation values are very close to their microcanonical ensemble averages.

For $^\forall \epsilon > 0$, we can prove

$$\mathrm{P}\left(\left|\langle\psi_E|\hat{A}|\psi_E\rangle - \langle\hat{A}\rangle^{\mathrm{ens}}_{E,V}\right| \le \epsilon \ \ \text{for } ^\forall \hat{A}\right) \ge 1 - \frac{1}{\epsilon^2}\boxed{\frac{N_{\mathrm{M}} \ \max_{\hat{A}}\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V}}{d}}$$

N_{M} : The number of the independent mechanical variables.

$\max_{\hat{A}}\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V}$: Maximum value of $\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V}$.

d : Dimension of the Hilbert space of the energy shell $[E-\Delta, E]$.

Typicality on Pure Quantum State

P. Bocchieri and A. Loinger (1959), A.Sugita (2007), P.Reiman (2007)

$$\mathrm{P}\left(\text{for } {}^{\forall}\hat{A},\ \left|\langle\psi_E|\hat{A}|\psi_E\rangle - \langle\hat{A}\rangle^{\mathrm{ens}}_{E,V}\right| \le \epsilon\right) \ge 1 - \frac{1}{\epsilon^2}\boxed{\frac{N_{\mathrm{M}}\ \max_{\hat{A}}\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V}}{d}}$$

N_{M} : The number of the independent mechanical variables.

$\max_{\hat{A}}\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V}$: Maximum value of $\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V}$.

d : Dimension of the Hilbert space of the energy shell $[E-\Delta, E]$.

We have

$$N_{\mathrm{M}} = O(V^m)$$

$$\max_{\hat{A}}\langle\hat{A}^2\rangle^{\mathrm{ens}}_{E,V} \le K^2 V^{2m}$$

(K : some constant)

$$d = \exp[O(V)]$$

Thus, we get

$$\frac{N_{\mathrm{M}}\ \max_{\hat{A}}\|\hat{A}\|^2}{d} \le \frac{O(V^{3m})}{\exp[O(V)]}$$

That is, when $\epsilon = O(1)$,

$$(\mathrm{RHS}) \ge 1 - \exp[-O(V)]$$

$|\psi_E\rangle$ gives correct equilibrium values for all mechanical variables simultaneously.

Direction of Our Work

We saw

$\boxed{\text{Typical states represent an equilibrium state.}}$

→ We call such states "thermal pure quantum (TPQ) states".

However …

- ✓ How can we realize such $|\psi_E\rangle$?

  Possible if we know all energy eigenstates $\{|n\rangle\}_n$,
  but it's as hard as the ensemble average…

- ✓ Can we obtain the genuine thermodynamic variables from a single pure state?

- ✓ Can we obtain such pure states corresponding to (grand)canonical ensemble?

We will solve these points and

Establish the formulation of statistical mechanics based on the **thermal pure quantum state**.

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Canonical Thermal Pure Quantum States

PRL 111, 010401 (2013)

The canonical thermal pure quantum (TPQ) state at temperature $1/\beta$ is defined by

$$|\beta, V\rangle \equiv \sum_i \underbrace{\boxed{z_i}}_{\text{Random phase}} \underbrace{\boxed{\exp\left[-\frac{1}{2}\beta\hat{H}\right]}}_{\text{High energy cut-off}} \underbrace{\boxed{|i\rangle}}_{\text{Arbitrary basis}}$$

$\{|i\rangle\}_i$: an arbitrary orthonormal basis of the Hilbert space (NOT a basis in the energy shell)

$\{z_i\}_i$: a set of random complex numbers

s.t. $z_i \equiv \frac{x_i + i y_i}{\sqrt{2}}$

(x_i and y_i obey normal distribution with mean = 0 and variance = 1)

- ✓ We don't have any resevoir.
- ✓ It's not the "purification" of the Gibbs state $Z(\beta, V)^{-1}\exp[-\beta\hat{H}]$.

Properties of Canonical TPQ State

We will show a single realization of $|\beta, V\rangle$ gives thermodynamic predictions correctly.

✓ Genuine Thermodynamic Variables

Free energy $F(\beta, V) = -\frac{1}{\beta}\ln Z(\beta, V)$ is obtained from the norm of $|\beta, V\rangle$!

$$F(\beta, V) \boxed{\simeq} -\frac{1}{\beta}\ln\langle\beta, V|\beta, V\rangle \left(= -\frac{1}{\beta}\ln\sum_{i,j} z_i^* z_j \langle i|\exp[-\beta\hat{H}]|j\rangle\right)$$

✓ Mechanical Variables

For ${}^\forall \hat{A} \in \text{Mechanical Variables},$

$$\langle\hat{A}\rangle^{\text{ens}}_{\beta,V} \boxed{\simeq} \langle\hat{A}\rangle^{\text{TPQ}}_{\beta,V} \equiv \frac{\langle\beta,V|\hat{A}|\beta,V\rangle}{\langle\beta,V|\beta,V\rangle}$$

$$\left(\simeq Z(\beta, V)^{-1}\sum_{i,j} z_i^* z_j \langle i|\exp[-\tfrac{1}{2}\beta\hat{H}]\hat{A}\exp[-\tfrac{1}{2}\beta\hat{H}]|j\rangle\right)$$

Moreover, $\simeq$ means
they are exponentially close!

$|\beta, V\rangle \equiv \sum_i z_i \exp\left[-\frac{1}{2}\beta\hat{H}\right]|i\rangle$

$Z(\beta, V)$: Partition function

Error Estimate for Canonical TPQ State

✔ Free energy

For ${}^\forall\epsilon > 0$,

$$\mathrm{P}\left(\left|\frac{\langle\beta,V|\beta,V\rangle}{Z(\beta,V)}-1\right|\le\epsilon\right)\ge 1-\frac{1}{\epsilon^2}\frac{1}{\exp[2V\beta\{f(2\beta;V)-f(\beta;V)\}]}$$

$$\ge 1-\frac{1}{\epsilon^2}\frac{1}{\exp[O(V)]}$$

[$Z(\beta,V)$: Partition function $\quad f(\beta;V)\equiv\frac{F(\beta,V)}{V}$: Free energy density]

✔ Mechanical Variables

For ${}^\forall\epsilon > 0$,

$$\mathrm{P}\left(\left|\langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,V}-\langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,V}\right|\le\epsilon\ \text{for}\ {}^\forall\hat{A}\right)$$

$$\ge\ 1-\frac{N_{\mathrm{m}}}{\epsilon^2}\frac{\langle(\Delta\hat{A})^2\rangle^{\mathrm{ens}}_{2\beta,V}+\left(\langle A\rangle^{\mathrm{ens}}_{2\beta,V}-\langle A\rangle^{\mathrm{ens}}_{\beta,V}\right)^2}{\exp[2V\beta\{f(2\beta;V)-f(\beta;V)\}]}$$

$$\ge\ 1-\frac{1}{\epsilon^2}\frac{V^{3m}}{\exp[O(V)]}$$

[N_{m}: The number of the independent mechanical variables. $\quad\langle(\Delta\hat{A})^2\rangle^{\mathrm{ens}}_{\beta,N}$:Variance of $\hat{A}$]

A single realization of the TPQ state gives equilibrium values of all macrocscopic quantities.

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Different Representations of the Same Equilibrium State

Conventional Formulation

$$\hat{\rho}_{\mathrm{can}} \ \left(\equiv \frac{1}{Z(\beta, V)} \exp(-\beta \hat{H}) \right)$$

TPQ States Formulation

$$|\beta, V\rangle$$

These formulations give the same thermodynamic predictions

Time invariance

P. Bocchieri and A. Loinger (1959), P.Reiman (2007)

Conventional Formulation

$$e^{-\frac{i}{\hbar}\hat{H}t}\rho_{\mathrm{can}}e^{\frac{i}{\hbar}\hat{H}t} = \rho_{\mathrm{can}} \qquad \left(\rho_{\mathrm{can}} \equiv \frac{\exp(-\beta\hat{H})}{Z(\beta,V)}\right)$$

$$\boxed{\text{Rigorously time invariant}}$$

TPQ States Formulation

$$e^{-\frac{i}{\hbar}\hat{H}t}|\beta,V\rangle = \sum_n e^{-\frac{i}{\hbar}E_n t} z_n \exp[-\beta\hat{H}]|n\rangle$$

$$\neq |\beta,V\rangle$$

Time invariance

P. Bocchieri and A. Loinger (1959),
P.Reiman (2007)

Conventional Formulation

$$e^{-\frac{i}{\hbar}\hat{H}t}\rho_{\mathrm{can}}e^{\frac{i}{\hbar}\hat{H}t} = \rho_{\mathrm{can}} \qquad \left(\rho_{\mathrm{can}} \equiv \frac{\exp(-\beta\hat{H})}{Z(\beta,V)}\right)$$

Rigorously time invariant

TPQ States Formulation

$$e^{-\frac{i}{\hbar}\hat{H}t}|\beta,V\rangle = \sum_n e^{-\frac{i}{\hbar}E_n t} z_n \exp[-\beta\hat{H}]|n\rangle$$

$$= \sum_n z'_n \exp[-\beta\hat{H}]|n\rangle$$

$$\left[z'_n \equiv e^{-\frac{i}{\hbar}E_n t} z_n\right]$$

$\longrightarrow \{z'_n\}_n$ is another realization of $\{z_n\}_n$

Macroscopically time invariant

Response Function

Cf) P.Reiman (2007)
C.Bartsch and J.Gemmer (2009)
T Monnai, A Sugita (2014)

When we apply an external field $-\hat{A}F(t)$ to system;

$$\hat{H}_{\mathrm{total}}(t) = \hat{H}_0 - \hat{A}F(t),$$

the response of a mechanical variable $\hat{B}$ is obtained by Green-Kubo relations,

$$\Delta B \ \left(\equiv \mathrm{Tr}(\hat{\rho}_{\mathrm{total}}(t)\hat{B}) - \mathrm{Tr}(\hat{\rho}_0\hat{B})\right)$$
$$= \tfrac{1}{i}\int_{-\infty}^{t} \mathrm{Tr}([\hat{A}, \hat{B}(t)]\hat{\rho}_0)$$

$\hat{\rho}_{\mathrm{total}}(t)$: Density matrix of the system

$$\hat{\rho}_0 \equiv Z(\beta, V)^{-1}\exp[-\beta\hat{H}_0], \qquad \hat{B}(t) \equiv e^{i\hat{H}_0 t}\hat{B}e^{-i\hat{H}_0 t}$$

Therefore, we need to evaluate $\langle \hat{A}e^{i\hat{H}t}\hat{B}e^{-i\hat{H}t}\rangle_{\beta,V}^{\mathrm{ens}}$ to know the response.

$\longrightarrow$ Using the TPQ state, this is evaluated by $\dfrac{\langle\beta,V|\hat{A}e^{i\hat{H}t}\hat{B}e^{-i\hat{H}t}|\beta,V\rangle}{\langle\beta,V|\beta,V\rangle}$.

Error of time correlation

Cf) P.Reiman (2007)
C.Bartsch and J.Gemmer (2009)
T Monnai, A Sugita (2014)

Error of $\hat{C} \equiv \hat{A} e^{i\hat{H}t} \hat{B} e^{-i\hat{H}t}$ using the canonical TPQ state is evaluated as

$$\mathrm{P}\left(\left| \langle \hat{C} \rangle^{\mathrm{TPQ}}_{\beta,N} - \langle \hat{C} \rangle^{\mathrm{ens}}_{\beta,N} \right| \geq \epsilon \right) \leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{C})^2 \rangle^{\mathrm{ens}}_{2\beta,V} + (\langle C \rangle^{\mathrm{ens}}_{2\beta,V} - \langle C \rangle^{\mathrm{ens}}_{\beta,V})^2}{\exp[2V\beta\{f(2\beta;V) - f(\beta;V)\}]}$$

$$\leq \frac{1}{\epsilon^2} \frac{V^{4m}}{\exp[O(V)]}$$

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

However, after waiting for exponentially long time, there can be a small period when $\left| \langle \hat{C} \rangle^{\mathrm{TPQ}}_{\beta,N} - \langle \hat{C} \rangle^{\mathrm{ens}}_{\beta,N} \right| \geq O(1)$.

$\longrightarrow$ We can evaluate $\langle \hat{C} \rangle^{\mathrm{ens}}_{\beta,N}$ correctly at most time t.

Fluctuation of Mixed state

In quantum statistical mechanics, fluctuation is the sum of "quantum fluctuation" and "thermal fluctuation" …… ???

For an arbitrary mixed state $\hat{\rho}$, fluctuation may be decomposed into two parts.

$$\mathrm{Tr}[\hat{A}^2\hat{\rho}] - \mathrm{Tr}[\hat{A}\hat{\rho}]^2 = \sum_i w_i \left\{ \langle i|\hat{A}^2|i\rangle - \langle i|\hat{A}|i\rangle^2 \right\}$$

Fluctuation

"Quantum fluctuation"

$$+ \sum_i w_i \left\{ \langle i|\hat{A}|i\rangle - \mathrm{Tr}[\hat{A}\hat{\rho}] \right\}^2$$

$$\hat{\rho} = \sum_i w_i |i\rangle\langle i|$$

"Thermal fluctuation"

However, since the basis $\{|i\rangle\}_i$ is not unique for mixed states $\hat{\rho}$, the decomposition of the fluctuation is not uniquely determined either.

→ We can't distinguish quantum and thermal fluctuations.

Fluctuation of TPQ state

Cf) Energy Eigenstate Themalization Hypothesis
M.Rigol, V.Dunjko & M.Olshanii (2008)

$$\mathrm{Tr}[\hat{A}^2\hat{\rho}] - \mathrm{Tr}[\hat{A}\hat{\rho}]^2 = \sum_i w_i \left\{ \langle i|\hat{A}^2|i\rangle - \langle i|\hat{A}|i\rangle^2 \right\}$$

Fluctuation

"Quantum fluctuation"

$$+ \sum_i w_i \left\{ \langle i|\hat{A}|i\rangle - \mathrm{Tr}[\hat{A}\hat{\rho}] \right\}^2$$

$$\hat{\rho} = \sum_i w_i |i\rangle\langle i|$$

"Thermal fluctuation"

By contrast, since $\hat{\rho}$ is a pure quantum state in TPQ formulation, the representation of $\hat{\rho}$ is unique, i.e., $\hat{\rho} = |\psi\rangle\langle\psi|$.

Therefore, in TPQ formulation, quantum and thermal fluctuations are well defined.

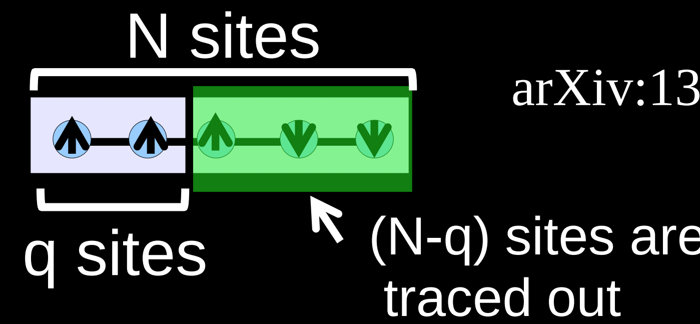
"Thermal fluctuation" $= 0$

"Quantum fluctuation" $= \langle(\Delta\hat{A})^2\rangle^{\mathrm{ens}}$

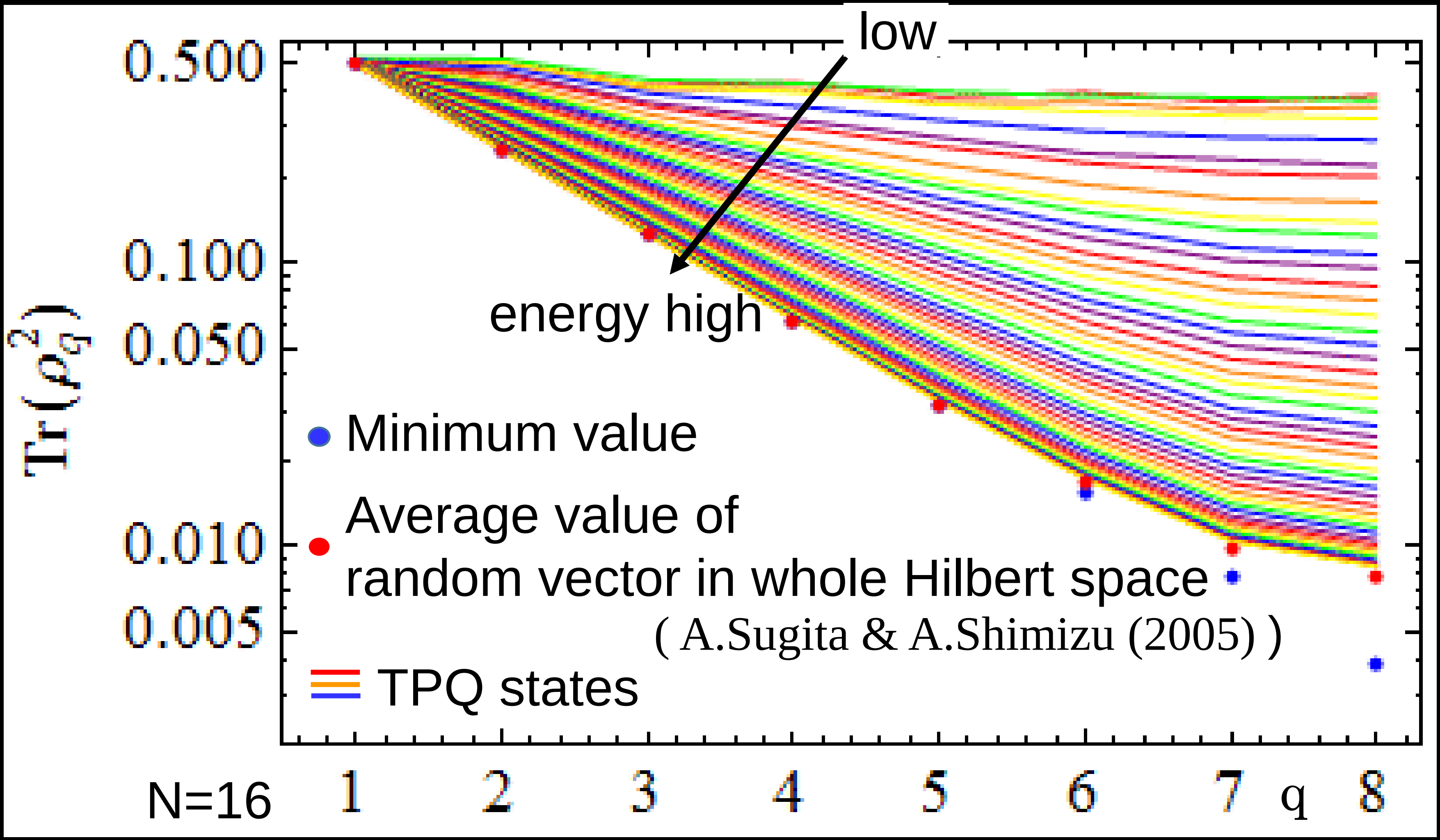
All fluctuation in ensemble formulation is squeezed into quantum fluctuation in TPQ formulation.

Entanglement -Purity

$$\hat{\rho}_q \equiv \mathrm{Tr}_{(N-q)}\left[|\beta, V\rangle\langle\beta, V|\right]$$



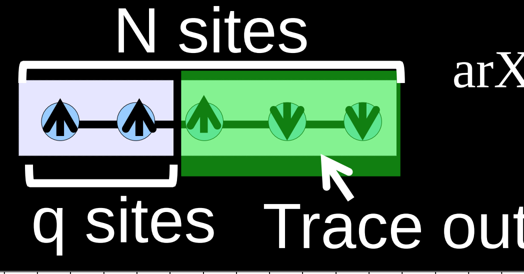
arXiv:1312.5145

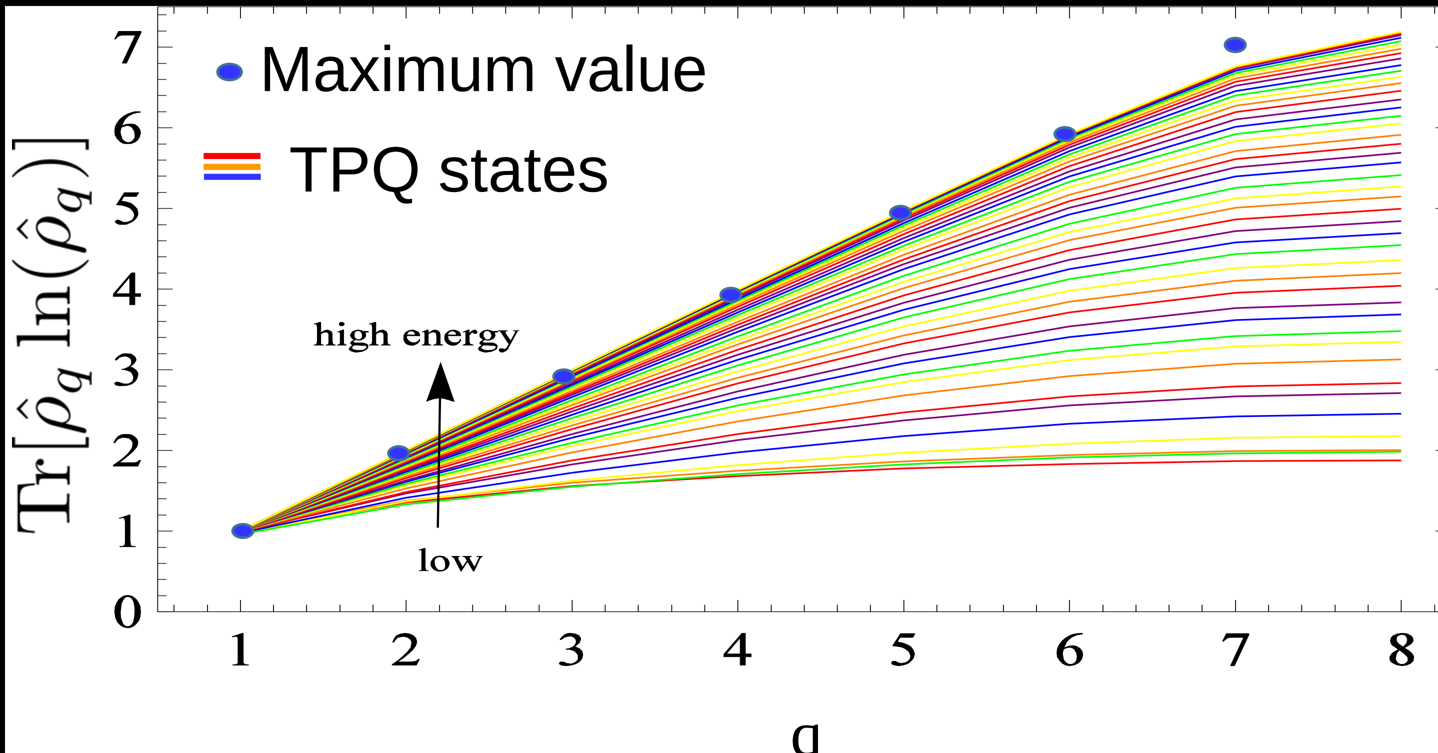


TPQ states are almost maximally entangled

Entanglement
-von Neumann's Entropy

arXiv:1312.5145





"When $q \ll N$, $\hat{\rho}_q$ is close to the Gibbs state."

("Canonical Typicality",
S.Goldstein, J.Lebowitz, R.Tumulka, N.Zanghi (2006)
S.Popescu, A.Short and A.Winter (2006))

⟶ von Neumann's entropy is close to the thermal entropy.

TPQ states are almost maximally entangled

Bipartite entanglement entropy

Conventional Formulation

$$\hat{\rho}_{\mathrm{can}} \ \left(\equiv \frac{1}{Z(\beta,V)} \exp(-\beta \hat{H}) \right)$$

$\longrightarrow$ At high temperature, they have little entanglement.

TPQ States Formulation

$$|\beta, N\rangle$$

$\longrightarrow$ TPQ states have almost maximum entanglement.

Microscopically completely different states represent the same equilibrium state.

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Application to Numerics (1)

PRL 111, 010401 (2013)

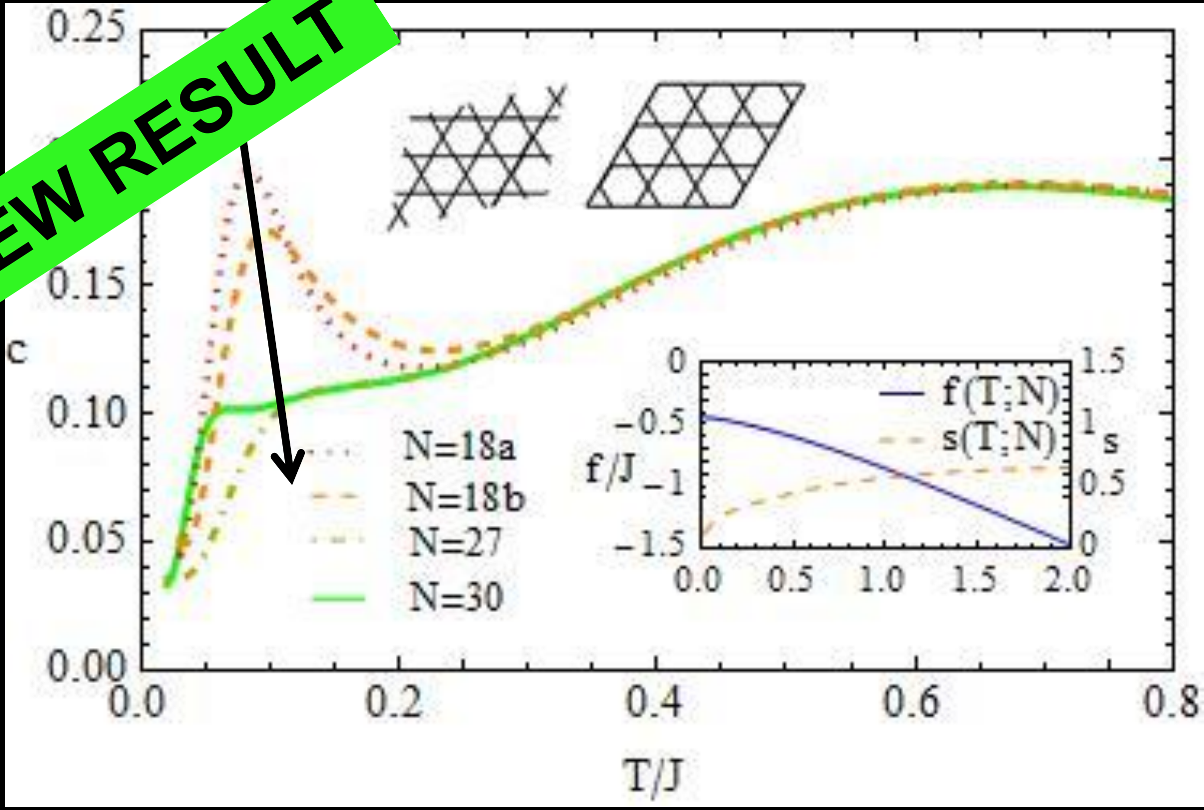
We replace

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

It is advantageous in practical applications.

S=1/2 kagome-lattice Heisenberg antiferromagnet $\hat{H} = \sum_{(i,j)} \vec{S}_i \vec{S}_j$

NEW RESULT



Second peak vanishesas as $V \to \infty$?

Application to Numerics (2)

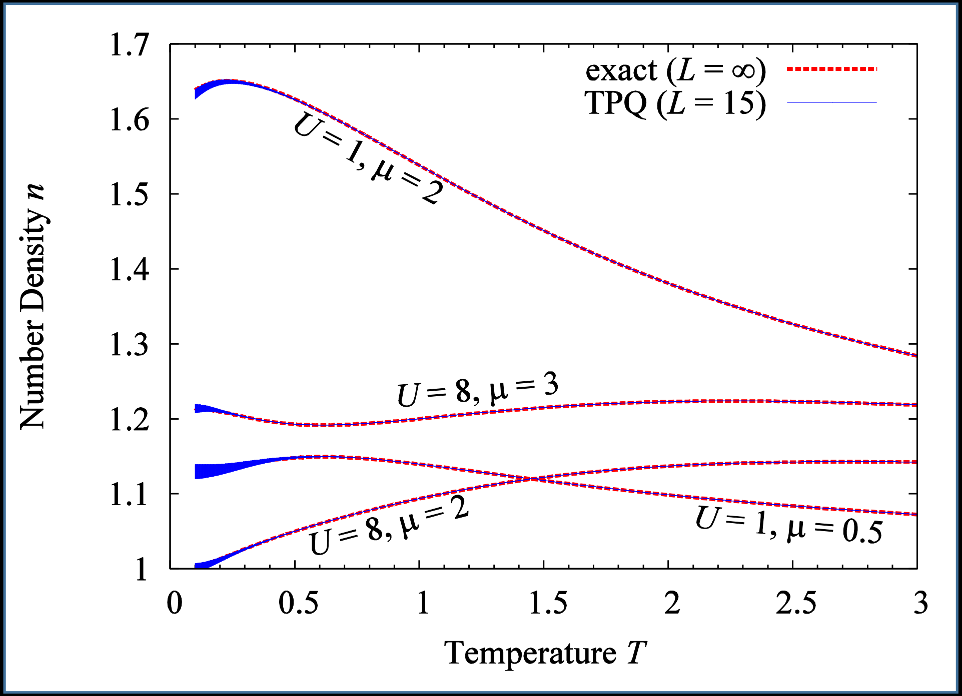
PRB 90, 121110(R) (2014)

1D Hubbard Model

$$\hat{H} = -t\sum_{i,\sigma}\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} + \text{h.c.} + U\sum_i(\hat{n}_{i,\uparrow}-\tfrac{1}{2})(\hat{n}_{i+1,\downarrow}-\tfrac{1}{2})$$

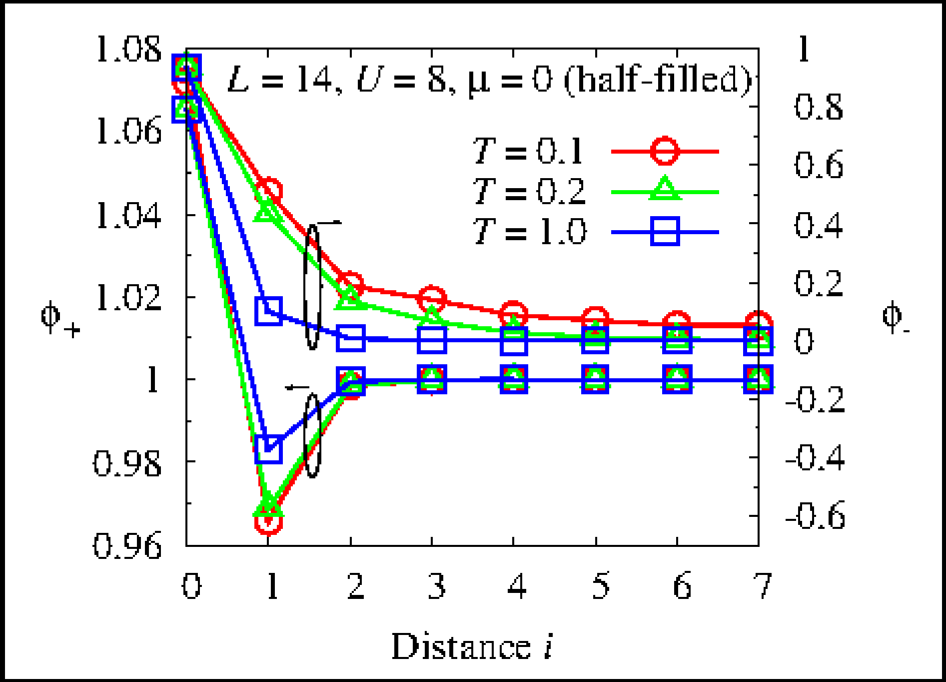
We use grandcanonical TPQ state : $\sum_i z_i \exp\left[-\frac{1}{2}\beta(\hat{H} - \nu\sum_i \hat{n}_i)\right] |i\rangle$

Number Density



Agree with exact results

Correlation Function



Correlation function can also be calculated

Application to Numerics (2)

PRB 90, 121110(R) (2014)

Hubbard Model

$$\hat{H} = -t \sum_{i,\sigma} \hat{c}^\dagger_{i,\sigma} \hat{c}_{i+1,\sigma} + \text{h.c.} + U \sum_i (\hat{n}_{i,\uparrow} - \tfrac{1}{2})(\hat{n}_{i+1,\downarrow} - \tfrac{1}{2})$$

Comparison

Canonical TPQ state

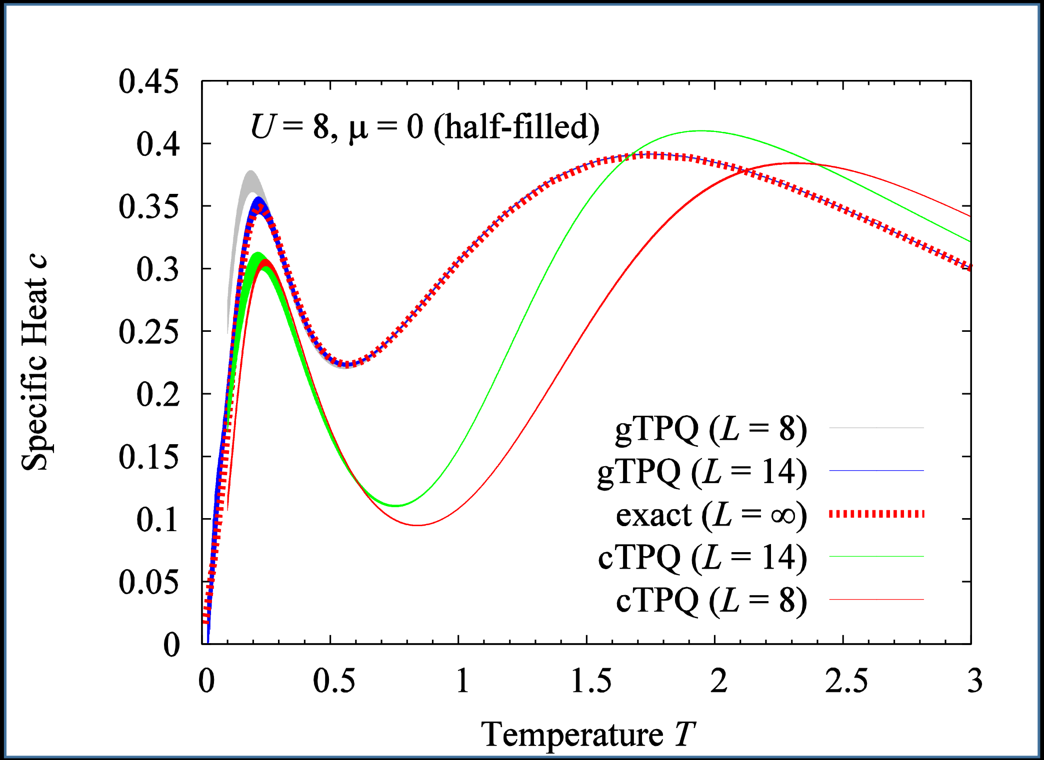
$$\sum_i z_i \ \exp\left[-\tfrac{1}{2}\beta \hat{H}\right] \ |i\rangle$$

V.S.

Grandcanonical TPQ state

$$\sum_i z_i \ \exp\left[-\tfrac{1}{2}\beta(\hat{H} - \nu \sum_i \hat{n}_i)\right] \ |i\rangle$$

Specific Heat



Although equivalence of ensembles holds in $V \to \infty$, grandcanonical ensemble is more accurate than canonical one in finite V.

Numerical Procedure

Canonical TPQ states are represented by superposition of equilibrium states $|k\rangle$.

$$\sum_i z_i \exp[-\beta \hat{H}/2]|i\rangle = e^{-\beta l/2} \sum_i z_i \sum_{k=0}^{\infty} \frac{(V\beta/2)^k}{k!}(l-\hat{h})^k|i\rangle$$

$$= e^{-\beta l/2} \sum_{k=0}^{\infty} \frac{(V\beta/2)^k}{k!}|k\rangle$$

$$\left(|k\rangle \equiv \sum_i z_i (l-\hat{h})^k|i\rangle\right)$$

Numerical Procedure

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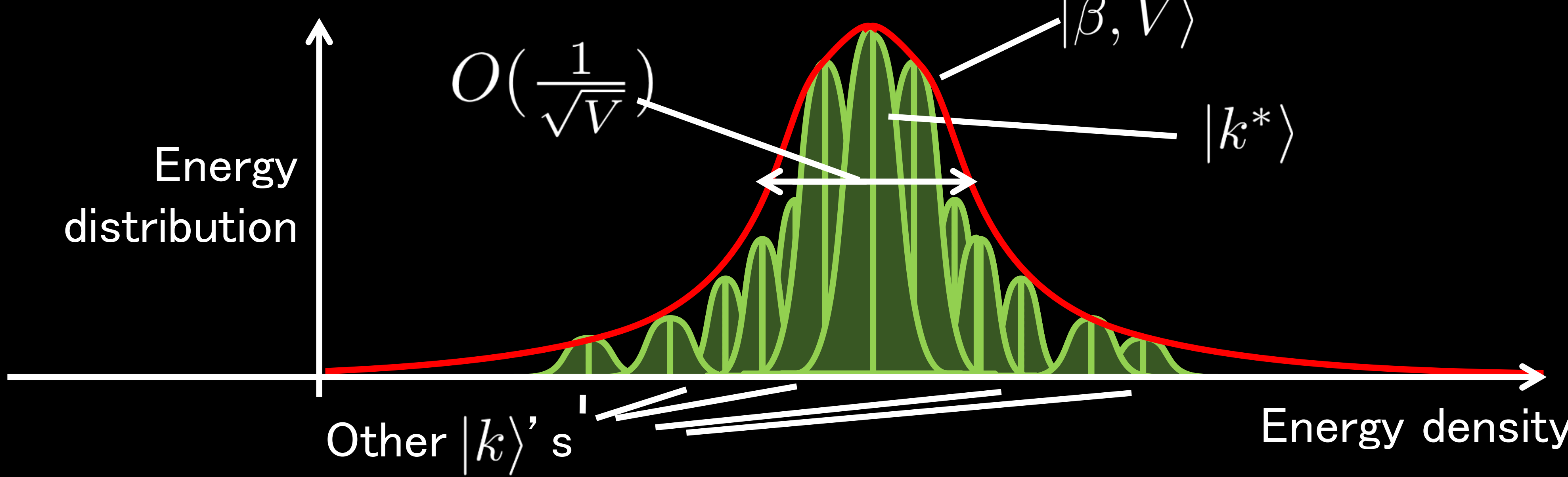

Practical Formula

Moreover, we don't need to construct $|\beta, V\rangle$'s for different temperatures one by one.

$$\langle \beta, V|\hat{A}|\beta, V\rangle = e^{-V\beta l} \sum_{k,k'} \frac{1}{k!k'!} \left(\frac{V\beta}{2}\right)^{k+k'} \langle k|\hat{A}|k'\rangle$$

$$= \sum_{k=0}^{\infty} \frac{(V\beta)^{2k}}{(2k)!} \boxed{\langle k|\hat{A}|k\rangle}$$

$$+ \sum_{k=0}^{\infty} \frac{(V\beta)^{2k+1}}{(2k+1)!} \boxed{\langle k|\hat{A}|k+1\rangle}$$

$+$ (Exponentially Small Error)

$$\left(|k\rangle \equiv \sum_i z_i (l - \hat{h})^k |i\rangle\right)$$

Equilibrium values are obtained only from $\langle k|\hat{A}|k\rangle$'s and $\langle k|\hat{A}|k+1\rangle$'s

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 spatial dimension and structure of Hamiltonian.

Applicable to 2D Frustrated/Fermion Systems
(Kagome) (Hubbard model)

- Almost Self-validating formulation

$$\mathrm{P}\left(\left|\langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,V} - \langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,V}\right| \leq \epsilon \text{ for } {}^{\forall}\hat{A}\right)$$

$$\geq 1 - \boxed{\frac{N_{\mathrm{m}}}{\epsilon^2}\frac{\langle(\Delta\hat{A})^2\rangle^{\mathrm{ens}}_{2\beta,V} + \left(\langle A\rangle^{\mathrm{ens}}_{2\beta,V} - \langle A\rangle^{\mathrm{ens}}_{\beta,V}\right)^2}{\exp[2V\beta\{f(2\beta;V) - f(\beta;V)\}]}}$$

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

Summary

SS and A.Shimizu, PRL 108, 240401 (2012)
SS and A.Shimizu, PRL 111, 010401 (2013)
SS and A.Shimizu, arXiv:1312.5145
M.Hyuga, SS, K.Sakai,and A.Shimizu, PRB 90, 121110(R) (2014)

✓ Thermal equilibrium state

$$\exp[-\beta \hat{H}] \qquad |\beta, N\rangle \equiv \sum_i c_i \exp\left[-\frac{1}{2}\beta\hat{H}\right]|i\rangle$$

Genuine thermodynamic variables $F(\beta, V) \simeq -\frac{1}{\beta}\ln\langle\beta, V|\beta, V\rangle$

Mechanical variables $\langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,N} \equiv \frac{\langle\beta,N|\hat{A}|\beta,N\rangle}{\langle\beta,N|\beta,N\rangle} \simeq \langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N}$

Errors are exponentially small!

✓ TPQ states reproduce many aspects of statistical mechanics

- TPQ states are time invariant.
- Time correlation can be caluculated
- All fluctuation is squeezed into quantum fluctuation

✓ TPQ states have large entanglement

✓ Advantageous to numerical applications