# 平衡化した量子純粋状態が持つ エンタングルメントエントロピーの普遍的な振る舞い arXiv: 1703.02993 (Nat. Comm. in press) 杉浦祥

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#### Ensemble average



#### ✓ Superposition of all realizable states

#### SS and A. Shimizu, PRL (2012) <u>Thermal Pure Quantum States</u> SS and A. Shimizu, PRL (2013) The canonical thermal pure quantum (cTPQ) state at temperature $1/\beta$ is $|\beta\rangle \equiv \frac{1}{\sqrt{Z}} \sum_{i} c_{ab} \exp\left[-\frac{1}{2}\beta \hat{H}\right] |i\rangle$ defined as Arbitrary basis Random number K High energy cut-off $Z \equiv \sum_{i} |c_i|^2 e^{-\beta E_i}, \{|a,b\rangle\}_{ab}$ : arbitrary orthonormal basis $\{c_i\}_i$ : random complex numbers s.t. $c_i \equiv \frac{x_i + iy_i}{\sqrt{2}}$ ( $x_i$ and $y_i$ obey normal distribution with mean = 0 and variance = 1)

$$\begin{array}{l} \checkmark \mbox{Equilibrium value} \\ \mbox{For } \forall \epsilon > 0, \\ P\left( \left| \langle \beta | \hat{A} | \beta \rangle - \langle \hat{A} \rangle_{\beta}^{\rm ens} \right| \geq \epsilon \right) \leq \frac{1}{\epsilon^2} \frac{\langle (\Delta \hat{A})^2 \rangle_{2\beta}^{\rm ens} + (\langle A \rangle_{2\beta}^{\rm ens} - \langle A \rangle_{\beta}^{\rm ens})^2}{\exp[2V\beta \{f(2\beta) - f(\beta)\}]} \\ \leq \frac{1}{\epsilon^2} \boxed{\frac{V^{3m}}{\exp[O(V)]}} \quad ``Typicality'' \\ f(\beta; V) \equiv \frac{F(\beta, V)}{V} : \mbox{Free energy density} \\ \langle \hat{A} \rangle_{\beta}^{\rm ens} : \mbox{Ensemble average, } \langle (\Delta \hat{A})^2 \rangle_{\beta}^{\rm ens} : \mbox{Variance of } \hat{A} \end{array}$$

#### Numerical Applications of TPQ state SS and A.Shimizu, arXiv (2013) M. Hyuga, SS, K. Sakai, A.Shimizu, PRB(2014)



Number Density

**Correlation Function** 



Specific Heat



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

#### Is such a state metaphysical?

No, such states are realized in ultracold atoms experiments.



By M.Greiner's Group (A.Kaufman,et.al, Science(2016)

"Quantum thermalization through entanglement in an isolated many-body system")





## **Bipartite Entanglement Entropy**

We consider isolated quantum systemHamiltonian:  $\hat{H}$ Time evolution:  $e^{-\frac{i}{\hbar}\hat{H}}|\psi\rangle$ 



<u>When a system is devided into A and B;</u> <u>Hilbert space:</u>  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ <u>Quantum state:</u>  $\hat{\rho}_A \equiv \operatorname{tr}_B[|\psi\rangle\langle\psi|]$ 

Renyi entanglement entropy  $S_n \equiv \frac{1}{1-n} \ln \left( \text{tr}_A[\hat{\rho}_A^n] \right)$ 

It quantifies a quantum correlation between A and B.

$$\xrightarrow{n \to 1} S_{\rm vN} \equiv {\rm tr}_A[\hat{\rho}_A \ln \hat{\rho}_A]$$

What is the role of the entanglement entropy in thermalization?

When we look locally, the thermodynamic entropy is recovered as the entanglement entropy

When we look grobally, quantum correlation breaks the correspondence between the thermal and entanglement entropy.

#### What is the role of the entanglement entropy in thermalization?



#### Experiment



#### Energy eigenstates



(Kaufman et.al., Science, 2016) (Garrison et.al, arXiv, 2015)

And more... (P. Calabrese and J. Cardy J. Stat Mech 2007 T.Takayanagi and T. Ugajin JHEP 2010 .....)

 In this talk, I focus on...
 ✓ Volume-law entanglement, i.e., the state has finite energy density
 ✓ The second (n = 2) Renyi entropy

#### <u>Renyi Entropy of TPQ state</u>

Let's calculate the Renyi entropy for the TPQ state;

$$|\beta\rangle \equiv \frac{1}{\sqrt{Z}} \sum_{a,b} c_{ab} \exp\left[-\frac{1}{2}\beta\hat{H}\right] |a,b\rangle \qquad Z \equiv \sum_{i} |c_{i}|^{2} e^{-\beta\hat{H}}$$

Reduced density matrix

$$\hat{\rho}_{A} \equiv \operatorname{tr}_{B} \left[ |\beta\rangle \langle \beta| \right] 
= \frac{1}{Z} \sum_{a_{1}, a_{2}, a_{3}, a_{4}, b_{1}, b_{2}, b_{3}} c_{a_{2}b_{2}} c_{a_{3}b_{3}}^{*} 
\times \langle a_{1}, b_{1}| e^{-\frac{1}{2}\beta \hat{H}} |a_{2}, b_{2}\rangle \langle a_{3}, b_{3}| e^{-\frac{1}{2}\beta \hat{H}} |a_{4}, b_{1}\rangle$$

Therefore, we can calculate  $\operatorname{tr}_A[\hat{\rho}_A^n]$ :

$$\begin{aligned} \operatorname{Tr}_{A}[\hat{\rho}_{A}^{n}] &= \frac{1}{Z^{n}} \sum_{\{a_{i}^{j}\}_{i,j},\{b_{i}^{j}\}_{i,j}} c_{a_{2}^{1}b_{2}^{1}} c_{a_{3}^{1}b_{3}^{1}}^{*} c_{a_{2}^{2}b_{2}^{2}} c_{a_{3}^{2}b_{3}^{2}}^{*} \cdots c_{a_{2}^{1}b_{2}^{n}} c_{a_{3}^{1}b_{3}^{n}}^{*} \\ &\times \langle a_{1}^{1}, b_{1}^{1} | e^{-\frac{1}{2}\beta\hat{H}} | a_{2}^{1}, b_{2}^{1} \rangle \langle a_{3}^{1}, b_{3}^{1} | e^{-\frac{1}{2}\beta\hat{H}} | a_{1}^{2}, b_{1}^{1} \rangle \\ &\times \langle a_{1}^{2}, b_{1}^{2} | e^{-\frac{1}{2}\beta\hat{H}} | a_{2}^{2}, b_{2}^{2} \rangle \langle a_{3}^{2}, b_{3}^{2} | e^{-\frac{1}{2}\beta\hat{H}} | a_{1}^{3}, b_{1}^{2} \rangle \\ &\cdots \times \langle a_{1}^{n}, b_{1}^{n} | e^{-\frac{1}{2}\beta\hat{H}} | a_{2}^{n}, b_{2}^{n} \rangle \langle a_{3}^{n}, b_{3}^{n} | e^{-\frac{1}{2}\beta\hat{H}} | a_{1}^{1}, b_{1}^{n} \rangle \end{aligned}$$

→ Just consider n=2 (&3) case in this talk.

## <u>Renyi Entropy</u>

## <u>2nd Renyi</u>

$$\begin{split} \overline{\mathrm{tr}_{A}[\hat{\rho}_{A}^{2}]} &= \frac{1}{Z^{2}} \sum_{\{a_{i}\}_{i},\{b_{i}\}_{i}} \overline{c_{a_{2}b_{2}}c_{a_{3}b_{3}}^{*}c_{a_{5}b_{5}}c_{a_{6}b_{6}}^{*}} \\ &\times \langle a_{1},b_{1}|e^{-\frac{1}{2}\beta\hat{H}}|a_{2},b_{2}\rangle\langle a_{3},b_{3}|e^{-\frac{1}{2}\beta\hat{H}}|a_{4},b_{1}\rangle \\ &\times \langle a_{4},b_{4}|e^{-\frac{1}{2}\beta\hat{H}}|a_{5},b_{5}\rangle\langle a_{6},b_{6}|e^{-\frac{1}{2}\beta\hat{H}}|a_{1},b_{4}\rangle \\ \end{split} \\ \\ \boxed{\mathsf{Using}} \qquad \qquad \mathsf{Rendomness in cTPQ state} \\ \overline{c_{a_{2}b_{2}}c_{a_{3}b_{3}}^{*}c_{a_{5}b_{5}}c_{a_{6}b_{6}}^{*}} = \delta_{(a_{2}b_{2}),(a_{3}b_{3})}\delta_{(a_{5}b_{5}),(a_{6}b_{6})} + \delta_{(a_{2}b_{2}),(a_{6}b_{6})}\delta_{(a_{5}b_{5}),(a_{3}b_{3})}, \end{split} \\ \mathsf{we get} \\ \hline{\mathrm{tr}_{A}[\hat{\rho}_{A}^{2}]} &= \frac{1}{Z^{2}} \sum_{\{a_{i}\}_{i},\{b_{i}\}_{i}} \langle a_{1},b_{1}|e^{-\beta\hat{H}}|a_{4},b_{1}\rangle\langle a_{4},b_{4}|e^{-\beta\hat{H}}|a_{1},b_{4}\rangle \\ &\quad + \langle a_{1},b_{1}|e^{-\beta\hat{H}}|a_{1},b_{4}\rangle\langle a_{4},b_{4}|e^{-\beta\hat{H}}|a_{4},b_{1}\rangle \\ &= \boxed{\frac{1}{Z^{2}} \left(\mathrm{tr}_{A} \left[\mathrm{tr}_{B}[e^{-\beta\hat{H}}]^{2}\right] + \mathrm{tr}_{B} \left[\mathrm{tr}_{A}[e^{-\beta\hat{H}}]^{2}\right]\right)} \end{split}$$

#### <u>2nd Renyi Entropy</u>

We evaluate 2<sup>nd</sup> Renyi entropy in statistical-mechanical way:

$$\overline{S_2} = -\ln\left[\frac{\operatorname{tr}_A\left[\operatorname{tr}_B\left[e^{-\beta\hat{H}}\right]^2\right] + \operatorname{tr}_B\left[\operatorname{tr}_A\left[e^{-\beta\hat{H}}\right]^2\right]}{Z(\beta)^2}\right]$$

Step1) For large  $Z(\beta)$ , by using transfer matrices, we can prove  $\operatorname{tr}_A\left[\operatorname{tr}_B[e^{-\beta\hat{H}}]^2\right] = P \times Z_A(2\beta)Z_B(\beta)^2$ , and  $Z(\beta) = Q \times Z_A(\beta)Z_B(\beta)$ P,Q: const.

Therefore, 
$$\overline{S_2} = -\ln\left(\frac{Z_A(2\beta)}{Z_A(\beta)^2} + \frac{Z_B(2\beta)}{Z_B(\beta)^2}\right) + \ln R \qquad R \equiv Q/P$$

Step2) For large *d*, the free energy is extensive, i.e.,  $\frac{Z_A(2\beta)}{Z_A(\beta)^2} = Sa^{-\ell}$ Extensivity of density matrix

Finally, we get 
$$\overline{S_2} = -\ln\left(a^{-\ell} + a^{-L+\ell}\right) + \ln K$$
  $K \equiv R/S$ 
$$= \ell \ln a - \ln\left(1 + a^{-L+2\ell}\right) + \ln K$$

#### <u>Analytical Result:</u> <u>2nd Renyi Entropy of cTPQ states</u>



#### Numerical calculation

Entanglement entropy of the cTPQ states

$$\overline{S_2} = \ell \ln a - \ln \left( 1 + a^{-L+2\ell} \right) + \ln K$$

Entanglement entropy of excited pure quantum states



(Garrison and Grover, arXiv, 2015)

We will use our analytical result for the cTPQ states as a fitting function for other excited pure states.

> It works when the state is scrambled, and doesn't when it isn't.

#### Numerical calculation 1: Energy eigenstates

Energyeigenstate Thermalization Hypothesis (ETH) (Deutsch, Srednicki, Rigol) :

In nonintegrable systems, a single energy eigenstate is expected to represent a thermal equilibrium state.

Popular expectation in ETH: At  $\ell \ll L$   $\operatorname{tr}_B[|n\rangle\langle n|] \simeq e^{-\beta \hat{H}}$ .

|n
angle: Energy eigenstate

 $\beta$ : Inverse temperature estimated from Energy

However,  ${
m tr}_B[|n
angle\langle n|]$  and  $e^{-eta\hat{H}}$  will be very different at  $\ell\sim L$ 

#### How about entanglement?

→ We will test our fitting function for energy eigenstates.

$$\overline{S_2} = \ell \ln a - \ln \left( 1 + a^{-L+2\ell} \right) + \ln K$$

#### Numerical calculation 1: Energy eigenstates

 $\hat{H} = \sum_{i} S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \Delta S_{i}^{z} S_{i+1}^{z} + J_{2} (S_{i}^{x} S_{i+2}^{x} + S_{i}^{y} S_{i+2}^{y} + S_{i}^{z} S_{i+2}^{z})$ 



Non-integrable  $\Delta = 0, J_2 = 0.45$ 

Integrable  $\Delta = 2, J_2 = 0$ 

Dots: numerical data Line: Fittings

Energy eigenstates agree with the function:  $\overline{S_2} = \ell \ln a - \ln (1 + a^{-L+2\ell}) + \ln K$ 

 $\checkmark\,$  At  $\,\ell \ll L\,$  , volume law. Consistent to Energy eigenstate thermalization hypothesis (ETH)

✓ At  $\ell \sim L$ ,  $S_2$  still exhibits generic behavior predictable by our formula

#### Numerical calculation 1: Energy eigenstates

 $\hat{H} = \sum_{i} S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \Delta S_{i}^{z} S_{i+1}^{z} + J_{2} (S_{i}^{x} S_{i+2}^{x} + S_{i}^{y} S_{i+2}^{y} + S_{i}^{z} S_{i+2}^{z})$ 



Non-integrable  $\Delta = 0, J_2 = 0.45$ 

Integrable  $\Delta = 2, J_2 = 0$ 



Dots: numerical data Line: Fittings

In the integrable model, there are a lot of energy eigenstates for which the fittings don't work.

→ Let's see this difference quantitatively.

# $$\begin{split} & \underline{\text{Numerical calculation 1: Energy eigenstates}} \\ & \hat{H} = \sum_{i} S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \Delta S_{i}^{z} S_{i+1}^{z} + J_{2} (S_{i}^{x} S_{i+2}^{x} + S_{i}^{y} S_{i+2}^{y} + S_{i}^{z} S_{i+2}^{z}) \\ & \text{Non-integrable} \quad \Delta = 0, J_{2} = 0.45 \end{split}$$



Vertical axis: Residues of fittings of energy eigenstates Horizontal axis: Index of eigenstates. Eigenstates are sorted in order of their residues, i.e., percentile.

Non-integrable: Fittings improves as L increases. Leads to typical behavior. Integrable: Fittings gets worse as L increases, maybe due to many conserved quantities. Cf) L.Vidmar,L.Hackl,E.Bianchi, M.Rigol PRL.119,020601(2017)

Effect of energy fluctuation in microcanonical energy shell Cf) T.Grover et.al, arXiv 1503.00729 &1709.08784, A.Dymarsky, N.Lashkari,& H.Liu, arXiv 1611.08764

#### Correction from energy fluctuation

$$\rho_{\rm mc/2} \equiv {\rm Tr}_B |n\rangle \langle n| \simeq \frac{e^{-\beta \hat{H}}}{Z}?$$

von Neumann Entropy

$$S_{\rm vN}(\hat{\rho}_{\rm mc}) = S_{\rm vN}(\frac{e^{-\beta \hat{H}}}{Z})$$

$$S_{\rm vN}(\hat{\rho}) \equiv -{\rm Tr}_A[\rho {\rm ln}\rho]$$

However, energy fluctuation is different

$$\langle n | (\Delta \hat{H})^2 | n \rangle = 0$$
  $\langle \beta | (\Delta \hat{H})^2 | \beta \rangle = O(L)$ 

Renyi entropy has the correction which comes from the energy fluctuation...

$$S_2(\hat{\rho}_{\rm mc}) \neq S_2(\frac{e^{-\beta \hat{H}}}{Z})$$

(T.Grover et.al, arXiv 1709.08784, A.Dymarsky, N.Lashkari,& H.Liu, arXiv 1611.08764)

# $$\begin{split} & \hat{H} = \sum_{i} S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \Delta S_{i}^{z} S_{i+1}^{z} + J_{2} (S_{i}^{x} S_{i+2}^{x} + S_{i}^{y} S_{i+2}^{y} + S_{i}^{z} S_{i+2}^{z}) \\ & \text{Non-integrable} \quad \Delta = 0, J_{2} = 0.45 \end{split}$$



This correction in non-integrable model is subtle effect only appear in eigenstates and in large L (and is easily fixable). By contrast, the behavior is completely different in integrable model

#### Numerical calculation 2: States after quantum quench

Quench protocol Initial state:  $|\uparrow\downarrow\uparrow\downarrow\cdots\uparrow\downarrow\rangle$ 

We suddenly change Hamiltonian from  $\hat{H} = \hat{1}$ to  $\hat{H} = \sum_{i} \vec{S}_{i} \cdot \vec{S}_{i+1}$ 

In integrable systems, a state after quench may relaxes to some stationary state, but it never thermalize.



How about entanglement?

# Numerical calculation 2: States after quantum quench

## Non-integrable $\hat{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + 0.5(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + S_i^z S_{i+2}^z)$



After the entanglement entropy saturates, it oscillates around our predicted curve.



#### Numerical calculation: States after quantum quench

Non-integrable  $\hat{H} = \sum_i \overrightarrow{S}_i \cdot \overrightarrow{S}_{i+1} + 0.5(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + S_i^z S_{i+2}^z)$ 





After the entanglement entropy saturates, it oscillates around our predicted curve.

## Integrable $\hat{H} = \sum_{i} \vec{S}_{i} \cdot \vec{S}_{i+1}$



# The time averages agree with our fitting.

Even the state has O(L) local integrables of motions,  $e^{-\beta \hat{H} + \sum_n \lambda_n I_n}$ ,  $2^{nd}$  Renyi entropy is still characterized only by two parameters!

10

12 14 16

#### Why it works?

Key of derivation✓ Randomness in cTPQ stateExtensivity of density matrix

In the case of a stationary state after a quench, the quantum state is

$$|\psi\rangle = \sum_{n} e^{-\frac{i}{\hbar}E_n} a_n |n\rangle$$

And the 2nd Renyi entropy is

$$S_{2} = -\ln\left(\operatorname{tr}_{A}\left(\sum_{i,j,k,l} e^{-\frac{i}{\hbar}(E_{i}-E_{j}+E_{k}-E_{l})} a_{i}a_{j}^{*}a_{k}a_{l}^{*}\operatorname{tr}_{B}\left(|i\rangle\langle j|\right)\operatorname{tr}_{B}\left(|k\rangle\langle l|\right)\right)\right).$$

$$\delta_{i,j}\delta_{k,l} + \delta_{i,l}\delta_{j,l}$$

If  $E_i \neq E_j$  for  $i \neq j$  and  $E_i - E_j \neq E_k - E_j$  for  $i \neq k$  and  $j \neq l$ ,

$$S_{2} = -\ln\left[\operatorname{tr}_{A}\left(\operatorname{tr}_{B}\left(\hat{\rho}_{\mathrm{dia}}\right)^{2}\right) + \operatorname{tr}_{B}\left(\operatorname{tr}_{A}\left(\hat{\rho}_{\mathrm{dia}}\right)^{2}\right)\right]$$

#### <u>Why it works?</u>

Key of derivation

Randomness in cTPQ state

Extensivity of density matrix

$$S_{2} = -\ln\left[\operatorname{tr}_{A}\left(\operatorname{tr}_{B}\left(\hat{\rho}_{\mathrm{dia}}\right)^{2}\right) + \operatorname{tr}_{B}\left(\operatorname{tr}_{A}\left(\hat{\rho}_{\mathrm{dia}}\right)^{2}\right)\right]$$

Since  $\langle \psi | (\Delta \hat{H})^2 | \psi \rangle = O(L)$ ,

 $\operatorname{tr}_{A}\left(\operatorname{tr}_{B}\left(\hat{\rho}_{\mathrm{dia}}\right)^{2}\right) = Ka^{-a}$ 

In the case of non-integrable model,

Thermal state (Gibbs ensemble)  $e^{-\beta \hat{H}}$ , characterized only by temperature  $1/\beta$ .

#### In the case of integrable model,

Generalized Gibbs Ensemble (GGE)  $e^{-\beta \hat{H} + \sum_n \lambda_n I_n}$ , characterized by temperature  $1/\beta$ , and

many integrals of motions  $I_n = \lambda_n^{-1}$  Lagrangian multiplier

#### Numerical calculation 3: Many-body Localization



$$\hat{H} = \sum_{i} \overrightarrow{S}_{i} \cdot \overrightarrow{S}_{i+1} + h_i S_z$$

 ${h_i}_i$ : drawn from a uniform distribution[-h, h]

#### It shows ETH-MBL transition. $h_c = 3.62, \; u = 0.80 \;$ (values at $\epsilon$ =0.5) (D. J. Luis, N. Laflorencie, and F. Alet, PRB(R) 2015)

#### ETH phase



It is an eigenstate transition (dynamical transition), which cannot be captured by the equilibrium values of ensembles.

### Numerical calculation 3: Many-body Localization

#### What kind of eigenstates?

#### ETH phase



0.01



(V.Khemani, S.P.Lim, D.N.Sheng. and D.A.Huse, PRB 2017)

(D. J. Luis, N. Laflorencie, and F. Alet, PRB(R) 2015)

 $\frac{10}{L|h-h_c|^{\nu}}$ 

#### Numerical calculation 3: Many-body Localization



$$\begin{split} \hat{H} &= \sum_{i} \overrightarrow{S}_{i} \cdot \overrightarrow{S}_{i+1} + h_i S_z \\ \{h_i\}_i \text{: drawn from a uniform distribution } [-h,h] \\ \text{It shows ETH-MBL transition.} \\ \text{At the middle of the spectrum,} \\ h_c &= 3.62, \ \nu = 0.80 \end{split}$$

(D. J. Luis, N. Laflorencie, and F. Alet, PRB(R) 2015)

Problem: Harris bound requires  $\nu \ge 2$ , and thus this result violates the bound... (A. Chandran, C. R. Laumann, and V. Oganesyan, arXiv, 2015)



Estimation of the critical exponent  $\nu$  is so improved that the value is very close to satisfy Harris bound  $\nu \ge 2$ .

## <u>Summary</u>

arXiv: 1703.02993

TPQ state: 
$$|\beta\rangle \equiv \frac{1}{\sqrt{Z}} \sum_{i} z_{i} \exp\left[-\frac{1}{2}\beta\hat{H}\right] |i\rangle$$
  
Renyi Entropy:  $S_{n} \equiv \frac{1}{1-n} \ln\left(\operatorname{tr}_{A}[\hat{\rho}_{A}^{n}]\right)$ 

Universal structure of Renyi entropy is obtained at finite temperature  $\overline{S_2} = \ell \ln a - \ln \left(1 + a^{-L+2\ell}\right) + \ln K$ 



<sup>2nd</sup> Renyi of Energy eigenstates obeys our prediction

<sup>2nd</sup> Renyi of State after Quench to integrable obeys our prediction





ETH-MBL transition is detected accurately