

Convex-roof entanglement measures
of density matrices block diagonal
in disjoint subspaces
for the study of thermal states

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Introduction

Density matrices block diagonal in disjoint subspaces

Convex roof entanglement measures in \uparrow

- The result: a simplified formula
- The proof for a qubit QS and E with two subspaces
- Generalization

Relevance

Examples

Conclusion

Introduction

Convex roof entanglement measures (bipartite systems)

[C. H. Bennett, et al., Phys. Rev. A 54, 3824 (1996)]

$$E(\hat{\rho}) = \min_{\alpha} \tilde{E}(\hat{\rho}) \quad \tilde{E}(\hat{\rho}) = \sum_n P_n E(|\psi_n\rangle)$$

Good pure state entanglement measure $E(|\psi\rangle)$

Minimization over all pure state decompositions $\hat{\rho} = \sum_n P_n |\psi_n\rangle\langle\psi_n|$

→ number of minimization parameters grows rapidly with system dimension

→ approximation of lower bounds

→ taking advantage of symmetries

→ variational methods

→ minimization over pure state extensions

→ random sampling

Density matrices block diagonal in disjoint subspaces

Bipartite system: QS + E

Block diagonal in some separable basis $\{|se\rangle \equiv |s\rangle \otimes |e\rangle\}$

→ the BD form is the result of the properties of E, so each block is built of QS-E states in which

- the whole range QS states can be present, but
- **the set of E states in each block is orthogonal to the states in any other block**

Decomposition into blocks $\hat{\rho} = \sum_n p_n \hat{\rho}_n$

where

$$\hat{\rho}_n = \sum_{ss'} \sum_{e_n e'_n} c_{ss'}^{ee'} |s\rangle \langle s'| \otimes |e_n\rangle \langle e'_n|$$

with $\langle e_n | e'_m \rangle = 0$ for all e_n and e'_m when $n \neq m$

It is not enough for the blocks to have orthogonal supports!

Example: qubit QS + E of dimension 4

$$\{|0\rangle, |1\rangle\} \quad \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$$

Mixed state

$$\hat{\rho} = \frac{1}{4} (|\Psi_{01}\rangle\langle\Psi_{01}| + |\Phi_{01}\rangle\langle\Phi_{01}| + |\Psi_{23}\rangle\langle\Psi_{23}| + |\Phi_{23}\rangle\langle\Phi_{23}|)$$

With Bell like components

$$|\Psi_{ij}\rangle = \frac{1}{\sqrt{2}} (|0i\rangle + |1j\rangle),$$

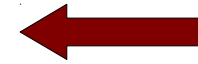
$$|\Phi_{ij}\rangle = \frac{1}{\sqrt{2}} (|1i\rangle + |0j\rangle),$$

$$\hat{\rho} = \frac{1}{8} \begin{pmatrix} \boxed{1} & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ \boxed{1} & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{1} & \boxed{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \boxed{1} & \boxed{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{1} & \boxed{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{1} & \boxed{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & \boxed{1} \\ 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & \boxed{1} \end{pmatrix}.$$

We will be working on states that have the red block-diagonal structure

Basis order: $|00\rangle, |11\rangle, |01\rangle, |10\rangle, |02\rangle, |13\rangle, |03\rangle, |12\rangle$

Convex roof entanglement measures in



The result: a simplified formula

For a bipartite density matrix which can be decomposed into blocks disjoint in the subspace of the environment

$$\hat{\rho} = \sum_n p_n \hat{\rho}_n$$

minimization over different blocks is not necessary, so

$$E(\hat{\rho}) = \sum_n p_n E(\hat{\rho}_n)$$

[<https://arxiv.org/abs/2202.09303>]

→ Blocks have lower dimension → less minimization parameters → reduction of numerical complexity

The proof for a qubit QS and E with two subspaces

Pure state entanglement measure:

Linear entropy of reduced density matrix of E (normalized)

The density matrix $\hat{\rho} = p_1\hat{\rho}_1 + p_2\hat{\rho}_2$

→ We assume that the pure state decomposition **of each block** that minimizes entanglement is known $\hat{\rho}_i = \sum_k q_i^k |\phi_i^k\rangle\langle\phi_i^k|$

→ so entanglement within each block is given by

$$E(\hat{\rho}_i) = \sum_k q_i^k E(|\phi_i^k\rangle)$$

We will show that there does not exist any decomposition of $\hat{\rho}$ for which entanglement is smaller than

$$E(\hat{\rho}) = p_1 E(\hat{\rho}_1) + p_2 E(\hat{\rho}_2)$$

Step 1: entanglement of any pure state

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle$$

→ superposition of states from different blocks

$$|\psi_i\rangle = x_i|0\rangle \otimes |\varphi_i^0\rangle + y_i|1\rangle \otimes |\varphi_i^1\rangle$$

$$\langle\varphi_i^0|\varphi_i^1\rangle \neq 0 \quad \text{same block}$$

$$\langle\varphi_1^a|\varphi_2^b\rangle = 0 \quad \text{different blocks}$$

Same state

$$|\psi\rangle = a|0\rangle \otimes |\psi_a\rangle + b|1\rangle \otimes |\psi_b\rangle$$

with

$$\begin{aligned} |\psi_a\rangle &= \frac{1}{a} (\alpha x_1 |\varphi_1^0\rangle + \beta x_2 |\varphi_2^0\rangle), & a &= \sqrt{|\alpha|^2 |x_1|^2 + |\beta|^2 |x_2|^2}, \\ |\psi_b\rangle &= \frac{1}{b} (\alpha y_1 |\varphi_1^1\rangle + \beta y_2 |\varphi_2^1\rangle). & b &= \sqrt{|\alpha|^2 |y_1|^2 + |\beta|^2 |y_2|^2}, \end{aligned}$$

not orthogonal

Reduced density matrix of E $\hat{\rho}_E = a^2 |\psi_a\rangle\langle\psi_a| + b^2 |\psi_b\rangle\langle\psi_b|$

Entanglement $E(|\psi\rangle) = 2(1 - \text{Tr} \hat{\rho}_E^2) = 4a^2 b^2 (1 - |\langle\psi_a|\psi_b\rangle|^2)$

with $|\langle\psi_a|\psi_b\rangle|^2 = \frac{1}{a^2 b^2} \left| |\alpha|^2 x_1^* y_1 \langle\varphi_1^0|\varphi_1^1\rangle + |\beta|^2 x_2^* y_2 \langle\varphi_2^0|\varphi_2^1\rangle \right|^2$

Block diagonality => simplified scalar product

Step 2: average of entanglement of block diagonal state

$$\hat{\rho}_{BD} = |\alpha|^2 |\psi_1\rangle\langle\psi_1| + |\beta|^2 |\psi_2\rangle\langle\psi_2|$$

$$\rightarrow \tilde{E}(\hat{\rho}_{BD}) = |\alpha|^2 E(|\psi_1\rangle) + |\beta|^2 E(|\psi_2\rangle)$$

$$\text{with } E(|\psi_i\rangle) = 4|x_i|^2|y_i|^2 \left(1 - |\langle\varphi_i^0|\varphi_i^1\rangle|^2\right)$$

Step 3: Comparison

$$\begin{aligned} E(|\psi\rangle) - \tilde{E}(\hat{\rho}_{BD}) &= 4|\alpha|^2|\beta|^2 \left[(|x_1|^2 - |x_2|^2)^2 \right. \\ &\quad \left. + |x_1^*y_1\langle\varphi_1^0|\varphi_1^1\rangle - x_2^*y_2\langle\varphi_2^0|\varphi_2^1\rangle|^2 \right] \geq 0. \end{aligned}$$

Entanglement present in a superposition of states from the different blocks is always greater than the average of entanglement contained in each block separately

Step 4: different decompositions of any block diagonal state

It is straightforward to show that entanglement present in $\hat{\rho} = p_1\hat{\rho}_1 + p_2\hat{\rho}_2$ is just an average over entanglement in each block.

Any pure state decomposition:

$$\begin{aligned}\hat{\rho} &= \hat{\rho}_A = \sum_i P_i |\psi_i\rangle\langle\psi_i| = \sum_i P_i |\alpha_i|^2 |\psi_{1i}\rangle\langle\psi_{1i}| + \sum_i P_i |\beta_i|^2 |\psi_{2i}\rangle\langle\psi_{2i}| \\ &\quad + \sum_i P_i \alpha_i \beta_i^* |\psi_{1i}\rangle\langle\psi_{2i}| + \sum_i P_i \alpha_i^* \beta_i |\psi_{2i}\rangle\langle\psi_{1i}|.\end{aligned}$$

Since the density matrix is BD, the last two terms must be zero, so

$$\hat{\rho} = \hat{\rho}_B = \sum_i P_i |\alpha_i|^2 |\psi_{1i}\rangle\langle\psi_{1i}| + \sum_i P_i |\beta_i|^2 |\psi_{2i}\rangle\langle\psi_{2i}|$$

is a different pure state decomposition.

Using (3) we get

$$\tilde{E}(\hat{\rho}_A) = \sum_i P_i E(|\psi_i\rangle) \geq \sum_i P_i |\alpha_i|^2 E(|\psi_{1i}\rangle) + \sum_i P_i |\beta_i|^2 E(|\psi_{2i}\rangle) = \tilde{E}(\hat{\rho}_B)$$

For any decomposition, there exists a BD decomposition with smaller (or equal) average entanglement

Generalization

Larger QS:

It is reasonably straightforward to prove that a difference analogous to step 3 is nonnegative also for larger QS than a qubit

[see appendix in <https://arxiv.org/abs/2202.09303>]

Then everything follows the qubit proof.

M subspaces:

Entanglement of the whole density matrix

can be found by averaging entanglement between one subspace and the remaining $M-1$, while the entanglement of the $M-1$ blocks can be found by averaging between one of them and the remaining $M-2$, and so on.

Relevance

Do there exist physical QS-E states that have the BD form?

yes

Thermal states have the same symmetry as the Hamiltonian

$$\rightarrow \hat{H} = \hat{H}_{\text{QS}} + \hat{H}_{\text{E}} + \hat{H}_{\text{QS-E}}$$

$\rightarrow [\hat{H}_{\text{E}}, \hat{A}] = 0 \Rightarrow$ Hamiltonian is block-diagonal in subspaces corresponding to a single eigenvalue of observable A
(e.g. Hubbard model commutes with operators:
number operator, total spin, and parity operator)

\rightarrow QS is affected by only one degree of freedom (same commutation)

\Rightarrow BD Hamiltonian

Examples: qubit + E of qubits

Hamiltonian is composed of 4x4 blocks

$$\hat{H}^m = \begin{pmatrix} E_{m1} & 0 & 0 & M_m \\ 0 & E_m & 0 & 0 \\ 0 & 0 & E_m & 0 \\ M_m^* & 0 & 0 & E_{m2} \end{pmatrix}$$

- two entangled eigenstates
- two separable eigenstates

$$\hat{H} = \sum_m \hat{H}^m$$

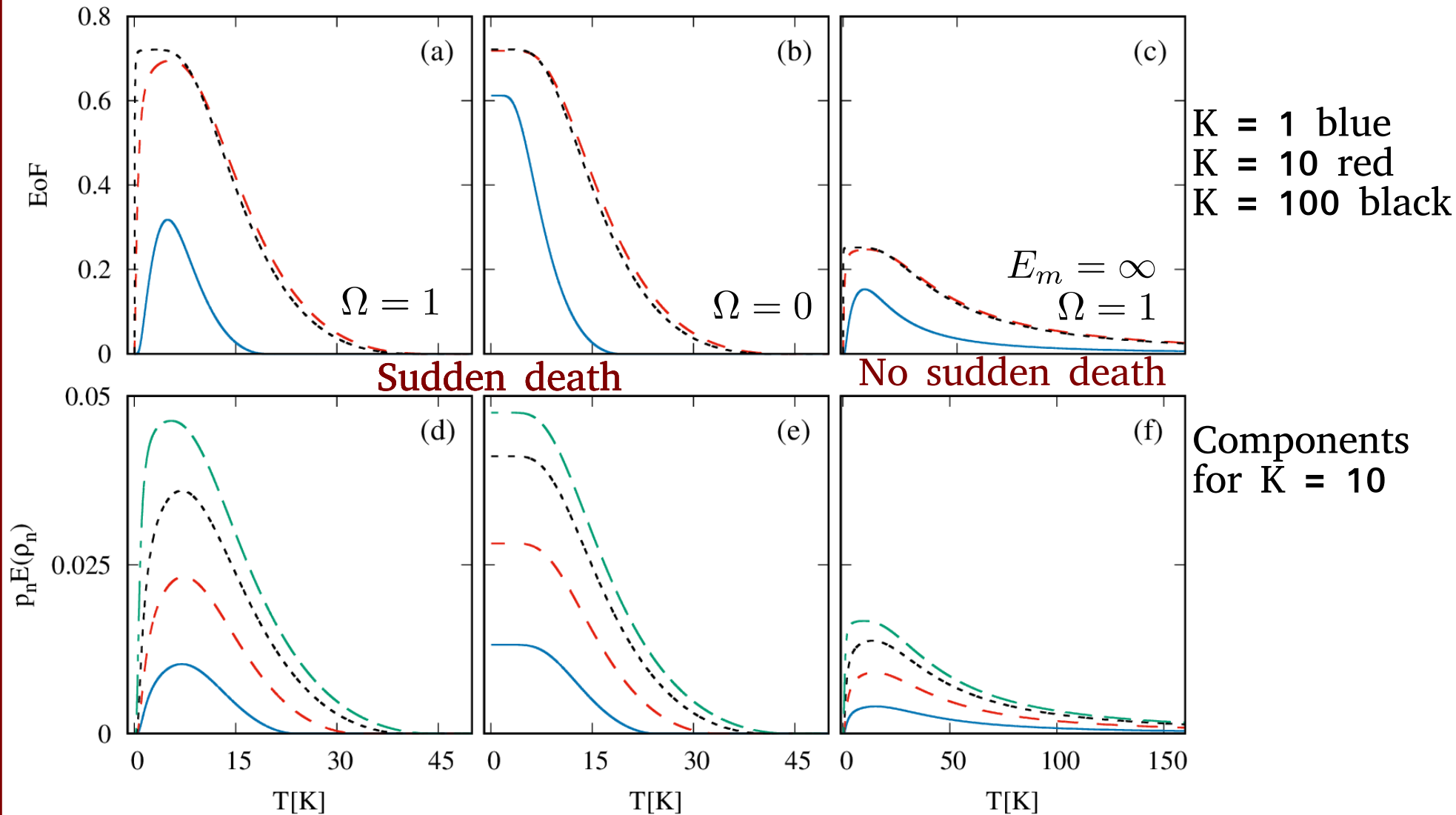
$$E_{m1} = \alpha \left(m + \frac{\Omega}{2} \right),$$

$$E_{m2} = -\alpha \left(m + 1 + \frac{\Omega}{2} \right),$$

$$M_m = \alpha \sqrt{K(K+1) - m(m+1)},$$

$$m = 0, \pm 1, \pm 2, \dots, \pm K$$

Temperature dependence of entanglement



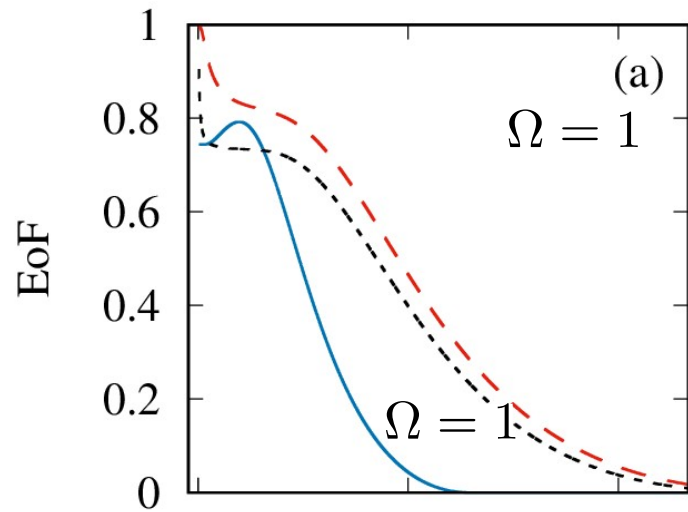
Highest and lowest state within block is entangled

No-degeneracy

Degeneracy between blocks

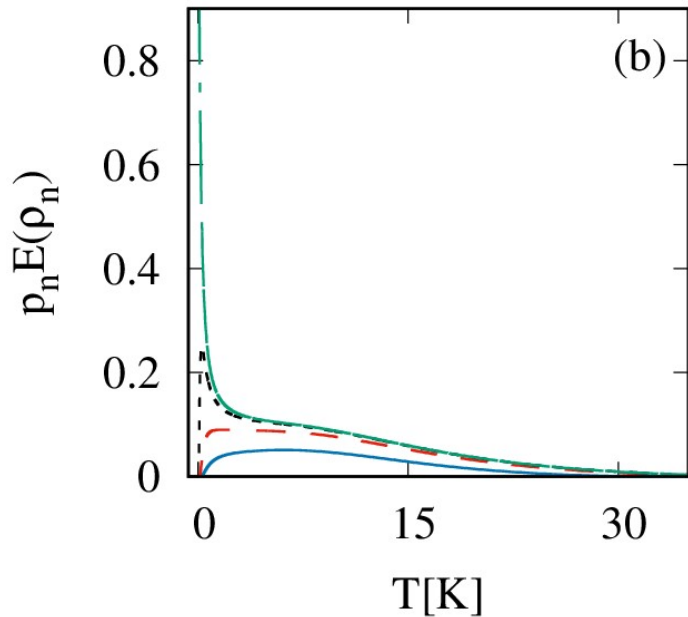
No separable eigenstates

Temperature dependence of entanglement: only negative m



Lowest energy state of the full Hamiltonian is entangled

$K = 1$ blue
 $K = 10$ red
 $K = 100$ black



Components
for $K = 10$

Nonmonotonous behavior!

Conclusion

- If a state is block-diagonal in such a way that the blocks are in different subspaces with respect to one of the subsystems
=> entanglement can be averaged over the blocks
- Block-diagonal Hamiltonians are abundant in nature
- Mixed state entanglement can show various temperature-dependences for very similar Hamiltonians (thermal equilibrium)