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CMQC

Many-Body Coherence in Quantum Thermodynamics

[The 3rd KIAS Workshop on Quantum Information and Thermodynamics]

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Contents

Introduction

- Thermodynamics in quantum system
  - Operational description of transformation between quantum states interacting with the thermal bath

- Equilibrium state (Gibbs state)

$$\hat{\gamma}_B = Z_B^{-1} e^{-\beta \hat{H}_B}$$

with the partition function $Z_B = \mathrm{Tr}[e^{-\beta \hat{H}_B}]$ and inverse temperature $\beta = (k_B T)^{-1}$

Q1. Quantum coherence (correlation) can do extra work?

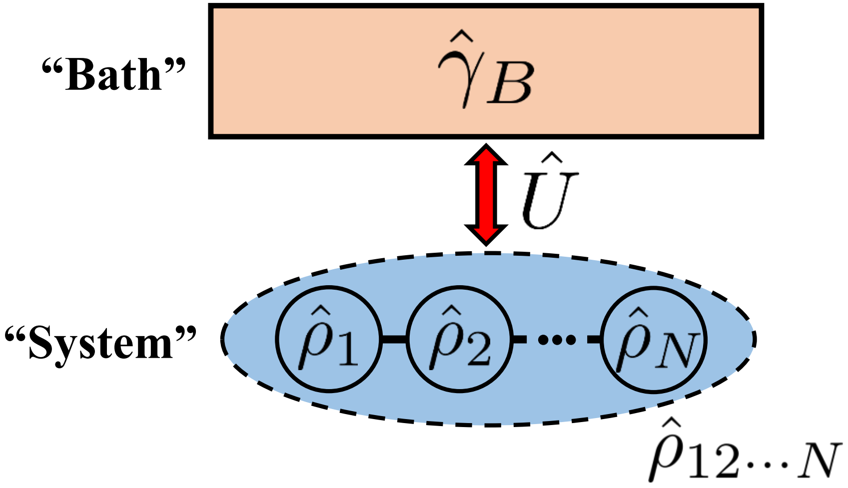
in "Many-body system"

Q2. Thermodynamic resource beyond work-yielding resource?

Contents

Thermal operation in quantum system

- Thermal operation :



$$\Lambda_\beta(\hat{\rho}_S) = \mathrm{Tr}_{B'}\left[\hat{U}(\hat{\rho}_S \otimes \hat{\gamma}_B)\hat{U}^\dagger\right]$$

✓ Energy preserving condition :

$$[\hat{U}, \hat{H}_S + \hat{H}_B] = 0$$

- (Quantum) Free energy : $F(\hat{\rho}) = k_B T S(\hat{\rho}||\hat{\gamma}) - k_B T \log Z_B = \langle \hat{H} \rangle_{\hat{\rho}} - k_B T S(\hat{\rho})$

  - Gibbs(equilibrium) state : $\hat{\gamma}_S = Z_S^{-1} e^{-\beta \hat{H}_S}$ where $Z_S = \mathrm{Tr}[e^{-\beta \hat{H}_S}]$

➔ **Minimum free energy : completely passive state**

Generalized free energies

- A family of free energies : $F_\alpha(\hat{\rho}) = k_B T S_\alpha(\hat{\rho}||\hat{\gamma}) - k_B T \log Z_B$

$$\text{Renyi Divergence : } S_\alpha(\hat{\rho}||\hat{\sigma}) = \begin{cases} \frac{1}{\alpha-1}\log \mathrm{Tr}[\hat{\rho}^\alpha \hat{\sigma}^{1-\alpha}], & \alpha \in [0,1) \\ \frac{1}{\alpha-1}\log \mathrm{Tr}\left[\left(\hat{\sigma}^{\frac{1-\alpha}{2\alpha}}\hat{\rho}\hat{\sigma}^{\frac{1-\alpha}{2\alpha}}\right)^\alpha\right], & \alpha > 1, \end{cases}$$

for $\alpha \to 1$ Renyi divergence becomes $S(\hat{\rho}||\hat{\sigma})$

- **Resource theory of thermodynamics (the 2nd law) :** $\Delta F_\alpha(\hat{\rho}_S) \leq 0$

Brandao et.al., PNAS (2015)

- Single-shot (deterministic) work extraction :

$$\hat{\rho} \otimes |0\rangle\langle 0|_W \xrightarrow{\Lambda_\beta} \hat{\sigma} \otimes |W\rangle\langle W|_W \quad \text{where} \quad \hat{H}_W = W|W\rangle\langle W|_W$$

  - **Work yield :** $W_{\hat{\rho}\to\hat{\sigma}} = k_B T \inf_\alpha [F_\alpha(\hat{\rho}) - F_\alpha(\hat{\sigma})]$ (for energy-diagonal states)

Brandao et.al., PNAS (2015)

Contents

Free energy correlation

- Free energy in many-body system : $F(\hat{\rho}_{12\cdots N}) = \sum_{i=1}^{N} F(\hat{\rho}_i) + k_B T I(\hat{\rho}_{1:2:\cdots:N}),$

  (total correlation)

- (Generalized) Free energy correlation :

$$C_\alpha(\hat{\rho}_{1:2:\cdots:N}) := (k_B T)^{-1}\left[F_\alpha(\hat{\rho}) - \sum_{i=1}^{N} F_\alpha(\hat{\rho}_i)\right]$$

$$\lim_{\alpha\to 1} C_\alpha(\hat{\rho}_{1:2:\cdots:N}) = S(\hat{\rho}) - \sum_{i=1}^{N} S(\hat{\rho}_i) := I(\hat{\rho}_{1:2:\cdots:N})$$

- For product state : $\hat{\rho}_1 \otimes \hat{\rho}_2 \otimes \cdots \otimes \hat{\rho}_N \Longrightarrow C_\alpha(\hat{\rho}_{1:2:\cdots:N}) = 0$

Free energy transfer from correlation

- Two-level system : $\hat{H}_{1(2)} = \omega_0 |1\rangle\langle 1|$

	$\lvert\psi\rangle = \lvert 0\rangle_1 \lvert 1\rangle_2$	$\lvert\phi\rangle = \frac{\lvert 0\rangle_1 \lvert 1\rangle_2 + \lvert 1\rangle_1 \lvert 0\rangle_2}{\sqrt{2}}$
• Local free energy :	$\sum_{i=1,2} F(\psi_i) = \omega_0$	$\sum_{i=1,2} F(\phi_i) = \omega_0 - 2k_B T$
• Free energy correlation :	$I(\psi_{1:2}) = 0$	$I(\phi_{1:2}) = 2k_B T$

$|\psi\rangle \xleftrightarrow{\text{TO}} |\phi\rangle$ **: Interconversion between local free energy and correlation**

Free energy change under thermal operations

- System interacting with bath $[\hat{U}, \hat{H}_S + \hat{H}_B] = 0$

$$\Delta F_\alpha(\hat{\rho}_S) + \Delta F_\alpha(\hat{\rho}_B) + k_B T \Delta C_\alpha(\hat{\rho}_{S:B}) = 0.$$

Regardless of the state of system-bath (not necessarily in Gibbs state & can be entangled)

- Free energy is additionally leaked through the system-bath correlation

- If the bath is initially in Gibbs state and uncorrelated with the system :

$$\Delta F_\alpha(\hat{\rho}_S) \leq 0$$ (The 2nd law of quantum thermodynamics)

Contents

Coherence in many-body system

- N-body quantum system : $\hat{\rho} = \sum_{\{E_i, E'_j\}} \rho^{E_1, E_2, \cdots, E_N}_{E'_1, E'_2, \cdots, E'_N} |E_1 E_2 \cdots E_N\rangle \langle E'_1 E'_2 \cdots E'_N|$

$$= \sum_{\boldsymbol{E}, \boldsymbol{E}'} \rho_{\boldsymbol{E}\boldsymbol{E}'} |\boldsymbol{E}\rangle \langle \boldsymbol{E}'| \quad \text{where} \quad |\boldsymbol{E}\rangle = |E_1 E_2 \cdots E_N\rangle, \quad \boldsymbol{E} = (E_1, E_2, \cdots, E_N)$$

- (Classical) Energy distribution : $P(\boldsymbol{E}) = \mathrm{Tr}\left[\hat{\Pi}_{\boldsymbol{E}} \hat{\rho}\right] = \rho_{\boldsymbol{E}\boldsymbol{E}}$ where $\hat{\Pi}_{\boldsymbol{E}} = |\boldsymbol{E}\rangle \langle \boldsymbol{E}|$

➔ **Classical thermodynamics**

- Coherence between Energy eigenstates : $|\boldsymbol{E}\rangle \langle \boldsymbol{E}'|$

✓ When $\mathcal{E}_{\boldsymbol{E}} = \mathcal{E}_{\boldsymbol{E}'}$: Equi-level coherence

✓ When $\mathcal{E}_{\boldsymbol{E}} \neq \mathcal{E}_{\boldsymbol{E}'}$: Inter-level coherence

✓ Total Energy : $\mathcal{E}_{\boldsymbol{E}} := \sum_{i=1}^{N} E_i$

Free energy and correlation for many-body system

- N-partite non-interacting system with non-degenerate local Hamiltonians

$$\hat{H}_{\text{tot}} = \sum_{i=1}^{N} \hat{H}_i$$

- Quantum contribution of free energy correlation :

$$\Delta C_\alpha(\hat{\rho}) := C_\alpha(\hat{\rho}) - C_\alpha(\Pi(\hat{\rho}))$$

  - Classical (diagonal) state with the same energy statistics : $\Pi(\hat{\rho}) = \sum_{\boldsymbol{E}} P(\boldsymbol{E}) |\boldsymbol{E}\rangle\langle\boldsymbol{E}|$

- Energy block-diagonal state $\hat{\rho} = \sum_{\mathcal{E}} p_{\mathcal{E}} \hat{\rho}_{\mathcal{E}}$

$$\Delta C_\alpha(\hat{\rho}) = \Delta F_\alpha(\hat{\rho}) \geq 0$$

All the free energy differences are contained in correlations

Contents

Extractable work from quantum coherence

- Work extraction without changing energy statistics :

$$\hat{\rho} \otimes |0\rangle\langle 0|_W \xrightarrow{\Lambda_\beta} \Pi(\hat{\rho}) \otimes |W\rangle\langle W|_W \quad \text{where} \quad \hat{H}_W = W|W\rangle\langle W|_W$$

$$\Pi(\hat{\rho}) = \sum_{\boldsymbol{E}} P(\boldsymbol{E})|\boldsymbol{E}\rangle\langle\boldsymbol{E}|$$

- Extracting work from quantum coherence :

$$W_{\text{ext}}(\hat{\rho}) = \inf_\alpha \left[F_\alpha(\hat{\rho}) - F_\alpha(\Pi(\hat{\rho}))\right]$$
$$= k_B T \inf_\alpha \left[\Delta C_\alpha(\hat{\rho})\right]. \quad \text{(for energy-diagonal states)}$$

Q1. Quantum coherence (correlation) can do extra work?

Possible if and only if $\Delta C_\alpha(\mathcal{D}(\hat{\rho})) > 0$ for all $\alpha \in [0, \infty)$

Extractable work from quantum coherence

- Work extraction without changing energy statistics :

$$\hat{\rho} \otimes |0\rangle\langle 0|_W \xrightarrow{\Lambda_\beta} \Pi(\hat{\rho}) \otimes |W\rangle\langle W|_W \quad \text{where} \quad \hat{H}_W = W|W\rangle\langle W|_W$$

$$\Pi(\hat{\rho}) = \sum_{\boldsymbol{E}} P(\boldsymbol{E})|\boldsymbol{E}\rangle\langle\boldsymbol{E}|$$

- Extracting work from quantum coherence :

Observation 1 *For an N-partite pure many-body quantum state with energy distribution $P(\boldsymbol{E})$, a single-shot extraction of non-zero work is possible without changing energy distributions if and only if the state contains equi-level coherence for $\mathcal{E}^*$ such that $\mathcal{E}^* = \operatorname{argmax}_{\mathcal{E}} p_{\mathcal{E}} e^{\beta\mathcal{E}}$, where $p_{\mathcal{E}} = \sum_{\mathcal{E}_{\boldsymbol{E}}=\mathcal{E}} P(\boldsymbol{E})$.*

$$|\boldsymbol{E}_1\rangle + |\boldsymbol{E}_2\rangle \rightarrow |\boldsymbol{E}_1\rangle\langle\boldsymbol{E}_1| + |\boldsymbol{E}_2\rangle\langle\boldsymbol{E}_2| + \text{“Work”}$$

For equi-level coherence $\mathcal{E}_{\boldsymbol{E}_1} = \mathcal{E}_{\boldsymbol{E}_2}$

“Classical energy distribution $P(\boldsymbol{E})$ unchanged”

➔ Purely quantum contribution on work extraction process

Extractable work from quantum coherence

- Interconversion between work and correlation(coherence) :

Observation 2 *Given a many-body system with N subsystems, a maximally coherent state $|\Psi\rangle = \sum_{\mathcal{E}_{\boldsymbol{E}}=\mathcal{E}_0} \frac{1}{\sqrt{d(\mathcal{E}_0)}} |\boldsymbol{E}\rangle$ within an energy eigenspace with energy $\mathcal{E}_0$ and degeneracy $d(\mathcal{E}_0)$ can be interconverted with the decohered state $\Pi(\hat{\rho}^{\Psi}) = \sum_{\mathcal{E}_{\boldsymbol{E}}=\mathcal{E}_0} d(\mathcal{E}_0)^{-1} |\boldsymbol{E}\rangle\langle\boldsymbol{E}|$ in a single-shot TO, with $k_B T \Delta I = k_B T \log d(\mathcal{E}_0)$ amount of work extracted/consumed.*

- Example : Dicke states (in N-partite two level systems)

$$|N,k\rangle = \binom{N}{k}^{-1/2} \sum_P P(|1\rangle^k |0\rangle^{N-k}) \quad \xleftrightarrow[\text{T.O.}]{} \quad \Pi(\hat{\rho}) = \binom{N}{k} \sum_P P(|1\rangle^k \langle 1|^k \otimes |0\rangle^{N-k} \langle 0|^{N-k})$$

$$\boxed{W = k_B T \Delta I = k_B T \log \binom{N}{k}}$$

When $N \gg 1$ and $r = k/N$,

$$W/N = k_B T H(r) = k_B T \left[-r \log r - (1-r)\log(1-r)\right]$$

Work-locking in coherence

- Inter-level coherence does not contribute to work extraction process

Theorem 3: for a general work extraction:

$$\rho \otimes |0\rangle\langle 0| \rightarrow \sigma \otimes \sum_w p(w)|w\rangle\langle w|,$$

the work distributions $p(w)$ that can be obtained from the states ρ and $\mathcal{D}_\mathrm{H}(\rho)$ through time-translation symmetric operations coincide.

$\mathcal{D}_H(\hat{\rho})$: energy block-diagonal state

Logtaglio *et.al.*, Nature Commun. (2015)

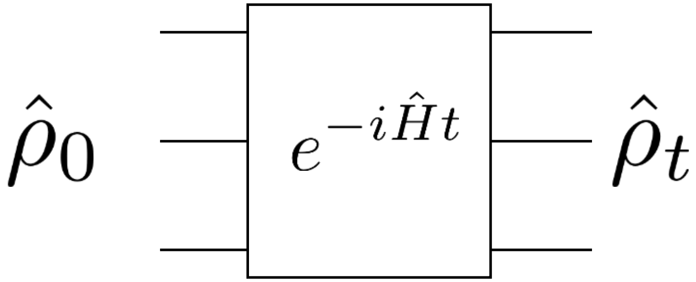
Q2. Thermodynamic resource beyond work-yielding resource?

(contained in inter-level coherence)

Contents

Coherence as a clock resource

- Quantum metrology: High-precision parameter estimation beyond classical shot-noise limit



✓ Estimator of the parameter : $\hat{t}$

➔ Variance of estimator : $(\Delta t)^2 = \langle (\hat{t} - t)^2 \rangle$

$$(\Delta t)^2 \geq \frac{1}{I_F(\hat{\rho}, \hat{H})}$$

(Quantum Cramer-Rao bound)

$$I_F(\hat{\rho}, \hat{H}) = 2 \sum_{i,j} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j} |\langle i | \hat{H} | j \rangle|^2$$

(Quantum Fisher Information)

- Time evolution of a quantum state with inter-level coherence :

$$|\psi_0\rangle = \sum_{\boldsymbol{E}} \sqrt{P(\boldsymbol{E})} |\boldsymbol{E}\rangle \rightarrow |\psi_t\rangle = \sum_{\boldsymbol{E}} \sqrt{P(\boldsymbol{E})} e^{i\mathcal{E}_{\boldsymbol{E}} t/\hbar} |\boldsymbol{E}\rangle$$

✓ Clock frequency : $\Delta\omega = (\mathcal{E}_{\boldsymbol{E}} - \mathcal{E}_{\boldsymbol{E}'})/\hbar$ ➔ "Time reference"

Coherence as a clock resource

- Coherent thermal state : $|\gamma\rangle = \sum_E \sqrt{\frac{e^{-\beta E}}{Z_S}}\,|E\rangle$ (No work can be extracted)

✓ High clock resolution : $I_F(|\gamma\rangle\,, \hat{H}_S) = 4\frac{\partial^2}{\partial\beta^2}\log Z_S = 4\omega_0^2\bar{n}(\bar{n}+1)$ → Heisenberg Limit

$$\hat{H}_S = \omega_0(\hat{a}^\dagger\hat{a} + \frac{1}{2})$$

- Clock resource does not increase under TO :

Observation 3 *Under a TO given by Λ_β, the quantum Fisher (skew) information $I_{F(\alpha)}$ of a quantum system always decreases, i.e.*

$$\Delta I_{F(\alpha)} = I_{F(\alpha)}(\Lambda_\beta(\hat{\rho}_S), \hat{H}_S) - I_{F(\alpha)}(\hat{\rho}_S, \hat{H}_S) \leq 0.$$

Contents

Coherence second law of thermodynamics

- Coherence second law in terms of QFI :

Observation 3 *Under a TO given by Λ_β, the quantum Fisher (skew) information $I_{F(\alpha)}$ of a quantum system always decreases, i.e.*

$$\Delta I_{F(\alpha)} = I_{F(\alpha)}(\Lambda_\beta(\hat{\rho}_S), \hat{H}_S) - I_{F(\alpha)}(\hat{\rho}_S, \hat{H}_S) \leq 0.$$

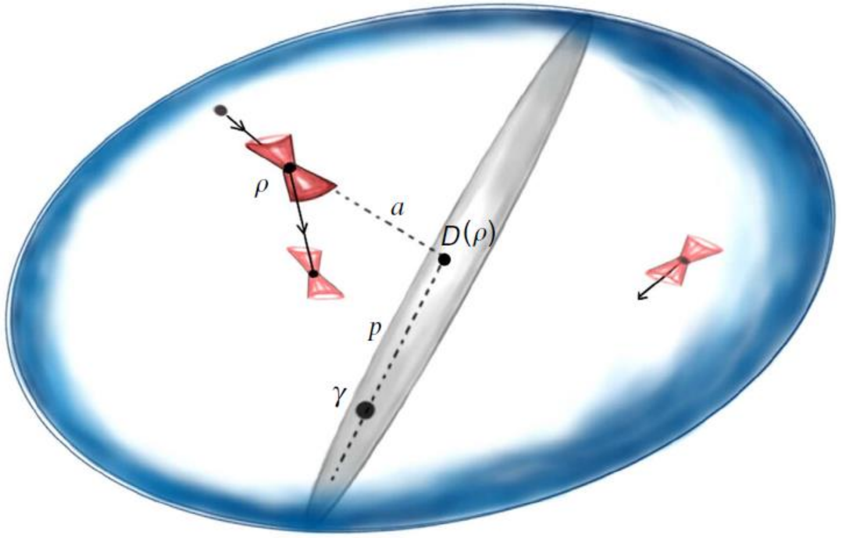
- Previously studied coherence restrictions :

$$A_\alpha(\hat{\rho}_S) = S_\alpha(\hat{\rho}_S || \mathcal{D}(\hat{\rho}_S))$$

(Asymmetry)

$$\sum_{\mathcal{E}_{\boldsymbol{E}} - \mathcal{E}_{\boldsymbol{E}'} = \omega} |\rho_{\boldsymbol{E}\boldsymbol{E}'}|$$

} Decreases under TO



Logtaglio *et.al.*, Nature Commun. (2015)
Logtaglio *et.al.*, Phys. Rev. X (2015)

QFI gives additional restriction for TO

- Four level Hamiltonian : $\hat{H} = \sum_{n=0}^{3} n\omega_0 |n\rangle\langle n|$

$$\hat{\rho} = \begin{pmatrix} 0.5 & 0 & 0.1 & 0.1 \\ 0 & 0.2 & 0 & 0 \\ 0.1 & 0 & 0.25 & 0.1 \\ 0.1 & 0 & 0.1 & 0.05 \end{pmatrix} \quad \overset{\text{T.O.?}}{\Longleftrightarrow} \quad \hat{\sigma} = \begin{pmatrix} 0.5 & 0.099 & 0.099 & 0.099 \\ 0.099 & 0.25 & 0 & 0 \\ 0.099 & 0 & 0.2 & 0 \\ 0.099 & 0 & 0 & 0.05 \end{pmatrix}$$

- Free energy: $F_\alpha(\hat{\rho}) \geq F_\alpha(\hat{\sigma})$
- Asymmetry: $A_\alpha(\hat{\rho}) \geq A_\alpha(\hat{\sigma})$

$$\sum_{\mathcal{E}_{\boldsymbol{E}} - \mathcal{E}_{\boldsymbol{E}'} = \omega} |\rho_{\boldsymbol{EE}'}| \geq \sum_{\mathcal{E}_{\boldsymbol{E}} - \mathcal{E}_{\boldsymbol{E}'} = \omega} |\sigma_{\boldsymbol{EE}'}|$$

For every energy difference $\omega = n\omega_0$

Possible…?

- QFI conditions :

$$I_{1/2}(\hat{\rho}, \hat{H}) = 0.153$$
$$I_{1/2}(\hat{\sigma}, \hat{H}) = 0.163$$
$$I_F(\hat{\rho}, \hat{H}) = 0.843$$
$$I_F(\hat{\sigma}, \hat{H}) = 0.959$$

$$I_{1/2}(\hat{\rho}) < I_{1/2}(\hat{\sigma})$$
$$I_F(\hat{\rho}) < I_F(\hat{\sigma})$$

Transition is impossible!

State transformation in many-copy

- Product state vs. GHZ-state : $I_{F(\alpha)}(\hat{\rho}^{\otimes N}, \hat{H}_{\rm tot}) = N I_{F(\alpha)}(\hat{\rho}, \hat{H}_0) \leq N||\hat{H}_0||^2$

$$I_{F(\alpha)}(\hat{\sigma}_{N-\rm GHZ}, \hat{H}_{\rm tot}) = O(N^2)$$

$$\hat{\sigma}_{N-\rm GHZ} = 2^{-1/2}(|0\rangle^{\otimes N} + |1\rangle^{\otimes N})$$

  - **GHZ-state cannot be generated from product state under TO**

- Many-body entanglement and QFI : $I_F(\hat{\rho}_N, \hat{H}_{\rm tot}) \leq kN||\hat{H}_0||^2$ for *k*-producible state

- Asymmetry vanishes on many-copy limit : $\lim_{n\to\infty} A_\alpha(\hat{\rho}^{\otimes n})/n = 0$
- QFI does not : $\lim_{n\to\infty} I_{F(\alpha)}(\hat{\rho}^{\otimes n}, \hat{H}_n)/n = I_{F(\alpha)}(\hat{\rho}, \hat{H}_0) \neq 0$

Catalytic transform

- State transformation rate in asymptotic limit $\hat{\rho}^{\otimes n} \to \hat{\sigma}^{\otimes Rn}$

$$R_{\mathrm{TO}}(\hat{\rho} \to \hat{\sigma}) = \sup\{R : \lim_{n\to\infty} \inf_{\Lambda_\beta} ||\Lambda_\beta(\hat{\rho}^{\otimes n}) - \hat{\sigma}^{\otimes Rn}||_1 = 0\}$$

- For pure gapless states : $R_{\mathrm{TO}}(|\psi\rangle \to |\phi\rangle) \leq R_{\mathrm{cov}}(|\psi\rangle \to |\phi\rangle) = \dfrac{\mathrm{Var}(\psi, \hat{H}_S)}{\mathrm{Var}(\phi, \hat{H}_S)}$

- Allowing catalytic transformation : $R^*_{\mathrm{TO}}(\hat{\rho} \to \hat{\sigma}) = S(\hat{\rho}||\hat{\gamma})/S(\hat{\sigma}||\hat{\gamma})$

Catalysis : $|\chi\rangle = |H|^{-1/2} \sum_{h\in H} |h\rangle$

$$H = \{0, \ldots, 2n^{2/3}\}$$

(sub-linear dimension)

$$I_F(\chi, \hat{H}_S) = (4/3)n^{2/3}(n^{2/3} + 1) \propto n^{4/3}$$

Catalysis itself requires super-linear amount of coherence resource

Contents

Many-body coherence in quantum thermodynamics