

微小系の非平衡熱力学と量子コヒーレンス

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based on:

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4. 結果:
散逸・熱流トレードオフ関係におけるコヒーレンスの効果
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有限パワー・カルノー効率の漸近的達成
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熱力学：マクロからミクロへ

マクロの領域で動作する熱機関

- 古典熱力学 (19th and 20th century)

- どのような熱機関であってもカルノー効率を超えた動作はできないことを予測
- 現実には動作のスピード(仕事率)も重要だが、古典熱力学は平衡状態に関する理論であり、時間や動力学へ言及することができない

熱力学：マクロからミクロへ

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- 古典熱力学 (19th and 20th century)

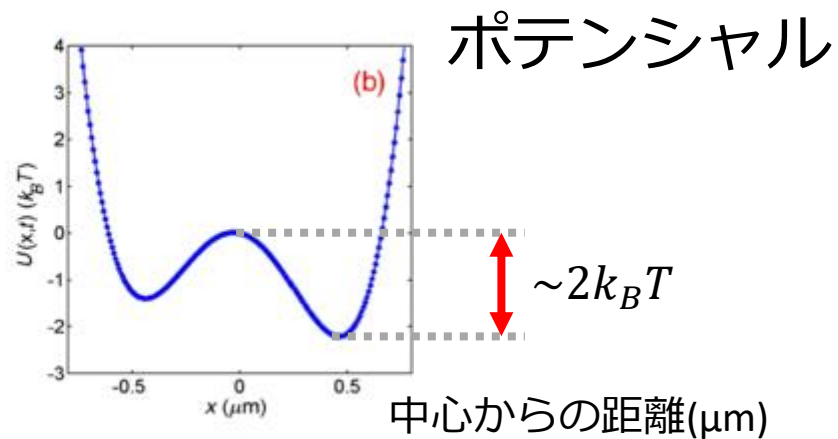
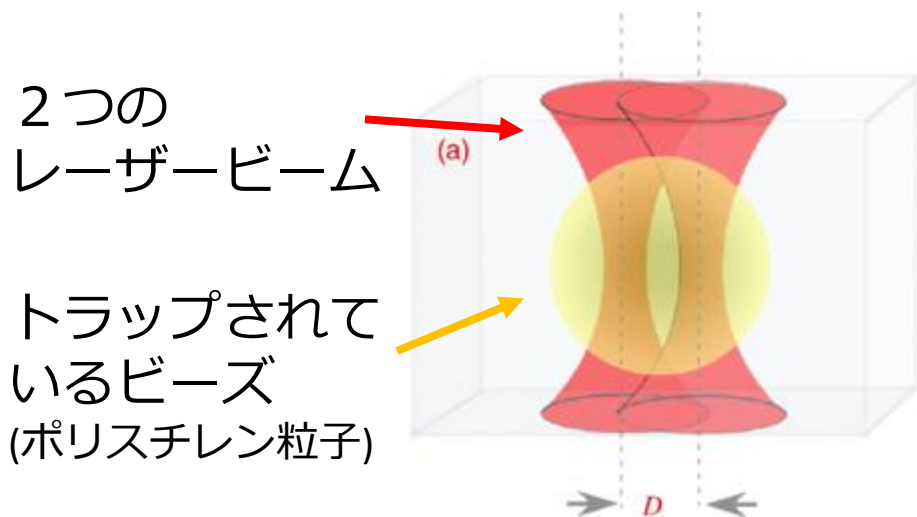
大きいスケール

一分子領域で動作する熱機関

- **ゆらぎの熱力学** (21st century ~)

熱ゆらぎ

関本謙「ゆらぎのエネルギー論」
U. Seifert, Rep. Prog. Phys. (2012)



S. Ciliberto, PRX (2017)

小さいスケール

熱力学：マクロからミクロへ

マクロの領域で動作する熱機関

- 古典熱力学 (19th and 20th century)

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一原子/キュービット領域で動作する熱機関

- 量子熱力学

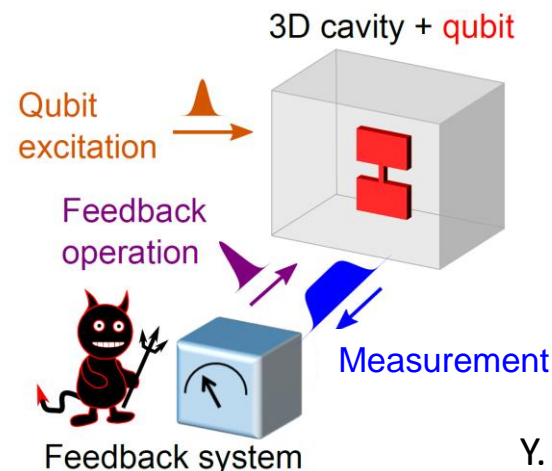
大きいスケール

熱ゆらぎ

量子ゆらぎ

小さいスケール

例：超電導量子ビット系



熱力学：マクロからミクロへ

マクロの領域で動作する熱機関

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一分子領域で動作する熱機関

- **ゆらぎの熱力学** (21st century ~)

一原子/キュービット領域で動作する熱機関

- **量子熱力学**

- 動力学とエネルギー学がコンシステントに融合した理論体系
- 非平衡・有限時間の熱力学的解析が可能

大きいスケール

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量子開放系のダイナミクス

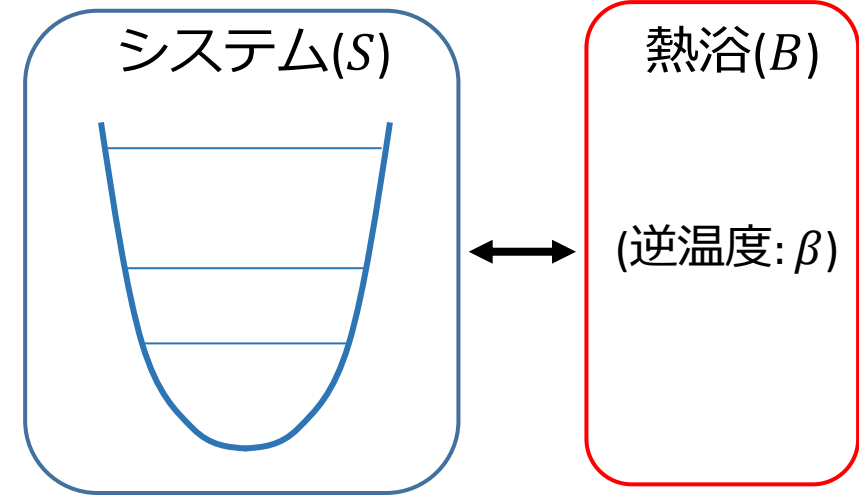
開放系の時間発展 (システム S +熱浴 B)

$$\rho_S(\tau) = \text{Tr}_B \left[\underbrace{U_\tau^{SB}}_{\text{全体系}(S+B)\text{の}} \left(\underbrace{\rho_S(0)}_{\text{システムの}} \otimes \underbrace{\rho_B^\beta}_{\text{熱浴の初期状態}} \right) \underbrace{(U_\tau^{SB})^\dagger}_{\text{ユニタリ時間発展}} \right]$$

全体系($S+B$)の
ユニタリ時間発展

システムの
初期状態

熱浴の初期状態
(逆温度 β のギブス分布)



- 厳密な記述だが、時間発展を解析的・数值的に解くのは困難 [cf. 非マルコフ効果]
- 多くの実験系では熱浴の影響はマルコフ的 (メモリー効果が無い)

“マルコフ的”なダイナミクスの最も一般的な形

→ Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) マスター方程式

$$\partial_t \rho_S(t) = \mathcal{L}(t) \rho_S(t)$$

物理的に妥当と思われる仮定 (弱結合、ボルン・マルコフ・セキュラー近似) から
GKSLの形になるマスター方程式が導かれる

量子開放系のダイナミクス

GKSLマスター方程式

ディシペーター

$$\partial_t \rho = \mathcal{L}(t) = -\frac{i}{\hbar} [H, \rho] + \mathcal{D}[\rho]$$

$$\mathcal{D}[\rho] = \sum_{\omega} \gamma(\omega) \left(L_{\omega} \rho L_{\omega}^{\dagger} - \frac{1}{2} \{ L_{\omega}^{\dagger} L_{\omega}, \rho \} \right)$$

ユニタリー時間発展の部分

熱浴によるデコヒーレンス・散逸の効果

GKSLマスター方程式は“マルコフ的”なダイナミクスの最も一般的な形を与える
 → 量子熱力学ではさらに**熱力学的にコンシステント**な条件を課す

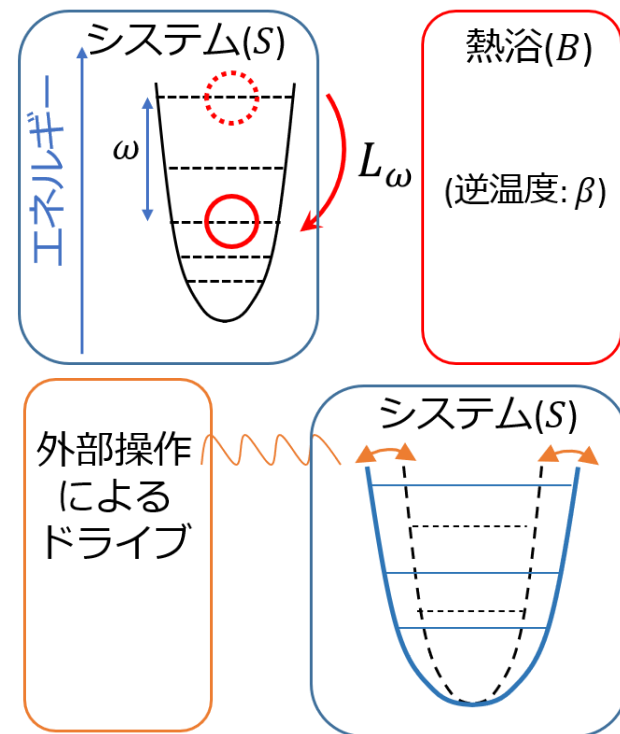
定常解が熱浴と同じ温度のギブス分布(平衡分布)

- L_{ω} : エネルギー固有状態 $\Pi_{e+\omega}$ から Π_e へのジャンプ
- 詳細釣り合い: $\gamma(\omega)/\gamma(-\omega) = \exp[\beta\omega]$

(通常の弱結合、ボルン・マルコフ・セキュラー近似による導出は上記の条件を満たす)

外部からの古典的な操作によってハミルトニアン $H(t)$ が時間的に変化する状況も取り扱う (この場合、各時刻ごとに上記の条件を課す)

→ **熱力学的にコンシステントなダイナミクスの構造の上に**
仕事・熱・エントロピー生成などのオブザーバブルを定義する

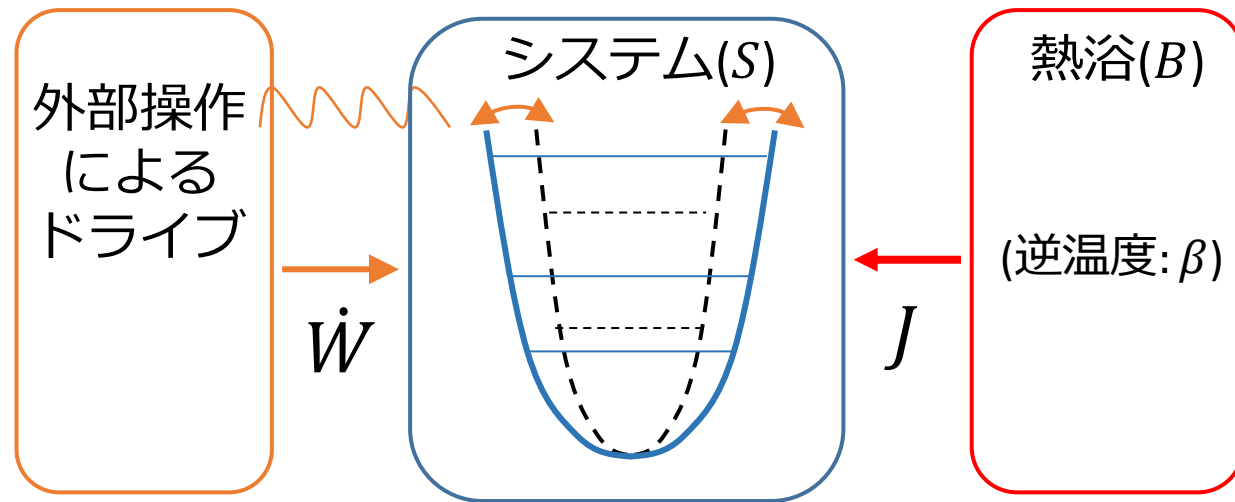


熱力学的なオブザーバブルと熱力学の法則

熱力学第一法則（エネルギー保存）

$$\frac{\partial_t(\text{Tr}[H\rho])}{\text{内部エネルギー変化 } \dot{E}} = \frac{\text{Tr}[(\partial_t H)\rho]}{\text{仕事流 } \dot{W}} + \frac{\text{Tr}[H\partial_t\rho]}{\text{熱流 } J}$$

内部エネルギー変化 \dot{E} 仕事流 \dot{W} 熱流 J



物理的解釈

- 仕事流 $\dot{W} = \text{Tr}[(\partial_t H)\rho]$
外部操作でハミルトニアンをドライブしたときのエネルギー変化

- 熱流 $J = \text{Tr}[H\partial_t\rho]$

マスター方程式

$$\partial_t\rho = -\frac{i}{\hbar}[H,\rho] + \mathcal{D}[\rho] \text{ を代入}$$

$J = \text{Tr}[H\mathcal{D}[\rho]]$: 熱浴と相互作用したときの散逸によるエネルギー変化

熱力学的なオブザーバブルと熱力学の法則

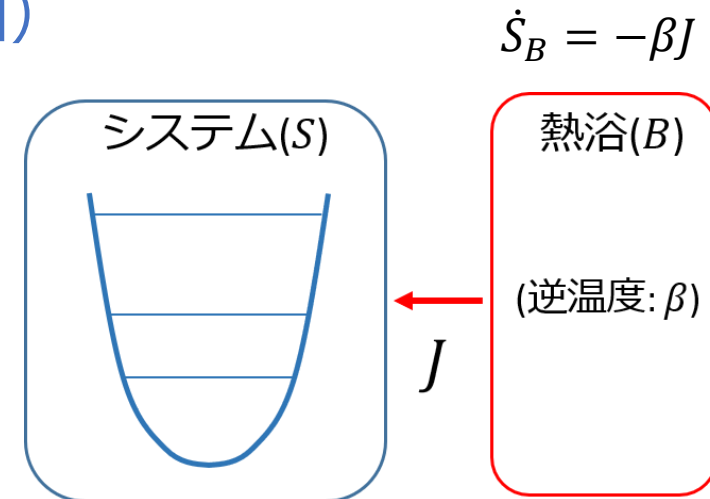
・ 熱力学第二法則 (エントロピー増大)

エントロピー生成率 ($S + B$ 全体系のエントロピー増加)

$$\dot{\sigma}(\rho) = \dot{S}(\rho) - \beta J(\rho)$$

システムの von Neumann エントロピー
 $S(\rho) = -\text{Tr}[\rho \ln \rho]$ の増加率

熱浴のエントロピー増加率
(cf. $\delta S = \delta E / T$)



- Spohn の表現 (の一般化)

$$\dot{\sigma}(\rho) = \lim_{dt \rightarrow 0} \frac{1}{dt} (D[\rho(t) \parallel \rho_{\text{Gibbs}}^\beta(t)] - D[\rho(t + dt) \parallel \rho_{\text{Gibbs}}^\beta(t)]) \geq 0$$

- $\rho_{\text{Gibbs}}^\beta(t)$: システムのハミルトニアン $H(t)$ に対応するギブス分布 (熱平衡状態)
- $D[\rho \parallel \sigma] = \text{Tr}[\rho(\ln \rho - \ln \sigma)]$: 相対エントロピー (2つの状態の“距離”)

熱平衡状態からのずれによる散逸、不可逆性の定量化

[$\dot{\sigma} \geq 0$ の証明には、時間発展がマルコフ的、 $\rho_{\text{Gibbs}}^\beta(t)$ が定常解であることと相対エントロピーの単調性を用いる]

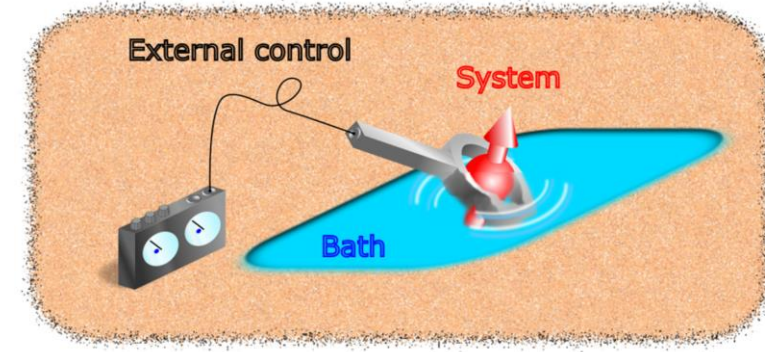
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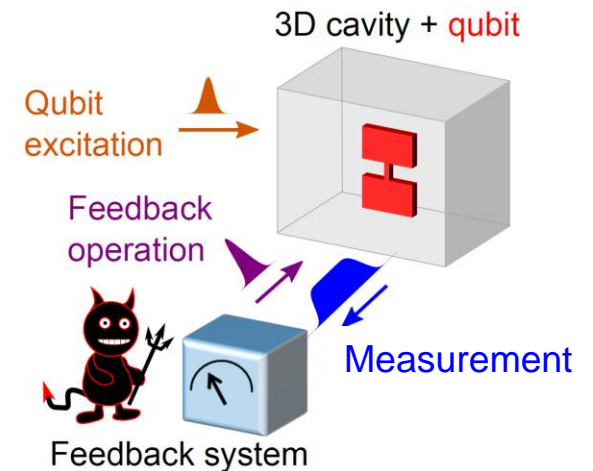
Understanding fundamental thermodynamic relations

Quantum thermodynamics:

- Understanding fundamental limits (no-go theorems) on the controllability and manipulation of quantum devices
- Understanding a deep connection between work, heat, and information in quantum systems
- Understanding potential quantum advantages in thermodynamics



from [PRE 95, 012136 (2017)]



from [Nat. Comm. 9, 1291 (2018)]

Quantum advantage in thermodynamics

- **Quantum coherence** improves the *performance of quantum devices* in many scenarios, e.g., superdense coding, Grover's algorithm, quantum sensing
- It is still unclear if there exists a nontrivial “**quantum advantages**” in thermodynamics
- Coherence that is built up during a heat engine cycle acts as quantum friction (**disadvantage**)
 - Linear response: Brandner, Bauer, Seifert, PRL (2017)
 - experimentally relevant model: Karimi and Pekola, PRB (2016)
- Some studies show that coherence improves the performance of heat engines (**advantage**)
 - Uzdin, Levy, Kosloff, PRX (2015)

classification of coherence advantages/disadvantages in thermodynamics

Main topic of this study

trade-off relations between “current” and “dissipation”

e.g. Joule heating $W = RI^2$

- thermodynamic uncertainty relations

Barato, Seifert, PRL 2015

(precision of) general current \Leftrightarrow entropy production

- open system quantum speed limits

probability current \Leftrightarrow entropy production

Shiraishi, Funo, Saito, PRL, 2018
Funo, Shiraishi Saito, NJP, 2019

- power-efficiency trade-off relation in heat engines

Shiraishi, Saito, Tasaki, PRL 2016

output power \Leftrightarrow thermodynamic efficiency

- trade-off relation between heat current and entropy production

coherence effect? not fully explored!

2 types of coherence

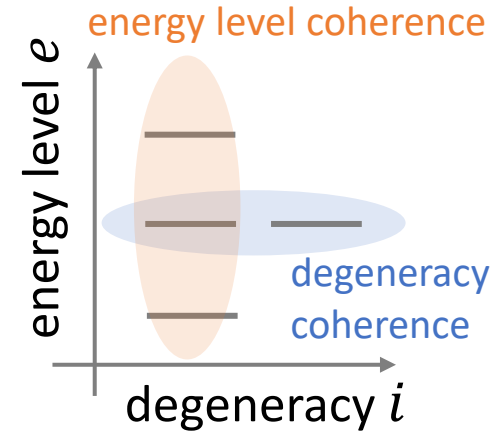
main aim of this research:

understand the effect of coherence on current-dissipation trade-off relation

for later purpose, we introduce 2 types of coherence:

1. coherence between different energy levels

2. coherence between degenerate states



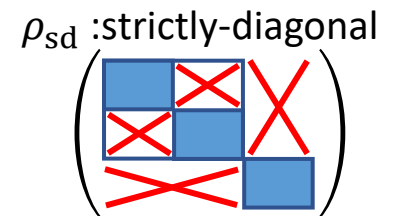
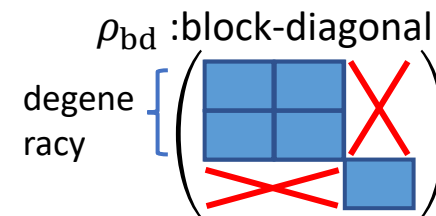
	general ρ	block-diagonal $\rho_{\text{bd}} = \sum_e \Pi_e \rho \Pi_e$	strictly-diagonal $\rho_{\text{sd}} = \sum_{e,i} \Pi_{e,i} \rho \Pi_{e,i}$
energy level coherence	✓	✗	✗
degeneracy coherence	✓	✓	✗

projection to energy level e

$$\Pi_e = \sum_i \Pi_{e,i}$$

projection to $|e, i\rangle$ state

$$\Pi_{e,i} = |e, i\rangle\langle e, i|$$



2 types of coherence

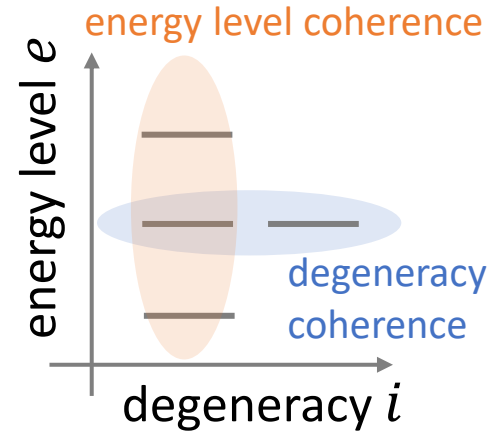
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compare these two states

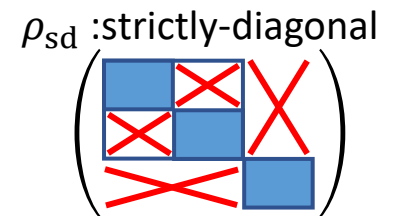
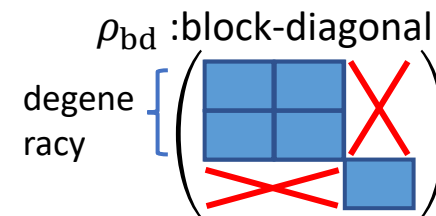
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2 types of coherence

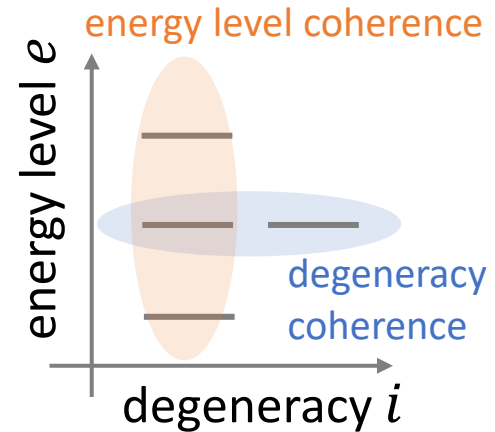
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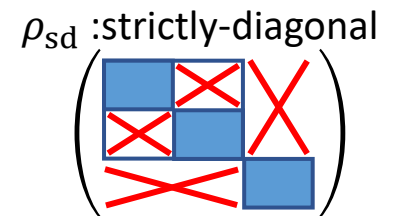
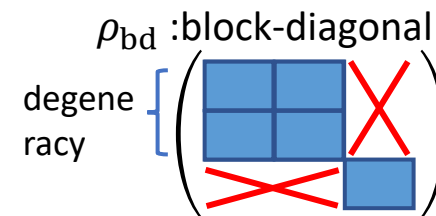
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Main results: coherence effect on current-dissipation ratio

current-dissipation (CD) ratio

$$\frac{J(\rho)^2}{\dot{\sigma}(\rho)}$$

← electrical conductance: $\frac{1}{R} = \frac{I^2}{W}$ (cf. Joule heating)

heat current: $J(\rho) = \text{Tr}[H\partial_t\rho]$

entropy production: $\dot{\sigma}(\rho) = \dot{S}(\rho) - \beta J(\rho)$

- we want **large heat current** and **small entropy production** for having high-performance thermodynamic devices (e.g. heat engines, refrigerators)
- higher CD ratio is preferred, but there exists an upper limit (CD trade-off relation)

	general ρ	block-diagonal $\rho_{\text{bd}} = \sum_e \Pi_e \rho \Pi_e$	strictly-diagonal $\rho_{\text{sd}} = \sum_{e,i} \Pi_{e,i} \rho \Pi_{e,i}$
energy level coherence	✓	✗	✗
degeneracy coherence	✓	✓	✗

In the following, we derive the CD trade-off relation and discuss how $J^2 / \dot{\sigma}$ depends on coherence ($\rho, \rho_{\text{bd}}, \rho_{\text{sd}}$)

Main results: coherence effect on current-dissipation (CD) ratio

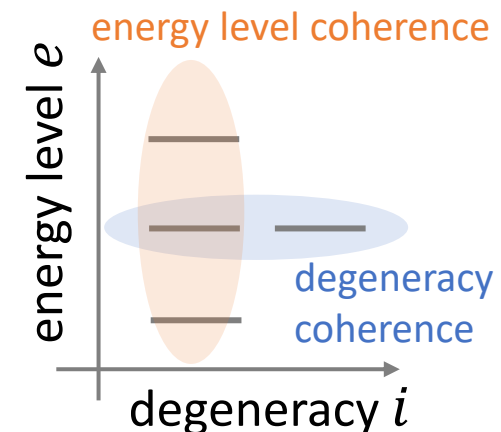
main result 1: energy level coherence *always* reduces the CD ratio → **disadvantage**

(e.g., conductance)

$$\frac{J(\rho)^2}{\dot{\sigma}(\rho)} \leq \frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})}$$

- note: a stronger relation can be obtained, $J(\rho) = J(\rho_{\text{bd}})$ and $\dot{\sigma}(\rho) \geq \dot{\sigma}(\rho_{\text{bd}})$
- heat bath cannot utilize and only destroys energy level coherence
- if the Hamiltonian is non-degenerate, coherence would always lower the performance

	general ρ	block-diagonal $\rho_{\text{bd}} = \sum_e \Pi_e \rho \Pi_e$	strictly-diagonal $\rho_{\text{sd}} = \sum_{e,i} \Pi_{e,i} \rho \Pi_{e,i}$
energy level coherence	✓	✗	✗
degeneracy coherence	✓	✓	✗



Main results: coherence effect on current-dissipation (CD) ratio

main result 1: energy level coherence *always* reduces the CD ratio → **disadvantage**

$$\frac{J(\rho)^2}{\dot{\sigma}(\rho)} \leq \frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})}$$

(e.g., conductance)

main result 2: degeneracy coherence allows increasing the CD ratio → **advantage**

$$\frac{J(\rho_{\text{sd}})^2}{\dot{\sigma}(\rho_{\text{sd}})} \leq \frac{A_{\text{cl}}}{2}$$

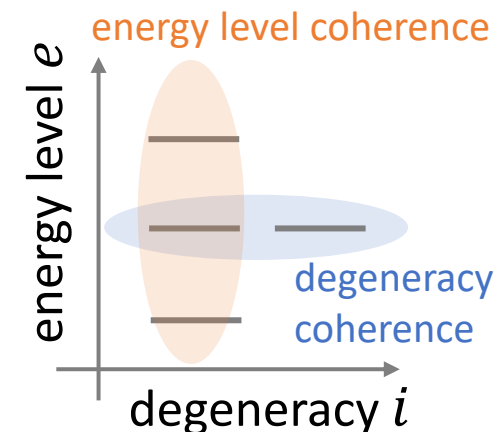
and

$$\frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})} \leq \frac{A_{\text{cl}} + A_{\text{qm}}}{2}$$

coherence effect!

also bounds CD ratio for ρ (using result 1)

	general ρ	block-diagonal $\rho_{\text{bd}} = \sum_e \Pi_e \rho \Pi_e$	strictly-diagonal $\rho_{\text{sd}} = \sum_{e,i} \Pi_{e,i} \rho \Pi_{e,i}$
energy level coherence	✓	✗	✗
degeneracy coherence	✓	✓	✗



Main results: coherence effect on current-dissipation (CD) ratio

main result 1: energy level coherence *always* reduces the CD ratio → **disadvantage**

$$\frac{J(\rho)^2}{\dot{\sigma}(\rho)} \leq \frac{J(\rho_{bd})^2}{\dot{\sigma}(\rho_{bd})}$$

(e.g., conductance)

main result 2: degeneracy coherence allows increasing the CD ratio → **advantage**

$$\frac{J(\rho_{sd})^2}{\dot{\sigma}(\rho_{sd})} \leq \frac{A_{cl}}{2}$$

and

$$\frac{J(\rho_{bd})^2}{\dot{\sigma}(\rho_{bd})} \leq \frac{A_{cl} + A_{qm}}{2}$$

coherence effect!

also bounds CD ratio for ρ (using result 1)

- physical interpretation of A : *instantaneous heat fluctuation*

classical (ρ_{sd} -dependent) part: A_{cl}

coherence effect part: $A_{qm} = (\text{collective jumps}) \times (\text{degeneracy coherence})$

- when bath *collectively* acts on *coherent* degenerate states, we can improve the CD ratio up to $A_{qm}/2$ → **advantage!**

Main results: scaling analysis of the current-dissipation ratio

$$\frac{J(\rho_{sd})^2}{\dot{\sigma}(\rho_{sd})} \leq \frac{A_{cl}}{2} \quad \text{and} \quad \frac{J(\rho_{bd})^2}{\dot{\sigma}(\rho_{bd})} \leq \frac{A_{cl} + A_{qm}}{2}$$

$O(N)$ points to the right-hand side of the second inequality.
 $O(1)$ points to the denominator of the second inequality.
 $O(N^2)$ points to the right-hand side of the second inequality, with A_{qm} highlighted in a blue box.

Next, we discuss the scaling behavior of the CD trade-off relation

- suppose that A_{qm} is an $O(N^2)$ quantity N: number of degeneracy or particle number

we find that $J = O(N)$ and $\dot{\sigma} = O(1)$ scaling is possible

when $A_{qm} = O(N^2)$ via ($O(N)$ degeneracy coherence \times $O(N)$ collective jumps)
 \Rightarrow $O(N)$ macroscopic heat flows but the $O(1)$ entropy production remains at microscopic order

In the following, we show a toy model example that realizes the above observation

example: 2N-state model that realizes $A_{\text{qm}} = O(N^2)$ scaling

system Hamiltonian:

$$H = \sum_{j=1}^N \hbar\omega |e, j\rangle \langle e, j|,$$

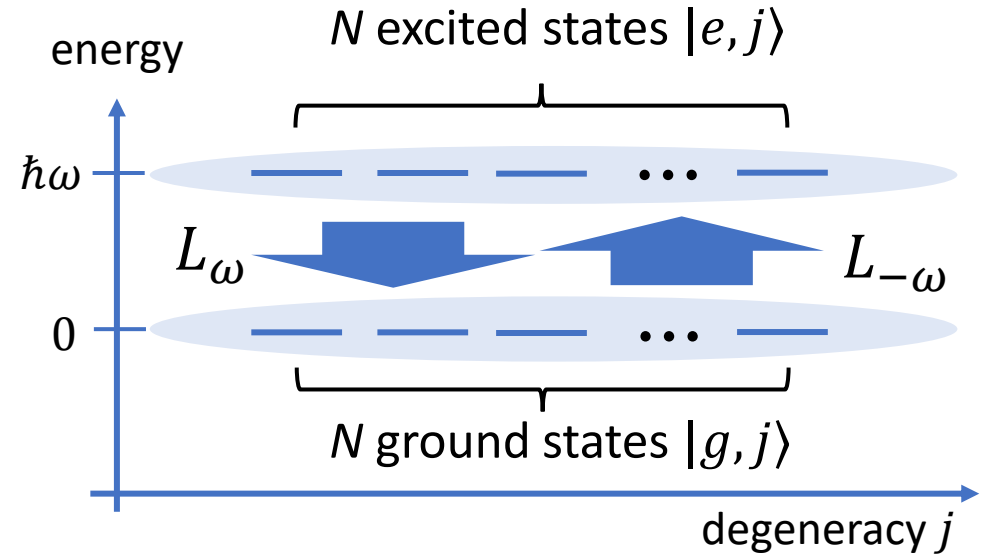
dissipator:

$$\mathcal{D}[\rho] = \sum_{\Omega=\omega, -\omega} \gamma(\Omega) (L_{\Omega} \rho L_{\Omega}^{\dagger} + \{L_{\Omega}^{\dagger} L_{\Omega}, \rho\})$$

jump operators: *correlated decays/excitation*

$$L_{\omega} = \sum_{j, j'} \sigma_{-}^{j, j'} \quad L_{-\omega} = \sum_{j, j'} \sigma_{+}^{j, j'}$$

$$\sigma_{+}^{j, j'} = |e, j\rangle \langle g, j'|, \quad \sigma_{-}^{j, j'} = |g, j\rangle \langle e, j'|$$



symmetric Dicke ladder



note: essential feature of this model can be captured by a n-qubit super-radiance model

use these two Dicke states
(via a technique called superabsorption)

example: 2N-state model that realizes $A_{\text{qm}} = O(N^2)$ scaling

system Hamiltonian:

$$H = \sum_{j=1}^N \hbar\omega |e, j\rangle \langle e, j|,$$

jump operators: *correlated decays/excitation*

$$L_\omega = \sum_{j,j'} \sigma_-^{j,j'} \quad L_{-\omega} = \sum_{j,j'} \sigma_+^{j,j'}$$

$$\sigma_+^{j,j'} = |e, j\rangle \langle g, j'|, \quad \sigma_-^{j,j'} = |g, j\rangle \langle e, j'|$$

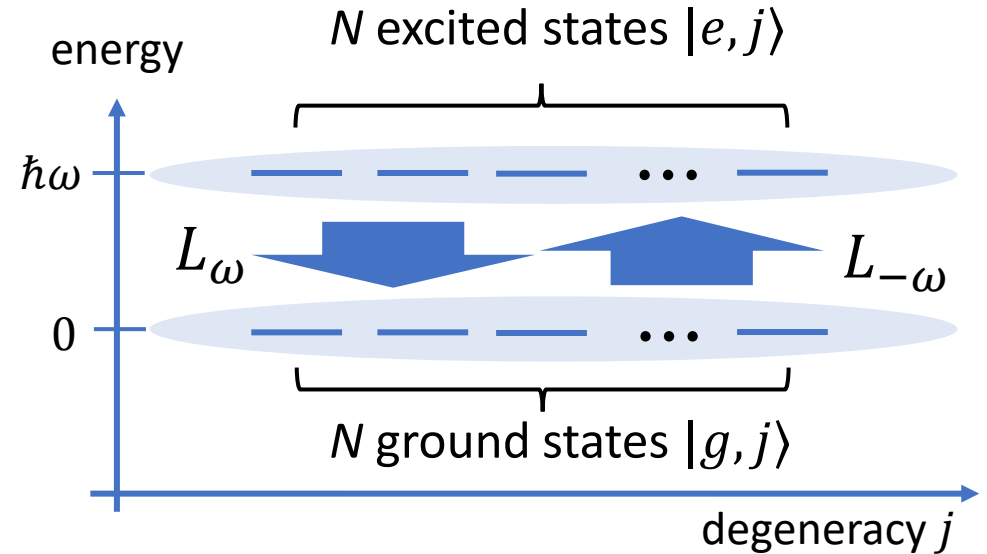
consider the following initial state (contains $O(N)$ coherence)

$$\rho_0 := p_g |g, +\rangle \langle g, +| + p_e |e, +\rangle \langle e, +|$$

straightforward calculation shows that

$$A_{\text{qm}} = O(N^2) \quad \& \quad J(\rho_0) = O(N)$$

$$\dot{\sigma}(\rho_0) = O(1)$$



$$|g, +\rangle := \frac{\sum |g, j\rangle}{\sqrt{N}} \quad |e, +\rangle := \frac{\sum |e, j\rangle}{\sqrt{N}}$$

$$\frac{p_g}{p_e} = \left(1 + \frac{1}{N}\right) e^{\beta\hbar\omega}$$

→ realization of a
“dissipation-less” heat current

example: $2N$ -state model that realizes $A_{\text{qm}} = O(N^2)$ scaling

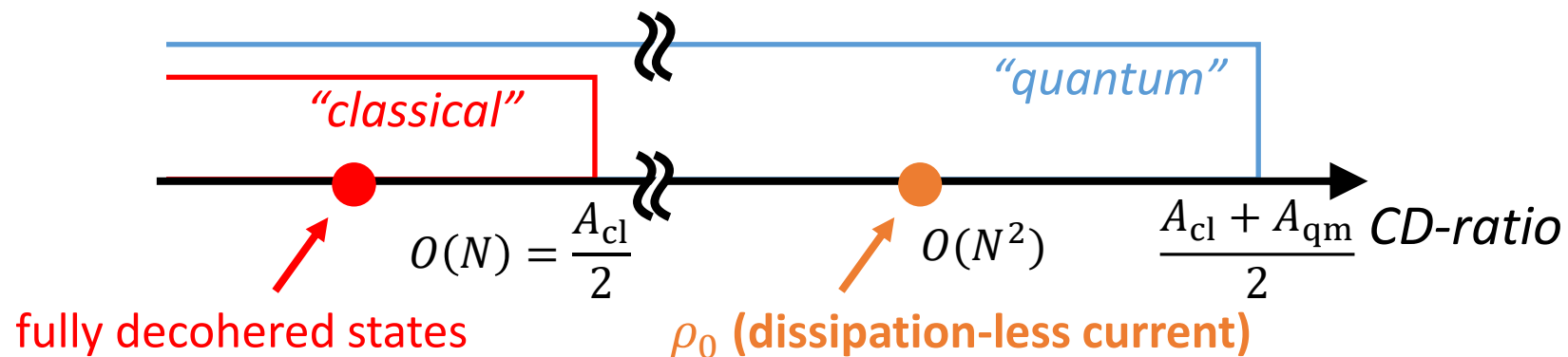
at least for this $2N$ -state model, we can rigorously show that

$$A_{\text{cl}} = O(N) \text{ for any state } \rho$$

- by noting the relation $\frac{J(\rho_{\text{sd}})^2}{\dot{\sigma}(\rho_{\text{sd}})} \leq \frac{A_{\text{cl}}}{2}$ the above statement implies that fully decohered states (i.e., ρ_{sd}) cannot produce a dissipation-less current:

$$J(\rho_{\text{sd}}) = O(N) \Rightarrow \dot{\sigma}(\rho_{\text{sd}}) = O(N)$$

- note that the CD ratio for the dissipation-less current is $J(\rho_0)^2 / \dot{\sigma}(\rho_0) = O(N^2)$, and it goes beyond the “classical” bound:



Summary of the main results

H. Tajima and K. Funo
Phys. Rev. Lett. **127**, 190604 (2021)

main result 1: energy level coherence *always* reduces the CD ratio (disadvantage)

(Current-Dissipation)

$$\frac{J(\rho)^2}{\dot{\sigma}(\rho)} \leq \frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})}$$

main result 2: degeneracy coherence allows increasing the CD ratio (advantage)

$$\frac{J(\rho_{\text{sd}})^2}{\dot{\sigma}(\rho_{\text{sd}})} \leq \frac{A_{\text{cl}}}{2} \quad \text{and} \quad \frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})} \leq \frac{A_{\text{cl}} + A_{\text{qm}}}{2}$$

coherence effect!

main result 3: large degeneracy coherence + collective jump mechanism

→ effective cancellation of the CD trade-off relation

macroscopic heat flows but the entropy production remains vanishingly small

$$J(\rho_0) = O(N) \quad \text{and} \quad \dot{\sigma}(\rho_0) = O(1)$$

in the following, we discuss how these results are related to the performance of heat engines

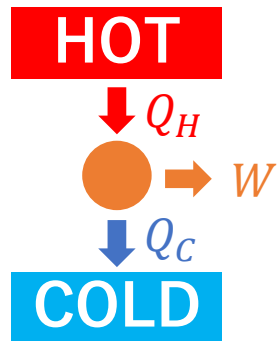
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Application to heat engines

Output power and heat-to-work conversion efficiency

Heat engines, refrigerators



$$P = \frac{W}{\tau} \quad \text{and} \quad \eta = \frac{W}{Q_H}$$

universal upper bound: Carnot efficiency

$$\eta \leq \eta_{\text{Car}} = \left(1 - \frac{T_C}{T_H} \right)$$

- Carnot efficiency can be reached for infinitely slow cycles
→ power vanishes

is it possible to produce finite power and reach Carnot efficiency?

classical limit: power-efficiency trade-off relation

power-efficiency trade-off relation

Shiraishi, Saito, Tasaki, PRL 2016

$$O(1) P \leq O(N) \bar{\Theta} \beta_C \eta (O(1/N) (\eta_{\text{Car}} - \eta))$$

from the above theorem, finite-time Carnot engine is not possible:

$$\eta = \eta_{\text{Car}} \implies P = 0$$

how about asymptotic realization of the Carnot efficiency with finite power? **No**

→ For classical models with reasonable assumptions, $\bar{\Theta}$ scales at most $O(N)$

$$\eta = \eta_{\text{Car}} - O(1/N) \implies P = \underline{O(1)}$$

cannot be $O(N)$, and producing finite power is not possible

➔ however, by using quantum effects, we could overcome this problem

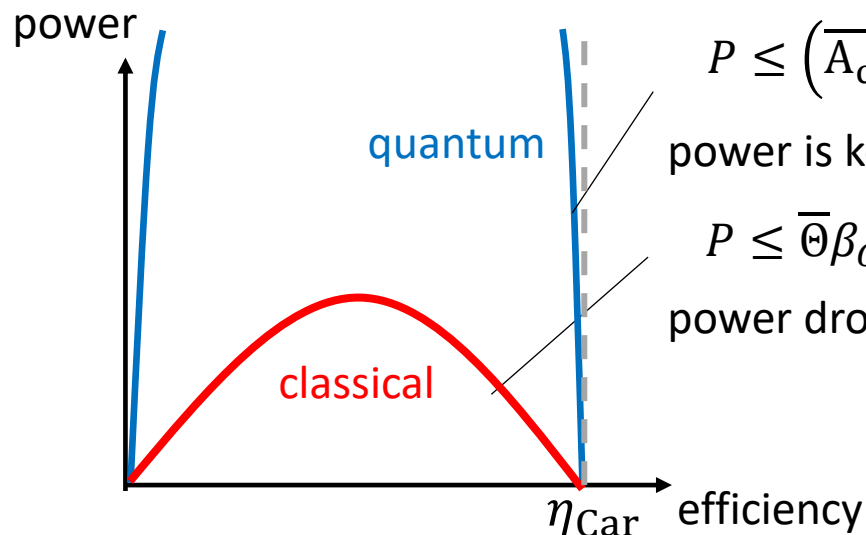
asymptotic realization of finite-power Carnot engine via coherence

In quantum systems, we can derive a power-efficiency trade-off relation

$$\boxed{P}_{O(N)} \leq \left(\overline{A}_{\text{cl}} + \boxed{\overline{A}_{\text{qm}}}_{O(N^2)} \right) c\beta_L \eta \boxed{(\eta_{\text{Car}} - \eta)}_{O(1/N)} \quad \text{Tajima, Funo, PRL 2021}$$

The coefficient \overline{A}_{qm} can grow $O(N^2)$ with coherence + collective jump effects
 → this would realize fundamental scaling difference between classical and quantum systems

$$\overline{A}_{\text{qm}} = O(N^2) \Rightarrow \eta = \eta_{\text{Car}} - O(1/N) \text{ and } P = O(N) \text{ is possible!}$$



$$P \leq (\overline{A}_{\text{cl}} + \overline{A}_{\text{qm}}) c\beta_C \eta (\eta_{\text{Car}} - \eta)$$

power is kept high even if η becomes close to η_{Car}

$$P \leq \overline{\Theta} \beta_C \eta (\eta_{\text{Car}} - \eta)$$

power drops down quickly to 0 as η becomes close to η_{Car}

asymptotic realization of a finite-power Carnot engine is possible in quantum systems [cf. 2N-state model]

Coherence effect on the performance of heat engines

larger value of the current-dissipation (CD) ratio is preferred for having good heat engines
(e.g., conductance)

from the obtained CD trade-off relation, we find the following intuitions:

1. Energy level coherence lowers the engine performance

➔ **for nondegenerate systems, coherence is always bad**

2. Degeneracy coherence can be utilized to improve the engine performance

- ✓ 2N-state model effective finite-time Carnot engine

- ✓ 2qubit super-radiance model heat engine (cf. Tajima-Funo 2021)

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$$\frac{J(\rho)^2}{\dot{\sigma}(\rho)} \leq \frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})}$$

main result 2: degeneracy coherence allows increasing the CD ratio (advantage)

$$\frac{J(\rho_{\text{sd}})^2}{\dot{\sigma}(\rho_{\text{sd}})} \leq \frac{A_{\text{cl}}}{2} \quad \text{and} \quad \frac{J(\rho_{\text{bd}})^2}{\dot{\sigma}(\rho_{\text{bd}})} \leq \frac{A_{\text{cl}} + A_{\text{qm}}}{2} \quad \text{coherence effect!}$$

main result 3: large degeneracy coherence + collective jump

→ *effective cancellation* of the CD trade-off relation

macroscopic heat flows but the entropy production remains vanishingly small

$$J(\rho_0) = O(N) \quad \text{and} \quad \dot{\sigma}(\rho_0) = O(1)$$

this scaling realizes **asymptotic finite-time Carnot engine**: $\eta = \eta_{\text{Car}} - O(1/N)$ and $P = O(N)$