Optimal performance of generalized heat engines with finite-size baths of arbitrary multiple conserved quantities beyond i.i.d.-scaling

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Introduction

- Various researches on quantum thermodynamics
  - thermodynamics of not macroscopic systems
- Performance of quantum heat engines is considered in many ways


...
Introduction

- Finiteness of the working body is mainly focused on
- However, effects of the finiteness of the baths have been less considered.

Restricted size of the baths may be accessible in small (mesoscopic) heat engines

Quantum devise, biological systems, chemical reactions, electrical batteries...

- Baths are treated as collections of i.i.d.-particles

Unphysical \(\rightarrow\) go beyond IID!
Finite size effect: Ordinary heat engine with heat baths composed of i.i.d. particles


- Heat baths are in the canonical state of i.i.d particles
- Finite-size effects for the optimal efficiency in terms of the number $n$ of particles

$$\frac{\Delta W}{\Delta Q_{H,n}} \leq 1 - \frac{\beta_H}{\beta_L} + c_1 \frac{\Delta Q_{H,n}}{n} + c_2 \frac{\Delta Q_{H,n}^2}{n^2} + o \left( \frac{\Delta Q_{H,n}^2}{n^2} \right)$$

- Optimal protocol with finite baths
Finite size effect: Ordinary heat engine with heat baths composed of i.i.d. particles


Not cover

- Arbitrary multiple conserved quantities (e.g. particle number)
  Chemical reactions, electric battery, biological systems, ...

- Non-i.i.d. scaling
  Scaling by volume, number of interacting particles
Beyond IID and single quantity

Characterize the optimal performance of QHE with non-i.i.d. finite baths with multiple conserved quantities.
Generalized heat engine

Unitary dynamics of the total system per unit process (not necessarily one stroke)

Battery (work storage)

A-type work extraction

\[ \Delta W_A = \Delta A_W \]
Baths with multiple conserved quantities

- We consider the quantum system $\mathcal{H}_B$ of two baths with two types A and B of conserved quantities (e.g. A stands for the energy and B stands for the particle number)

<table>
<thead>
<tr>
<th>Type A</th>
<th>Type B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bath 1</td>
<td>$X_{1,\lambda} = A_{1,\lambda}$</td>
</tr>
<tr>
<td>Bath 2</td>
<td>$X_{2,\lambda} = A_{2,\lambda}$</td>
</tr>
</tbody>
</table>

Observables of the baths’ Hilbert space depending on the scale parameter $\lambda$

Not needed to mutually commute

Baths can be correlated
Generalized thermal state

• Initial state as the generalized thermal state


\[ \tau_{\theta_0}^{(\lambda)} := \exp \left[ - \sum_{i=1}^{2} (\beta_i A_{i,\lambda} + \gamma_i B_{i,\lambda}) - \phi_\lambda(\theta_0) \right] \]

• Free entropy (Massieu potential) : \( \phi_\lambda(\theta_0) = \log \text{tr} e^{-\sum_{i=1}^{2}(\beta_i A_{i,\lambda} + \gamma_i B_{i,\lambda})} \)

\( \beta_i, \gamma_i \) : generalized inverse temperature conjugate to \( A_{i,\lambda}, B_{i,\lambda} \)

Coordinate expression \( \theta_0 = (\theta_0^1, \theta_0^2, \theta_0^3, \theta_0^4) := (\beta_1, \beta_2, \gamma_1, \gamma_2) \)

Initial inverse temperature
Beyond IID based on asymptotic extensivity

Assume asymptotic extensivity for neighborhood of $\theta_0$:

- **Free entropy**
  $$\phi_\lambda(\theta) = \lambda \phi(\theta) + o(\lambda)$$

- **Asymptotic density**
  Deviation from the extensivity

- **Expectation values**
  $$\eta_{\lambda,i}(\theta) := -\frac{\partial \phi_\lambda}{\partial \theta^i}(\theta) = \text{tr} X_{i,\lambda} \tau_\theta^{(\lambda)} = \lambda \eta_i(\theta) + o(\lambda)$$

- **Canonical correlation**
  $$J_{\lambda,i,j}(\theta) := \frac{\partial^2 \phi_\lambda}{\partial \theta^i \partial \theta^j}(\theta)$$

  $$\quad = \int_0^1 ds \, \text{tr} \left[ \left( \tau_\theta^{(\lambda)} \right)^{1-s} X_{i,\lambda} \left( \tau_\theta^{(\lambda)} \right)^s X_{j,\lambda} \right] - \eta_{\lambda,i}(\theta) \eta_{\lambda,j}(\theta)$$

  $$\quad = \lambda g_{ij}(\theta) + o(\lambda)$$

Asymptotic extensivity is expected from the extensivity in thermodynamics.
Generalized heat engine

We do not fix the protocol of the engine a priori

- Conservation law of each type among the whole system

\[
\Delta A_{1,\lambda} + \Delta A_{2,\lambda} + \Delta A_W = 0
\]
\[
\Delta B_{1,\lambda} + \Delta B_{2,\lambda} + \Delta B_W = 0
\]

Generalized heat

\[
\Delta Q_{A,1} = -\Delta A_{1,\lambda}
\]
\[
\Delta Q_{A,2} = -\Delta A_{2,\lambda}
\]
\[
\Delta Q_{B,1} = -\Delta B_{1,\lambda}
\]
\[
\Delta Q_{B,2} = -\Delta B_{2,\lambda}
\]

- A-type work extraction

\[
\Delta W_A = \Delta Q_{A,1} + \Delta Q_{A,2}
\]

Fundamental bound of the A-type work extraction

In response to generalized heat
Constraint on the reduced dynamics $\Gamma$ on the baths and working body

$\Gamma$ : implicit battery operations as CPTP maps on the systems of the baths and working body

- **Unitalness**
  \[ \Gamma(I_{BC}) = I_{BC} \]

  Increasing of the von Neumann entropy

  Corresponding to the adiabaticity

- **Cyclicity**
  \[ \text{tr}_C \Gamma(\tau^{(\lambda)}_\theta \otimes \rho_C) = \rho_C \]

The unitary operations are of course included
Second law for multiple conserved quantities


• The following follows from the increasing of the von Neumann entropy

\[
\sum_{i=1}^{2} (\beta_i \Delta A_{i,\lambda} + \gamma_i \Delta B_{i,\lambda}) \geq D(\rho'_{\lambda} \| \tau^{(\lambda)}_{\theta_0})
\]

Difference in the expectation value

Relative entropy between the final and initial states

\(=\) difference in the free entropy

\[
\Delta X_{i,\lambda} := \text{tr}(\rho'_{\lambda} - \tau^{(\lambda)}_{\theta_0})X_{i,\lambda}
\]

• \(D(\rho'_{\lambda} \| \tau^{(\lambda)}_{\theta_0}) \geq 0\) implies \(\sum_{i=1}^{2} (\beta_i \Delta A_{i,\lambda} + \gamma_i \Delta B_{i,\lambda}) \geq 0\)

Thermodynamic constraint
Generalized Carnot bound (GCB) without finite-size effects (thermodynamic limit)

- Type A work extraction

\[ \Delta W_A = - (\Delta A_{1, \lambda} + \Delta A_{2, \lambda}) \]

Based on the conservation of the average value

- Generalization of the original Carnot bound

\[ \Delta Q_A \text{ and } \Delta Q_{B,i} \text{ "Generalized heat" are given as } -\Delta A_{2, \lambda} \text{ and } -\Delta B_{i, \lambda} (i = 1, 2) \]

Then,

\[ \sum_{i=1}^{2} (\beta_i \Delta A_{i, \lambda} + \gamma_i \Delta B_{i, \lambda}) \geq 0 \text{ implies} \]

\[ \Delta W_A \leq \left( 1 - \frac{\beta_2}{\beta_1} \right) \Delta Q_{A, 2} - \sum_{i=1}^{2} \frac{\gamma_i}{\beta_1} \Delta Q_{B,i} \]

GCB
Finite-size effects

\[ \sum_{i=1}^{2} (\beta_i \Delta A_{i,\lambda} + \gamma_i \Delta B_{i,\lambda}) \geq 0 \quad \leftrightarrow \quad \Delta W_A \leq \left( 1 - \frac{\beta_2}{\beta_1} \right) \Delta Q_{A,2} - \sum_{i=1}^{2} \frac{\gamma_i}{\beta_1} \Delta Q_{B,i} \]

- The equality is achieved only in thermodynamic limit since

\[ \sum_{i=1}^{2} (\beta_i \Delta A_{i,\lambda} + \gamma_i \Delta B_{i,\lambda}) \geq D\left( \rho_B' \parallel \tau_{\theta_0}^{(\lambda)} \right) > 0 \]

GCB is not tight in finite regime

We should focus on how the relative entropy can be small under the fixed heat amounts in finite regime to incorporate the finite-size effect to GCB
Asymptotic expansion of the entropy

- Legendre transform \( S_\lambda(\eta) := \min_{\tilde{\theta}} \left[ \sum_{i=1}^{4} \tilde{\theta}^i \eta_i + \phi_\lambda(\tilde{\theta}) \right] \)

\[
S(\tau_{\theta'}^{(\lambda)}) - S(\tau_{\theta_0}^{(\lambda)}) \\
= S_\lambda(\eta_\lambda(\theta')) - S_\lambda(\eta_\lambda(\theta_0)) \\
= \sum_{i=1}^{4} \theta_0^i \Delta \eta_{\lambda,i} - \frac{1}{2} \sum_{i,j=1}^{4} J_{\lambda}^{ij}(\theta_0) \Delta \eta_{\lambda,i} \Delta \eta_{\lambda,i} + O\left( \frac{\|\Delta \eta_{\lambda}\|^3}{\lambda^2} \right) \\
= \sum_{i=1}^{4} \theta_0^i \Delta \eta_{\lambda,i} - \frac{1}{2} \sum_{i,j=1}^{4} g_{\lambda}^{ij}(\theta_0) \frac{\Delta \eta_{\lambda,i} \Delta \eta_{\lambda,i}}{\lambda} + o\left( \frac{\|\Delta \eta_{\lambda}\|^2}{\lambda} \right) \\
\geq S(\rho_B') - S(\tau_{\theta_0}^{(\lambda)}) \geq 0, \quad \text{where} \quad \rho_B' := \Gamma(\tau_{\theta_0}^{(\lambda)}) \quad \theta' := \tilde{\theta}_\lambda(\rho_B')
Main result: fine-grained GCB (FGCB)

\[ \Delta W_A \leq \left(1 - \frac{\beta_2}{\beta_1}\right) \Delta Q_{A,2,\lambda} - \sum_{i=1}^{2} \frac{\gamma_i}{\beta_1} \Delta Q_{B,i,\lambda} - C_{AA} \frac{\Delta Q_{A,2,\lambda}^2}{\lambda} - \sum_{i=1}^{2} C_{AB}^i \frac{\Delta Q_{A,2,\lambda} \Delta Q_{B,i,\lambda}}{\lambda} \]

\[ - \sum_{1 \leq i \leq j \leq 2} C_{BB}^{i,j} \frac{\Delta Q_{B,i,\lambda} \Delta Q_{B,j,\lambda}}{\lambda}. \]

Finite-size effect

Universal characterization beyond IID heat bath

\[ C_{AA} = \frac{1}{2} \left[ g_{11}^{(\theta_0)} \beta_2^2 \frac{1}{\beta_1^3} + \frac{g_{22}^{(\theta_0)}}{\beta_1} - 2 g_{12}^{(\theta_0)} \beta_2 \right], \]

\[ C_{AB}^i = \frac{1}{2} \left[ g_{11}^{(\theta_0)} \beta_2 \gamma_i \frac{1}{\beta_1^3} + \frac{g^{2(i+2)}(\theta_0)}{\beta_1} - \frac{g^{1(i+2)}(\theta_0) \beta_2}{\beta_1^2} - \frac{g^{12}(\theta_0) \gamma_i}{\beta_1^2} \right], \]

\[ C_{BB}^{i,j} = \frac{1}{2} \left[ g_{11}^{(\theta_0)} \gamma_i \gamma_j \frac{1}{\beta_1^3} + \frac{g^{(i+2)(j+2)}(\theta_0)}{\beta_1} - \frac{g^{1(i+2)}(\theta_0) \gamma_j}{\beta_1^2} - \frac{g^{1(j+2)}(\theta_0) \gamma_i}{\beta_1^2} \right] \]

\[ g^{i,j}(\theta_0) : \]

Inverse of the canonical correlation matrix
Finite-size effect coefficients

- The coefficients reflect the effects of the fluctuation and correlation of the baths through the canonical correlation.

- Fine structure, the canonical correlation, are relevant in FGCB, differently from GCB, where just the temperatures are relevant.

\[
C_{AA} = \frac{1}{2} \left[ \frac{g^{11}(\theta_0)\beta_2^2}{(\beta_1)^3} + \frac{g^{22}(\theta_0)}{\beta_1} - 2\frac{g^{12}(\theta_0)\beta_2}{\beta_1^2} \right], \quad C_{AB}^i = \frac{1}{2} \left[ \frac{g^{11}(\theta_0)\beta_2\gamma_i}{(\beta_1)^3} + \frac{g^{2(i+2)}(\theta_0)}{\beta_1} - \frac{g^{1(i+2)}(\theta_0)\beta_2}{\beta_1^2} - \frac{g^{12}(\theta_0)\gamma_i}{\beta_1^2} \right],
\]

\[
C_{BB}^{ij} = \frac{1}{2} \left[ \frac{g^{11}(\theta_0)\gamma_i\gamma_j}{(\beta_1)^3} + \frac{g^{(i+2)(j+2)}(\theta_0)}{\beta_1} - \frac{g^{1(i+2)}(\theta_0)\gamma_j}{\beta_1^2} - \frac{g^{1(j+2)}(\theta_0)\gamma_i}{\beta_1^2} \right],
\]

Inverse of the canonical correlation:

\[
g^{ij}(\theta_0) := \frac{\text{tr} \left[ \left( \tau^{(\lambda)}_{\theta} \right)^{1-s} X_{i,\lambda} \left( \tau^{(\lambda)}_{\theta} \right)^s X_{j,\lambda} \right] - \eta_{\lambda,i}(\theta)\eta_{\lambda,j}(\theta)}{\lambda} \rightarrow g_{i,j}(\theta_0)
\]

**Correlation between two quantities reflecting non-commutativity (even between different baths):**

- The coefficients reflect the effects of the fluctuation and correlation of the baths through the canonical correlation.

- Fine structure, the canonical correlation, are relevant in FGCB, differently from GCB, where just the temperatures are relevant.
To show that FGCB is really achievable in physical sense

• We should verify
  ✓ Existence of the battery
  ✓ That no hidden heat source is cheatingly included in the battery

• Unitalness is just a necessary condition on the reduced dynamics on the baths to be allowed

Explicitly construct the unitary operation on the whole system
Battery system

- Corresponding Type A and B quantities are given by

\[ A_W = c_a \hat{x}_a, \quad B_W = c_b \hat{x}_b \]

The coefficient gives the correct unit of each quantity

- Shift operators

\[ \Delta^\epsilon_A := \exp(-i\epsilon \hat{p}_a) \quad \Delta^\epsilon_B := \exp(-i\epsilon \hat{p}_b) \]

Doubly infinite spectrum

Neglecting the length of the string suspending the weight in thermodynamics
Just focus on the finiteness of the baths
Commutative case

Constraints (*) on the allowed operations for commutative case

Only global unitary operation $\mathbf{U}$ satisfying the following is allowed

- **Strict conservation law** (not only average conservation)

\[
\left[ \sum_{j=1}^{2} A_{j,\lambda} + A_{W,\lambda} \right] = 0
\]

- **Cyclicity**

\[
\text{tr}_{BW} \mathbf{U} (\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_{W,1})\mathbf{U}^\dagger = \rho_C
\]

- **Do not use the battery as a resource**


- **No cheating condition**

  - Independence of the initial state of the battery

\[
\text{tr}_W \mathbf{U} (\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_{W,2})\mathbf{U}^\dagger = \text{tr}_W \mathbf{U} (\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_{W,1})\mathbf{U}^\dagger
\]

  - **Shift invariance**

\[
[\Delta^\epsilon_A, \mathbf{U}] = [\Delta^\epsilon_B, \mathbf{U}] = 0
\]
Ideal final state

The thermal state at the ideal inverse temperature $\theta_\lambda$ defined by the following conditions attains the FGCB

$$S(\tau^{(\lambda)}_{\theta_\lambda}) = S(\tau^{(\lambda)}_{\theta_0})$$

$$\beta_\lambda \beta_1 \geq 0$$

$$\text{tr} \ A_{2,\lambda}(\tau^{(\lambda)}_{\theta_0} - \tau^{(\lambda)}_{\theta_\lambda}) = \Delta Q_{A,2,\lambda}$$

$$\text{tr} \ B_{i,\lambda}(\tau^{(\lambda)}_{\theta_0} - \tau^{(\lambda)}_{\theta_\lambda}) = \Delta Q_{B,i,\lambda} \quad (i = 1, 2)$$

• However, such a thermal state is generally not achievable by an allowed operation

We instead construct a protocol to achieve ‘nearly’ this ideal final state $\tau^{(\lambda)}_{\theta_\lambda}$
Commumative case

Protocol

- We label the simultaneous eigenstates of all the conserved quantities via the diagonalization depending on $\theta, \lambda$

$$\tau^{(\lambda)}_{\theta} =: \sum_{i} p^{(\lambda)}_{\theta}(i) \langle \omega_{i}^{\theta, \lambda} | \omega_{i}^{\theta, \lambda} \rangle$$

so that

$$p^{(\lambda)}_{\theta}(1) \geq p^{(\lambda)}_{\theta}(2) \geq \ldots$$

- Map the eigenbasis based on the relabeling

$$\theta_{0} \rightarrow \theta_{\lambda}$$
Commutative case

Realization by a unitary satisfying the conditions (*)

- This protocol is achieved by the following unitary operation

\[ U_{\text{opt}} := \sum_i \left| \omega_i^{\theta_0,\lambda} \right\rangle \left\langle \omega_i^{\theta_0,\lambda} \right| \]

\[ \otimes \Delta_{A}^{c_i^{-1}}(a_1, \lambda (\omega_i^{\theta_0,\lambda}) + a_2, \lambda (\omega_i^{\theta_0,\lambda}) - a_1, \lambda (\omega_i^{\theta_0,\lambda}) - a_2, \lambda (\omega_i^{\theta_0,\lambda})) \]

\[ \otimes \Delta_{B}^{c_i^{-1}}(b_1, \lambda (\omega_i^{\theta_0,\lambda}) + b_2, \lambda (\omega_i^{\theta_0,\lambda}) - b_1, \lambda (\omega_i^{\theta_0,\lambda}) - b_2, \lambda (\omega_i^{\theta_0,\lambda})) \]

Indeed,

\[ \text{tr}_W U_{\text{opt}}(\tau_{\theta_0}^{(\lambda)} \otimes \rho_W) U_{\text{opt}}^\dagger = \rho_{\text{opt}}^{(\lambda)} \]

- Regardless of the state of the battery
- Shift invariant
- Satisfies strict conservation
- The dynamics on the working body is just the identity – no catalytic effect
Asymptotic optimality: evaluation of closeness

- $\tau_{\theta_{\lambda}}^{(\lambda)}$ attains the optimal performance

If the expectation values of $\rho_{\text{opt}}^{(\lambda)}$ is sufficiently close to those of $\tau_{\theta_{\lambda}}^{(\lambda)}$

$\rho_{\text{opt}}^{(\lambda)}$ attains asymptotic optimal performance
Asymptotic optimality: evaluation of closeness

\[ \xi_\lambda = \tilde{\theta}_\lambda (\rho_{\text{opt}}^{(\lambda)}) \]

Effective temperature

Related to the expectation values

**Information geometry: Pythagorean theorem**

\[ D(\rho_{\text{opt}}^{(\lambda)} \| \tau_{\theta_\lambda}^{(\lambda)}) = D(\rho_{\text{opt}}^{(\lambda)} \| \tau_{\xi_\lambda}^{(\lambda)}) + D(\tau_{\xi_\lambda}^{(\lambda)} \| \tau_{\theta_\lambda}^{(\lambda)}) \geq D(\tau_{\xi_\lambda}^{(\lambda)} \| \tau_{\theta_\lambda}^{(\lambda)}) \]
Asymptotic optimality: evaluation of closeness

Our unitary operation indeed achieves the equality in FGCB

• \(2D(\tau^{(\lambda)}_{\hat{\xi}_\lambda} \| \tau^{(\lambda)}_{\theta_\lambda}) \max_{t \in [0,1]} \| (J_{\lambda,i,j}(s(t)))_{ij} \| \)

\(\geq \| \eta_{\lambda}(\theta_\lambda) - \eta_{\lambda}(\xi_\lambda) \|^2\)

• Pythagorean theorem

\(D(\rho^{(\lambda)}_{\text{opt}} \| \tau^{(\lambda)}_{\theta_\lambda}) = D(\rho^{(\lambda)}_{\text{opt}} \| \tau^{(\lambda)}_{\hat{\xi}_\lambda}) + D(\tau^{(\lambda)}_{\hat{\xi}_\lambda} \| \tau^{(\lambda)}_{\theta_\lambda}) \)

\(\geq D(\tau^{(\lambda)}_{\hat{\xi}_\lambda} \| \tau^{(\lambda)}_{\theta_\lambda}) \)

The relation between difference in the average and the relative entropy & Fisher information

Reduction to the estimation of the relative entropy and Fisher information
Extension of CLT to asymptotic extensive case

Theorem:

Let \((X_\lambda)_{\lambda \in \mathbb{R}_+}\) be a family of random variables with each finite sample space \(\Omega_\lambda\). If the cumulant generating functions \(\psi_\lambda(t) := \mathbb{E}[e^{tX_\lambda}]\) of \(X_\lambda\) satisfy the asymptotic extensivity \(\psi_\lambda(t) = \lambda \psi(t) + o(\lambda)\ (\lambda \to \infty)\) pointwise on some interval including 0, then we have

\[
\sup_x |F_\lambda(x) - \mathcal{N}(x)| = O(\lambda^{-\frac{1}{2}}) \quad (\lambda \to \infty),
\]

where \(F_\lambda\) and \(\mathcal{N}\) are the cumulative distribution functions of normalized \(X_\lambda\) and the standard Gaussian distribution.

• This theorem makes IID-like asymptotic analysis possible for our asymptotic extensive case
Evaluation of the relative entropy

Our unitary operation indeed achieves the equality in FGCB

• By definition,\[ D(\rho_{\text{opt}}^{(\lambda)} \| \tau_{\theta_{\lambda}}^{(\lambda)}) = \sum_j p_{\theta_0}^{(\lambda)}(j)(\log p_{\theta_0}^{(\lambda)}(j) - \log p_{\theta_{\lambda}}^{(\lambda)}(j)) \]

Problem is reduced to the analysis of classical probabilities

• Applying the strong large deviation by making use of the extension of CLT


In a similar method as in


\[ D(\rho_{\text{opt}}^{(\lambda)} \| \tau_{\theta_{\lambda}}^{(\lambda)}) = O\left(\frac{\|Q_{\lambda}\|^2}{\lambda^2}\right) + O(\lambda^{-\frac{1}{2}}) \]
FGCB is tight in the asymptotic sense

- This protocol satisfies

\[ \text{tr } X_i,\lambda \rho^{(\lambda)}_{\text{opt}} = \text{tr } X_i,\lambda \tau^{(\lambda)}_{\theta_\lambda} + o \left( \frac{||Q_\lambda||^2}{\lambda} \right) \]

\[ i = 1, 2, 3, 4 \]

- Expectation values are asymptotically the same as those of the ideal final state

- Ideal final state attains the FGCB

FGCB is asymptotically achieved by our constructed protocol
Example 1: Ising spin chain as the baths one type quantity (energy) with non-i.i.d.

- Hamiltonian
  \[ H_{n}^{(b)} = -J_{b} \left( \sum_{i=1}^{n-1} \hat{s}_{i}^{(b)} \hat{s}_{i+1}^{(b)} + \hat{s}_{n}^{(b)} \hat{s}_{1}^{(b)} \right), \quad (b = \hbar, c) \]

- Scale: The number \( n \) of the spins

- Type A: energy, Type B: none

- Asymptotic extensivity
  \[ \phi_{n}(\beta_{\hbar}, \beta_{c}) = n(\log[2 \cosh \beta_{\hbar}J_{\hbar}] + \log[2 \cosh \beta_{c}J_{c}]) + o(1) \]

\( \beta_{\hbar}, \beta_{c} \) Inverse temperatures

Applicable
Example 1: Ising spin chain as the baths

\[
\Delta W \leq \left(1 - \frac{\beta_h}{\beta_c}\right) \Delta Q_{h,\lambda} - C \frac{\Delta Q_{h,\lambda}^2}{\lambda} + \mathcal{O}\left(\frac{\Delta Q_{h,\lambda}^3}{\lambda^2}\right).
\]

\[
C = \frac{\beta_h^2 \cosh^2 \beta_c J_c}{2\beta_c^3 J_c^2} + \frac{\cosh^2 \beta_h J_h}{2\beta_c J_h^2}
\]

- For fixed rate of inverse temperatures, it takes minimum when
  \[
  2\beta_b J_b \sinh 2\beta_b J_b - \cosh 2\beta_b J_b - 1 = 0 \quad (b = c, h)
  \]
  holds.
- Symmetric with respect to the sign of the coupling constants
Example 2: Free fermions inside the 1D-well potential

- The heat engine with particle transport
- We use ideal gas composed of free fermions inside the 1D-well potential as the baths

Baths are in the grand canonical state
Example 2:
Free fermions inside the 1D-well potential

\[ \phi_\lambda(\beta, \mu) = \int_0^\infty \frac{\lambda \sqrt{2m}}{2\pi \hbar} \epsilon^{-\frac{1}{2}} \log(1 + e^{\beta \mu - \beta \epsilon}) d\epsilon + O(1) \]

\[ = \lambda \phi(\beta, \mu) + O(1) \]
Example 2: Free fermions inside the 1D-well potential

- FGCB

$$\Delta W \leq \left(1 - \frac{\beta_h}{\beta_c}\right) \Delta Q_\lambda + \mu_c \Delta N_{c,\lambda} + \frac{\beta_h}{\beta_c} \mu_h \Delta N_{h,\lambda}$$

$$- C_{HH} \frac{\beta_h^2}{\beta_c} \frac{\Delta Q_\lambda^2}{\lambda} - \sum_{b=c,h} C_{NN}^{b,b} \frac{\beta_b^2}{\beta_c} \frac{\Delta N_{b,\lambda}}{\lambda} - C_{NN}^{c,h} \frac{\beta_h \mu_h \mu_c}{\beta_c} \frac{\Delta N_{c,\lambda} \Delta N_{h,\lambda}}{\lambda} - \sum_{b=c,h} C_{HN}^{b} \frac{\beta_h \beta_b \mu_b}{\beta_c} \frac{\Delta Q_\lambda \Delta N_{b,\lambda}}{\lambda}$$

$$+ o \left( \frac{\Delta Q_\lambda^2 + \Delta N_{c,\lambda}^2 + \Delta N_{h,\lambda}^2}{\lambda} \right)$$

- Coefficients $C^{**} \propto \hbar / \sqrt{m}$ Explicitly dependence on the mass
Appearance of Planck constant

Heavier particle has better optimal performance
Conclusion

✓ Generic non-i.i.d. scaling of heat baths based on the asymptotic extensivity
✓ Universal characterization of optimal performance of QHE with multiple conserved quantities beyond IID regime
  : **Fine-grained generalized Carnot bound**
✓ Finite-size effect is characterized not only by the temperatures but also correlations between the quantities
✓ General protocol to achieve FGCB
✓ Some examples show finer structure of the optimal performance with finite-size baths
Thank you for your attention!
Assumption: Order of the heat

We consider the case when generalized heat $Q_\lambda := (\Delta Q_{A,2,\lambda}, \Delta Q_{B,1,\lambda}, \Delta Q_{B,2,\lambda})$ satisfies $\Delta Q_{A,2,\lambda} = o(\lambda), \Delta Q_{B,i,\lambda} = o(\lambda)$

- The final temperature (in terms of the effective inverse temperature) converges to the initial inverse temperature in thermodynamic limit
- The baths converges to infinite baths in thermodynamic limit
- The baths are used just as the ‘baths’ in thermodynamic sense

Final temperature in terms of the effective inverse temperature $\tilde{\theta}_\lambda(\rho)$ for a generic state $\rho$

\[
\begin{align*}
\text{tr } A_{i,\lambda} \tau_{\tilde{\theta}_\lambda(\rho)}^{(\lambda)} &= \text{tr } A_{i,\lambda} \rho \\
\text{tr } B_{i,\lambda} \tau_{\tilde{\theta}_\lambda(\rho)}^{(\lambda)} &= \text{tr } B_{i,\lambda} \rho \quad (i = 1, 2)
\end{align*}
\]
Non-Commutative case

Conditions (*) on the allowed operations for non-commutative case

Only global unitary operation $U$ satisfying the following is allowed

With the same battery system

• Just average conservation law

$$\text{tr} \left( U (\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W) U^\dagger \right) \left( \sum_{j=1}^{2} A_{j,\lambda} + A_W \right) = \text{tr} \left( \tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W \right) \left( \sum_{j=1}^{2} A_{j,\lambda} + A_W \right),$$

$$\text{tr} \left( U (\tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W) U^\dagger \right) \left( \sum_{j=1}^{2} B_{j,\lambda} + B_W \right) = \text{tr} \left( \tau_{\theta_0}^{(\lambda)} \otimes \rho_C \otimes \rho_W \right) \left( \sum_{j=1}^{2} B_{j,\lambda} + B_W \right).$$

• The others are the same
Construction of the protocol

• Diagonalization (not simultaneous)

\[ \tau^{(\lambda)}_{\theta_0} = \sum_i p^{(\lambda)}_{\theta_0}(i) |\psi_i\rangle\langle\psi_i| \]

\[ \tau^{(\lambda)}_{\theta_\lambda} = \sum_i p^{(\lambda)}_{\theta_\lambda}(i) |\varphi_i\rangle\langle\varphi_i| \]

• Protocol

\[ U_{\text{opt}} := \sum_i |\varphi_i\rangle\langle\psi_i| \]

\[ \bigotimes A \Delta^{-1}_a \left( \langle\psi_i| \sum_{l=1}^2 A_{l,\lambda}\psi_i \rangle - \langle\varphi_i| \sum_{l=1}^2 A_{l,\lambda}\varphi_i \rangle \right) \]

\[ \bigotimes B \Delta^{-1}_b \left( \langle\psi_i| \sum_{l=1}^2 B_{l,\lambda}\psi_i \rangle - \langle\varphi_i| \sum_{l=1}^2 B_{l,\lambda}\varphi_i \rangle \right) \]

This unitary satisfies the conditions for non-commutative case, though fails to satisfy the strict conservation.
Implicit- vs Explicit-battery formulation

There are two ways to treat the battery system and the dynamics:

- **Implicit-battery formulation:**
  - Focus on the baths and working body
  - Similar as the macroscopic thermodynamics

- **Explicit-battery formulation:**
  - Focus on the total system including the battery
Implicit-battery formulation:

- Focus on the quantum system composed of the baths and working body
- Macroscopic thermodynamics

We employ it in derivation of the upper bound on the performance for wide applicability

Explicit-battery formulation:

- Focus on the total system including the battery
Implicit-battery formulation:
- Focus on the quantum system composed of the baths and working body
- Macroscopic thermodynamics

Explicit-battery formulation:
- Focus on the total system including the battery

We finally fix an explicit battery to verify the achievability of the optimal performance truly as work-like extraction
Example 3: A Toy model of two level system bath

two types of quantities, i.i.d. scaling

• We consider just one bath with the Hamiltonian

\[ H = \hbar \omega \sigma_z \]

\[ \sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1| \]

• Suppose that the other non-commutative conserved quantity (for global dynamics not just for the bath)

\[ \sigma_\theta = \cos \theta (|0\rangle\langle 0| - |1\rangle\langle 1|) + \sin \theta (|0\rangle\langle 1| + |1\rangle\langle 0|) \]

exists

• Assume that the initial state of the bath is

\[ \tau_{\beta,\gamma}^{(n)} = \left( \frac{e^{-\beta H - \gamma \sigma_\theta}}{Z} \right)^\otimes n \]

Scale: \( n \) with corresponding generalized inverse temperature \( \gamma \)
Example 3: A Toy model of two level system bath

- Asymptotic extensivity is trivial

FGCB: \[ \Delta W_n \leq -\frac{\gamma}{\beta} \Delta Q_{\sigma, n} - C(\beta, \gamma, \omega, \theta) \frac{(\Delta Q_{\sigma, n})^2}{n} + O \left( \frac{(\Delta Q_{\sigma, n})^3}{n^2} \right) \]

\( \Delta Q_{\sigma, n} \) : Generalized heat of \( \sigma \theta \)

\[ C(\beta, \gamma, \omega, \theta) = \frac{\left( (\beta \hbar \omega)^2 + \gamma^2 + 2\gamma \beta \hbar \omega \cos \theta \right)^{\frac{3}{2}}}{2\beta^3 (\hbar \omega)^2 \sin^2 \theta \tanh \sqrt{(\beta \hbar \omega)^2 + \gamma^2 + 2\gamma \beta \hbar \omega \cos \theta}} \]
Example 3: A Toy model of two level system bath

- We should fix $\eta = \gamma / \beta$ to see the minimization of the second order

$$C(\beta, \omega, \theta; \eta) := C(\beta, \beta \eta, \omega, \theta) = \frac{((\hbar \omega)^2 + \eta^2 + 2\hbar \omega \eta \cos \theta)^{\frac{3}{2}}}{2(\hbar \omega)^2 \sin^2 \theta \tanh \left( \beta \sqrt{(\hbar \omega)^2 + \eta^2 + 2\hbar \omega \eta \cos \theta} \right)}$$

FIG. The graph of $C(\beta, \omega, \frac{\pi}{2}; \eta)$ at $T = 1K$, and $\eta = 1J$ as a function of $\omega$. It takes its minimum at $\hbar \omega \approx \sqrt{2J} = \sqrt{2} \eta$.

FIG. The graph of $C(\beta, \omega, \theta; \eta)$ at $T = 1K$, and $\eta = 1J$ with $\hbar \omega = 10J$ (blue) and $\hbar \omega = \sqrt{2}J$ (red).