Measurement-based Formulation of Quantum Heat Engine and Optimal Efficiency with Finite-Size Effect

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http://arxiv.org/abs/1504.06150
1st part: Measurement-based Formulation of Quantum Heat Engine

- Two scenarios for work extraction from quantum system
- CP-work extraction
- FQ-work extraction
- Trade-off relation for semi-classical model
- How to resolve the problem: Shift-invariant model
- Classical model
Work extraction
Extracting energy from thermal energy in a bath system as a dynamical energy to an outer system.

However, there are several formulations for quantum mechanical work extraction.

Two scenarios for work extraction from quantum system

**Semi-Classical scenario**

I: Baths and heat engine

\[ U_I = \exp[-i \int_0^\tau \hat{H}_I(t) dt] \]

\[ W := \text{Tr}[\rho_I \hat{H}_I(0) - U_I \rho_I U_I^\dagger \hat{H}_I(\tau)] \]


**Full-Quantum(FQ) scenario**

E: work storage

\[ [U, \hat{H}_I + \hat{H}_E] = 0 \]

\[ W := \text{Tr}[\Lambda_E(\rho_E) \hat{H}_E - \rho_E \hat{H}_E] \]


CP-work extraction

\[
\{ \mathcal{E}_j \}_j : CP\text{-map valued measure}
\]

\[
\{ \mathcal{E}_j, w_j \}_j : CP\text{-work extraction}
\]

\[ w_j \] Amount of extracted work

\[ \rho_I \rightarrow \text{Work extraction device} \rightarrow \mathcal{E}_j (\rho_I) / \text{Tr} \mathcal{E}_j (\rho_I) \]

Initial state

Final state with probability \( \text{Tr} \mathcal{E}_j (\rho_I) \)

Energy conservation law:

\[
\mathcal{E}_j (\langle x | x \rangle) = P_{h_x - w_j} \mathcal{E}_j (\langle x | x \rangle) P_{h_x - w_j}
\]

\[ |x\rangle : \text{Energy eigenstate with eigenvalue } h_x \]

\[ \hat{H} = \sum_h hP_h \] Spectral decomposition of Hamiltonian

Unital condition: \( \sum_j \mathcal{E}_j (I) = I \)
FQ-work extraction with measurement

Initial state

Internal system $\rho_I$ \rightarrow Work extraction Device (unitary $U$) \rightarrow Final state $\rho_I' \rightarrow \rho_{I|H=h}'$

External system \( \rho_E \rightarrow \rho_E' \rightarrow \rho_{E|H=h}' \)

Correlated state

Energy conservation law:

$$[U, \hat{H}_I + \hat{H}_E] = 0$$

Unitary $U$ + Measurement + eigenstate $\rho_E$ Amount of extracted work $w_h := h - \text{Tr} \rho_E \hat{H}_E$

$$\mathcal{E}_h(\rho_I) := \text{Tr}_E U(\rho_I \otimes \rho_E)U^\dagger P_h$$

$$\{\mathcal{E}_h, w_h\}_h : \text{CP-work extraction}$$
FQ-work extraction with measurement

Initial state

Internal system $\rho_I$ → Work extraction Device (unitary $U$) → Final state $\rho_I' \rightarrow \rho_I|H=h'\rangle$

External system (work storage) $\rho_E$ $\otimes$ $\rho_E'$

Correlated state

Energy conservation law:

$$[U, \hat{H}_I + \hat{H}_E] = 0$$

Unitary $U$ + Measurement + eigenstate

$\exists \rho_E$ Amount of extracted work

$w_h := h - \text{Tr} \rho_E \hat{H}_E$

$E_h(\rho_I) := \text{Tr}_E U(\rho_I \otimes \rho_E)U^\dagger P_h$

$\forall \{E_h, w_h\}_h : CP$-work extraction
Inconsistency between two scenarios

If two scenarios are equivalent as follows:

\[ \rho_I U_I U_I \rho_I U_I^\dagger = \Lambda_I(\rho_I) \]

Relation \[ U = U_I \otimes U_E \] holds.

\[ \Rightarrow \text{Internal and External systems are evolved independently.} \]
\[ \Rightarrow \text{No energy is transferred.} \]
Approximation?

\[ \rho_I \xrightarrow{U_I} U_I \rho_I U_I^\dagger \approx \rho_I \xrightarrow{\Lambda_I(\rho_I)} U \]

Semi-classical scenario

\[ \otimes \]

\[ \rho_E \rightarrow \rho'_E \]

Fully quantum(FQ) scenario

To realize this approximation,

[1] Unitary \( U \) needs to conserve the energy in the total system \( IE \).

[2] Time evolution \( \Lambda_I \) needs to approximate unitary \( U \).

[3] It is required to estimate the amount of extracted work based on the measurement for the external system.

Our result:

Conditions [2] and [3] are not compatible even approximately.
Trade-off relation 1/2

\[ U \otimes \rho_E \xrightarrow{\Lambda_I(\rho_I)} \rho_E' \]
Trade-off relation 1/2

\[ |\Psi_{IR}\rangle: \text{purification of } \rho_I \]
\[ \text{Tr}_R[|\Psi_{IR}\rangle\langle\Psi_{IR}|] = \text{Tr}_I[|\Psi_{IR}\rangle\langle\Psi_{IR}|] = \rho_I \]

\( R: \text{Reference system, which preserves initial state of } I. \)
Trade-off relation 1/2

\[ |\Psi_{IR}\rangle \otimes \rho_E \xrightarrow{U} \Lambda_{I}(\rho_I) \]

\[ |\Psi_{IR}\rangle : \text{purification of } \rho_I \]

\[ \text{Tr}_R[|\Psi_{IR}\rangle \langle \Psi_{IR}|] = \text{Tr}_I[|\Psi_{IR}\rangle \langle \Psi_{IR}|] = \rho_I \]

\( R: \text{Reference system, which preserves initial state of } I. \)
Trade-off relation 1/2

\begin{equation}
\hat{H}_R - \hat{H}_I = \sum_z z F_z
\end{equation}

\[\begin{array}{c}
\rho_I \\
\otimes
\rho_E
\end{array}\rightarrow U \rightarrow \Lambda_I(\rho_I) \rightarrow
\begin{array}{c}
\rho_I \\
\otimes
\rho_E
\end{array}\rightarrow U \rightarrow \rho_E'

\begin{array}{c}
|\Psi_{IR}\rangle
\end{array}
:purification of \rho_I

\begin{align}
\text{Tr}_R[|\Psi_{IR}\rangle\langle\Psi_{IR}|] &= \text{Tr}_I[|\Psi_{IR}\rangle\langle\Psi_{IR}|] = \rho_I
\end{align}

R:Reference system, which preserves initial state of I.
Trade-off relation 1/2

\[ |\Psi_{IR}\rangle \otimes \rho_E \xrightarrow{U} \{F_z\} \]  
\[ \hat{H}_R - \hat{H}_I = \sum_z zF_z \]  
\[ P_z(z) : \text{work distribution} \]

\[ \rho_I \otimes \rho_E \xrightarrow{U} \Lambda_I(\rho_I) \]

\[ |\Psi_{IR}\rangle : \text{purification of } \rho_I \]
\[ \text{Tr}_R[|\Psi_{IR}\rangle \langle \Psi_{IR}|] = \text{Tr}_I[|\Psi_{IR}\rangle \langle \Psi_{IR}|] = \rho_I \]

*R*: Reference system, which preserves initial state of *I.*
Trade-off relation 1/2

\[ \hat{H}_R - \hat{H}_I = \sum_z zF_z \]

\[ \rho'' = \sum_z P_z(z) |z\rangle\langle z| \otimes \rho_{E|Z=z} \]

\[ \rho_I \]

\[ \rho_E \]

\[ \rho_I \]

\[ \Lambda_I(\rho_I) \]

\[ \Psi_{IR} \rangle \text{: purification of } \rho_I \]

\[ \text{Tr}_R[|\Psi_{IR}\rangle\langle\Psi_{IR}|] = \text{Tr}_I[|\Psi_{IR}\rangle\langle\Psi_{IR}|] = \rho_I \]

R: Reference system, which preserves initial state of I.
Trade-off relation 1/2

\[ \begin{align*} 
\hat{H}_R - \hat{H}_I &= \sum_z z F_z \\
\rho'' &= \sum_z P_z(z) |z\rangle \langle z| \otimes \rho_{E|Z=Z} \\
I_{\rho''}(Z; E) &= \text{Correlation between E and amount of extracted work} \\
\end{align*} \]

\[ \Psi_{IR} \] : purification of \( \rho_I \)

\[ \text{Tr}_R[|\Psi_{IR}\rangle \langle \Psi_{IR}|] = \text{Tr}_I[|\Psi_{IR}\rangle \langle \Psi_{IR}|] = \rho_I \]

\( R \) : Reference system, which preserves initial state of \( I \).
Trade-off relation 2/2

Time evolution of internal system is close to a unitary evolution.

⇒ It is impossible to read out the amount of extracted work!

\[
S_e (\Lambda, \rho_I) + \Delta I_{\rho''} (Z; E) \geq S(P_Z)
\]

\[
S_e (\Lambda, \rho_I) := S(\Lambda\left(\left\vert \Psi_{IR}\right\rangle\left\langle \Psi_{IR}\right\vert\right))
\]

\[
\Delta I_{\rho''} (Z; E) := S(P_Z) - I_{\rho''} (Z; E)
\]

Imperfectness of information gain

Demolition of coherence

Correlation between E and amount of extracted work
How to resolve the problem:

**Shift-invariant model**

\[ \{ |x\rangle \} : \text{CONS of internal system} \quad \hat{H}_I = \sum_x h_x |x\rangle\langle x| \]

\[ \{ |y\rangle \} : \text{CONS of external system} \quad \hat{H}_E = \sum_y y |y\rangle\langle y| \]

Unitary \( U \) on composite system is *shift invariant*

\[
\langle y + l | U | y \rangle = \langle y' + l | U | y' \rangle \quad \forall y', \forall y
\]

\[
U_I = \sum_{x,x'} u^{x'}_x |x\rangle\langle x'| : \text{Internal unitary}
\]

One-to-one

\[
F[U_I] = \sum_{y,x,x'} u^{x'}_x |x\rangle\langle x'| \otimes |y + h_x, -h_x\rangle\langle y|
\]

: Shift-invariant and energy-conservative unitary

This unitary generates unital CP-work extraction.
Classical work extraction (Jarzynski)

\( X, h \) : Classical system with Hamiltonian

**Deterministic case**

\[ h(x) - h(f(x)) : \text{Amount of extracted work} \]

\[ x \rightarrow \text{Work extraction device} \rightarrow f(x) \]

Initial state \( f \) Final state

**Probabilistic case**

\( P_{X|X'}(x | x') \) : Probability transition matrix

\( P_{X'}(x') \) : Input distribution

Average amount of extracted work

\[ \sum_{x,x'} (h(x') - h(x)) P_{X|X'}(x | x') P_{X'}(x') \]

**Bi-stochastic case**

\[ P_{X|X'}(x | x') = \sum_f P_F(f) \delta_{x,f(x')} \]
Relation between Classical and CP work extraction

\[ \rho_I = \sum_x P_{x'}(x') |x'\rangle\langle x'|, \quad \hat{H}_I = \sum_x h(x) |x\rangle\langle x| \]

\( \{\mathcal{E}_j, w_j\}_j : \) Unital and energy conservative CP-work extraction

Bi-stochastic Probability transition matrix

\[ P_{x|x'}(x | x') = \langle x | \sum_j \mathcal{E}_j (| x'\rangle\langle x'|) | x \rangle \]

Average of amount of extracted work

\[ \sum_{x,x'} (h(x') - h(x)) P_{x|x'}(x | x') P_{x'}(x') \]

\[ = \sum_j w_j \text{Tr} \mathcal{E}_j (\rho_I) \]
Relation between Classical and CP work extraction

\[ \rho_I = \sum_{x'} P_{x'}(x') |x'\rangle\langle x'|, \quad \hat{H}_I = \sum_{x} h(x) |x\rangle\langle x| \]

\[ \exists \{ \mathcal{E}_j, w_j \}_j : \text{Unital and energy conservative CP-work extraction} \]

Bi-stochastic Probability transition matrix

\[ \forall P_{x|x'}(x|x') \overset{s.t.}{=} \langle x | \sum_j \mathcal{E}_j (|x\rangle\langle x'|) |x\rangle \]

It is enough to optimize the performance among classical work extractions, bi-stochastic transition matrices.
History of semi-classical model


Classical work extraction model


Semi-classical work extraction model


Work distribution

2014 Batalhão *etal.* *Phys. Rev. Lett.* **113**, 140601

Experimental reconstruction of work distribution

However, this experiment does not extract work!
Summary: 1\textsuperscript{st} part

- We have formulated work extraction process as a measuring process in two different ways (CP and FQ work extractions).
- We have derived a trade-off relation for the coherence and information acquisition for amount of work extraction.
- We also have clarified the relationships among the fully quantum work extraction, the CP-work extraction.

These results have the following meanings.

- The incompatibility of the coherence of the internal system and information acquisition for the amount of extracted work.
- The reduction of analysis for quantum work extraction to the classical model.
2\textsuperscript{nd} part:
Optimal Efficiency with Finite-Size Effect

- Setup: Heat Engine with two heat baths
- Optimal Efficiency
- Our optimal operation
- Summary
- Appendix: Derivation
Set up with CP-work extraction

Based on the measurement-based formulation, we give the set up for the quantum heat engines with finite-size heat baths.

We assume the baths are in Gibbs states:

$$\rho_I = (Ce^{-\beta_1 \hat{H}_1} \otimes e^{-\beta_2 \hat{H}_2})^\otimes n$$
Set up with FQ-work extraction

- Hot bath with n particles
- Cold bath with n particles
- Work storage
- Energy
  - Conservative
  - Unitary
  - Evolution on Total System

- Hot bath with n particles
- Cold bath with n particles
- Work storage
- Measurement of Hamiltonian

\( h \)
Contents

• Setup: Heat Engine with two heat baths
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Efficiency

We consider thermal states on two heat baths.

\[ \rho_I = (Ce^{-\beta_1 \hat{H}_1} \otimes e^{-\beta_2 \hat{H}_2})^\otimes n \]

Hot bath’s Hamiltonian
Cold bath’s Hamiltonian

We define the efficiency of the CP-work extraction:

\[ \eta(\{\mathcal{E}_j, w_j\}) = \frac{W(\{\mathcal{E}_j, w_j\})}{Q(\{\mathcal{E}_j, w_j\})} \]

Average amount of extracted work

\[ W(\{\mathcal{E}_j, w_j\}) := \sum_j w_j \text{Tr}\mathcal{E}_j(\rho_I) \]

\[ = \text{Tr}(\hat{H}_1^{(n)} + \hat{H}_2^{(n)})(\rho_I - \sum_j \mathcal{E}_j(\rho_I)) \]

Endothermic energy amount

\[ Q(\{\mathcal{E}_j, w_j\}) := \text{Tr}\hat{H}_1^{(n)}(\rho_I - \sum_j \mathcal{E}_j(\rho_I)) \]
Optimal efficiency

\[ \max_{\{E_j, w_j\}: Q(\{E_j, w_j\}) = Q_n} \eta(\{E_j, w_j\}) \]

\[ = 1 - \frac{\beta_1}{\beta_2} - C_1 \frac{Q_n}{n} - C_2 \left(\frac{Q_n}{n}\right)^2 + O\left(\frac{Q_n}{n^2}\right) \]

\[ C_1 := \left( \frac{1}{2 \beta_1^2 \sigma_1^2} + \frac{1}{2 \beta_2^2 \sigma_2^2} \right) \frac{\beta_1^2}{\beta_2} \]

\[ C_2 := \left( -\frac{\gamma_1}{6 \beta_1^3 \sigma_1^3} + \frac{\gamma_2}{6 \beta_2^3 \sigma_2^3} + \frac{1}{2 \beta_2^4 \sigma_2^4} + \frac{1}{2 \beta_1^2 \beta_2^2 \sigma_1^2 \sigma_2^2} \right) \frac{\beta_1^3}{\beta_2} \]

\[ \sigma_i : \text{energy variance} \]

\[ \gamma_i : \text{Skewness of energy (3}^{\text{rd}} \text{cumulant)} \]
Finite-size effect of heat baths decrease the optimal efficiency!
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optimal work extraction (Outline)

Our optimal work extraction consists of three steps. See the schematic diagram in the next page.

**Step 1:** we first reorder the diagonal elements of $\rho_I$ on the diagonal basis into the decreasing order. Then, the particles which are near to the $n$-th particle are almost in the ground state, i.e., they are extremely cold. Similarly, the particles which are near to the first particle is almost in maximally mixed state, which is the Gibbs state of the infinite temperature, i.e., they are extremely hot.

**Step 2:** we reorder the positions of particles as the schematic diagram.

**Step 3:** we perform the inverse process of the first step.

The detail is in pages 26-28 of arXiv:1504.06150.
Schematic diagram of our optimal work extraction

\[ m_n := \left[ \frac{\beta X Q_n + \frac{Q_n^2}{2n\sigma_X^2(\beta_X)}}{\log d} \right] \]

**Hot**

\[ \beta \approx 0 \]

\[ m_n \quad n - m_n \text{ particles} \]

**Cold**

\[ \beta \approx \infty \]

\[ n - m_n \text{ particles} \quad m_n \]

**Relaxation**

\[ \beta \approx 0 \]

\[ \beta \approx \infty \]
The entropy gain of the work storage is so negligibly small as compared with the energy gain of the work storage!
Relation with thermodynamics

\[ \frac{Q}{n} \]: This term can be treated by thermodynamics

\[ \frac{1}{n} \]: This term cannot be treated by thermodynamics

\[
\max \eta(\{E_j, w_j\})
\]

\[= 1 - \frac{\beta_1}{\beta_2} - C_1 \frac{Q}{n} - C_2 \left( \frac{Q}{n} \right)^2 + O\left( \frac{Q}{n^2} \right)\]

*can be derived by thermodynamics*  *cannot be derived by thermodynamics*
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Summary of 2\textsuperscript{nd} part

- We have considered the work extraction when from the pair of hot and cold baths.

- We have showed that the optimal efficiency converges the Carnot efficiency when the hot and cold baths are \( n \) particles with \( n \to \infty \).

- In the above results, we have derived the higher order terms of the optimal efficiency in the asymptotic expansion. These expansions clarifies the difference between the microscopic and the macroscopic characterizations.

- We can also construct the optimal work extraction as an energy-preserving unitary time evolution among the heat baths and the work storage. During the optimal work extraction, the entropy gain of the work storage is so negligibly small as compared with the energy gain of the work storage.
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Derivation I

Optimality part (Impossibility part):

General upper bound

$$\eta(\{E_j, w_j\})$$

$$\leq 1 - \frac{\beta_1}{\beta_2} n(D(\rho_{\beta_1}', \| \rho_{\beta_1}) + D(\rho_{\beta_2}', \| \rho_{\beta_2}))$$

where $\beta_1'$ and $\beta_2'$ are chosen as

$$Q = n\text{Tr}((\rho_{\beta_1}' - \rho_{\beta_1})\hat{H}_1$$

$$S(\rho_{\beta_1}) + S(\rho_{\beta_2}) = S(\rho_{\beta_1}') + S(\rho_{\beta_2}')$$

$$D(\rho \| \rho') := \text{Tr}\rho(\log \rho - \log \rho')$$

Information-geometry method

$\rightarrow$ Asymptotic expansion
Derivation II

Possibility part (lower bound):

Strong Large Deviation:

\[ \log P_c \{ \log P^n_\beta \geq nR \} = -n(\psi(R)R - \phi(\psi(R))) \]

\[ -\log \sqrt{2\pi n\phi'''(\psi(R))}\psi(R) + \frac{f_1(R)}{n} + \frac{f_2(R)}{n^2} + ... \]

where

\[ \phi(s) := \log E_x (P_\beta(X))^s \]

\[ \psi(R) := (\phi')^{-1}(R) \]

Cumulant generating function of \( \log P_\beta(X) \)

\[ \rho_\beta = \sum_x P_\beta(x) \left| x \right\rangle \left\langle x \right| \]

Strong Large Deviation yields the evaluation of the efficiency of our optimal operation.
Detail of Derivation II

For the evaluation, we introduce the following quantity:

\[
D_\beta(m) := \sum_{j=1}^{d^{m-n}} P^n_\beta(j) \left( \log P^n_\beta(j) - \log \frac{P^n_\beta(j)}{d^m} \right)
\]

The efficiency of our protocol is given as

\[
\eta(\text{Our protocol}) = 1 - \frac{\beta_1}{\beta_2 (\beta_2 Q)} \cdot D_{\beta_1}(m) + D_{\beta_2}(-m)
\]

where \( m \) is chosen as

\[
\beta_1 Q = m \log d - D_{\beta_1}(m)
\]
For the evaluation, we need to treat the following quantity:

\[ D_\beta (m) := \sum_{j=1}^{d^{m-n}} P_\beta^n(j)(\log P_\beta^n(j) - \log \frac{P_\beta^n\downarrow\{d^{-m}j\}}{d^m}) \]

For our evaluation, we introduce the function

\[ \log F(Z) := \log P_c\{\log P_\beta^n \geq -nS + \sqrt{n}Z\} \]

where \( S := S(\rho_\beta) \) and the quantity \( \Delta Z \) as

\[ F(Z + \Delta Z)d^m = F(Z) \]

Then, we have

\[ D_\beta (m) = E_Z[m \log d - \sqrt{n}\Delta Z] \]

where \( E_Z \) denotes the expectation under the distribution \( P_\beta^n\downarrow(j) \)
Using the perturbation theory, we have

\[ m \log d - \sqrt{n \Delta Z} \]

\[ = m \log d \left[ n^{-\frac{1}{2}} \psi'(-S)Z \right. \]

\[ - n^{-1} \left( - \frac{\psi''(-S)}{2} + \psi'(-S)^2 \right) \left( Z^2 - \frac{1}{\psi'(-S)} \right) \]

\[ - n^{-\frac{3}{2}} \left( a_1 Z + a_3 Z^3 \right) - n^{-2} \left( b_0 + b_2 Z^2 + b_4 Z^4 \right) \]

\[ + (m \log d)^2 \left[ n^{-1} \frac{\psi'(-S)}{2} \right. \]

\[ + n^{-\frac{3}{2}} \left( - \frac{3\psi'(-S)^2}{2} + \frac{\psi'''(-S)}{2} \right) Z \]

\[ + n^{-2} \left( c_0 + c_2 Z^2 \right) \] + 

where \( a_1, a_3, b_0, b_2, b_4, c_0, c_2 \) are constants.
Detail of Derivation II

Finally, we find that $Z$ obeys the normal distribution asymptotically.

Substituting the previous expansion and this fact, we have

$$D_\beta (m) = E_Z [m \log d - \sqrt{n} \Delta Z]$$

$$= (m \log d)^2 [n^{-1} \frac{\psi'(-S)}{2} + n^{-2} (c_0 + \frac{c_2}{\psi'(-S)})] + \ldots$$
Using the relations:

\[ \eta(\text{Our protocol}) = 1 - \frac{\beta_1}{\beta_2} - \frac{D_{\beta_1}(m) + D_{\beta_2}(-m)}{\beta_2 Q} \]

\[ \beta_1 Q = m \log d - D_{\beta_1}(m), \]

we obtain

\[ \eta(\text{Our protocol}) = 1 - \frac{\beta_1}{\beta_2} - C_1 \frac{Q}{n} - C_2 \left(\frac{Q}{n}\right)^2 + O\left(\frac{Q}{n^2}\right) \]