Efficiency at optimal performance: Quantum and mesoscopic heat engines with prior information

Ramandeep S. Johal

Indian Institute of Science Education and Research Mohali
Punjab, India

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Outline of the talk

- Inference and Prior Information
- Heat Engines
- Internal optimization
- Prior based estimates of optimal behaviour
- Conclusions

Inference and Prior information

In inductive reasoning, the premises or hypotheses seek to suggest in favour of (not absolute proof of) the truth of the conclusion. While the conclusion of a deductive argument is understood to be certain, the truth of an inductive argument is supposed to be probable, based upon the evidence given.

Prior information is the piece of information which is assumed to be given—as part of the model, before, say, the data are considered.

Maximum entropy principle

Prior information:
Prior information in the form of constraints on mean values.

$$\sum_i E_i p_i = U, \quad \sum_i p_i = 1.$$

Maximize Shannon entropy S subject to constraints.

$$S = -\sum_i p_i \ln p_i.$$

Optimal solution:

$$p_i = \exp(-\beta E_i) / \sum_i \exp(-\beta E_i).$$

Bayes' Theorem

Updating probabilities in the light of new information:

$$P(X|D) = \frac{p(D|X)\pi(X)}{p(D)}$$

$$p(D) = \sum_{\{X\}} p(D|X)\pi(X).$$

$\pi(X)$: Prior Probability

$p(D|X)$: Likelihood function

$p(X|D)$: Posterior Probability

Heat Engines

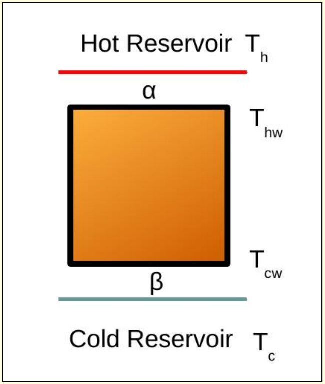
Classical heat cycles

Reversible cycle has the maximum efficiency, $\eta_C = 1 - \frac{T_c}{T_h}$.

Maximum work extraction, but power output

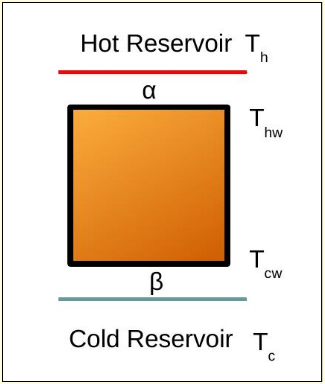
$$P = \frac{\text{Work}}{\text{Cycle period}} \to 0.$$

Finite-time models of heat engines



Endoreversible Model

Finite-time models of heat engines



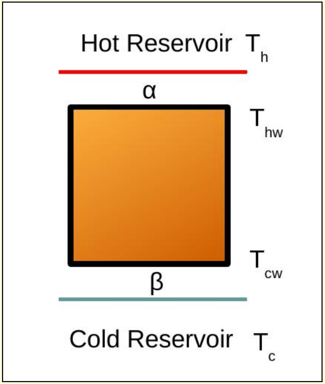
Endoreversible Model

$$
\begin{aligned}
q_h &= \alpha(T_h - T_{hw}) \\
q_c &= \beta(T_{cw} - T_c)
\end{aligned}
$$

Power output:

$$P = \frac{Q_h - Q_c}{t_c + t_h}.$$

Finite-time models of heat engines



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Efficiency at maximum power (EMP)

$$\eta_{\mathrm{CA}} = 1 - \sqrt{\frac{T_c}{T_h}}$$

F. L. Curzon and B. Ahlborn, Am. J. Phys. **43**, 22 (1975)

EMP

TABLE I. Theoretical bounds and observed efficiency η_{obs} of thermal plants

Plant	$T_h(K)$	$T_c(K)$	η_C	η_-	η_+	η_{obs}
Doel 4 (Nuclear, Belgium)[5]	566	283	.5	.25	.33	.35
Almaraz II (Nuclear, Spain)[5]	600	290	.52	.26	.35	.34
Sizewell B (Nuclear, UK)[5]	581	288	.5	.25	.34	.36
Cofrentes (Nuclear, Spain)[5]	562	289	.49	.24	.32	.34
Heysham (Nuclear, UK)[5]	727	288	.60	.30	.43	.40
West Thurrock (Coal,UK)[1]	838	298	.64	.32	.48	.36
CANDU (Nuclear,Canada)[1]	573	298	.48	.24	.32	.30
Larderello (Geothermal,Italy)[1]	523	353	.32	.16	.19	.16
Calder Hall (Nuclear,UK)[5]	583	298	.49	.24	.32	.19
(Steam/Mercury,US)[5]	783	298	.62	.31	.45	.34
(Steam,UK)[5]	698	298	.57	.29	.40	.28
(Gas Turbine, Switzerland)[5]	963	298	.69	.35	.53	.32
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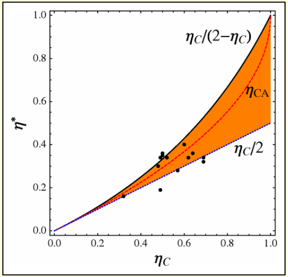

Low-dissipation model

M. Esposito, R. Kawai, K. Lindenberg, and C. Van den Broeck, Phys. Rev. Lett. **105**, 150603 (2010).

EMP

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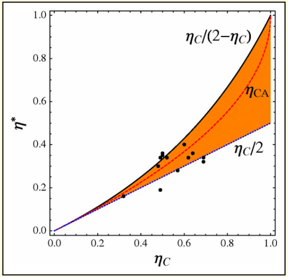

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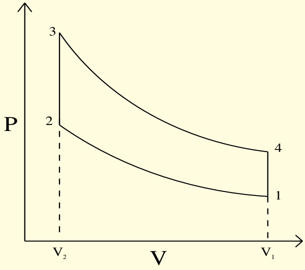
Universality near equilibrium

$$\eta^* = \frac{\eta_C}{2} + \frac{\eta_C^2}{4(1+\sqrt{\Sigma_-/\Sigma_+})} + \mathcal{O}(\eta_C^3)$$

Otto cycle

4-step cycle:

- Two isochoric processes
- Two adiabatic processes



Quantum Heat Cycle

- Two heat reservoirs with $T_1 > T_2$.
- Quantum working medium: $H(a) = \sum_i E_i |i\rangle\langle i|, E_i = \epsilon_i a$.
- Heat exchange with reservoirs; a is kept constant.
- Work performed by changing a; occupation probabilities stay constant.

Statistical Definitions of Heat and Work

Quantum state ρ.

Mean energy: $U = \mathrm{Tr}[\rho H]$.

Change in mean energy: $\delta U = \mathrm{Tr}[\rho\, \delta H] + \mathrm{Tr}[\delta\rho\, H]$,

First law of thermodynamics: $\delta U = \delta Q + \delta W$.

Quantum Otto Cycle

Initial state: $a = a_1$, $\rho = \sum_i p_i |i\rangle\langle i|$.

$$p_i = \exp(-\epsilon_i a_1 / k_{\rm B} T_1)/Z.$$

(i) Ist adiabatic process: $a_1 \to a_2$, without any transition between the levels. The system continues to occupy its initial state.

The work done *by* the system: $W_1 = \mathrm{Tr}[\rho\, \Delta H]$

$$W_1 = \sum_i (E_i - E_i') p_i.$$

(ii) Ist Isochoric process: The system with $a = a_2$ in thermal contact with the cold bath ($T = T_2$). The average heat dissipated

$$Q_2 = \sum_i E_i' (p_i' - p_i).$$

The Quantum Cycle

(iii) 2nd adiabatic process: The system is now detached from the cold bath and made to undergo $a_2 \to a_1$. Work done *on* the system:

$$W_2 = \sum_i (E_i' - E_i) p_i';$$

(iv) 2nd Isochoric Process: Finally, the system in thermal contact with the hot bath again. Heat absorbed by the system

$$Q_1 = \sum_i E_i (p_i - p_i').$$

Total work in one cycle

$$W = \sum_i (E_i - E_i')(p_i - p_i').$$

Two-levels System

$$
\begin{aligned}
Q_1 &= a_1 \left[\frac{1}{1+\exp(a_1/T_1)} - \frac{1}{1+\exp(a_2/T_2)} \right] \\
W &= (a_1 - a_2) \left[\frac{1}{1+\exp(a_1/T_1)} - \frac{1}{1+\exp(a_2/T_2)} \right]
\end{aligned}
$$

$$\text{Efficiency : } \boxed{\eta = 1 - \frac{a_2}{a_1}}.$$

The operation as a heat engine: $W \geq 0$ and $Q_1 \geq 0$,

$$\frac{a_2}{T_2} > \frac{a_1}{T_1} \implies \eta < 1 - \frac{T_2}{T_1}.$$

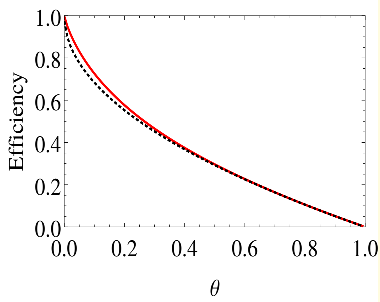
Work Extraction: Internal optimization

For given temperatures:

$$\left(\frac{\partial W}{\partial a_1}\right)_{a_2} = 0; \quad \left(\frac{\partial W}{\partial a_2}\right)_{a_1} = 0.$$

Efficiency at Optimal Work:

$$\eta^* = 1 - \frac{{a_2}^*}{{a_1}^*}$$



Prior based approach

Engine with a known efficiency:

$$W(a_1, \eta) = a_1 \eta \left[\frac{1}{\left(1 + e^{a_1/T_1}\right)} - \frac{1}{\left(1 + e^{a_1(1-\eta)/T_2}\right)} \right].$$

Known			Unknown
T_1	T_2	η	a_1 (a_2)

What can we say about the expected performance of the engine?

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Known			Unknown
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What can we say about the expected performance of the engine?

Expected value:

$$\overline{X} = \int X(a_1)\, \pi(a_1) da_1.$$

How to assign a suitable prior distribution for a_1?

Choice of the prior

Prior should be proper.

Choice of the prior

Prior should be proper.

If there is no reason to prefer one value of a_1 over another, then a uniform density ($\pi(a_1) =$ constant) seems a natural choice.

Choice of the prior

Suppose the efficiency is specified, $\eta = 1 - \frac{a_2}{a_1}$.

Rule

The prior in terms of a_1 or in terms of a_2, should be the same, because a change of scale should not be reflected in the prior as the two problems are equivalent.

$$\pi(a_1)da_1 = \pi(a_2)da_2.$$

$$\pi(a_1) = \frac{N}{a_1},$$

$$N = \left[\ln\left(\frac{a_{\max}}{a_{\min}}\right)\right]^{-1}$$

$$\overline{W}(\eta) \equiv \int_{a_{\min}}^{a_{\max}} W(a_1, \eta)\, \pi(a_1) da_1$$

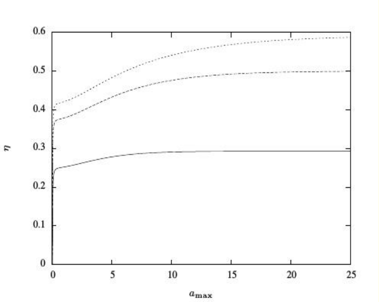
$$\overline{W}(\eta) = N\eta \left[\frac{T_2}{(1-\eta)} \ln \left(\frac{1 + e^{a_{\max}(1-\eta)/T_2}}{1 + e^{a_{\min}(1-\eta)/T_2}} \right) - T_1 \ln \left(\frac{1 + e^{a_{\max}/T_1}}{1 + e^{a_{\min}/T_1}} \right) \right].$$

$\overline{W}$ vanishes when (i) $\eta = 0$, (ii) $\eta = \eta_c$.

In between, the expected work exhibits a maximum.

The efficiency at maximum expected work:

$$\frac{\partial \overline{W}}{\partial \eta} = 0 \longrightarrow \hat{\eta}(a_{\min}, a_{\max}).$$



The curves correspond to $T_2 = 1$ and T_1 taking values $2, 4, 6$ respectvely, from bottom to top.

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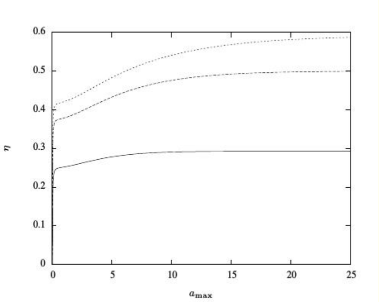


The curves correspond to $T_2 = 1$ and T_1 taking values $2, 4, 6$ respectvely, from bottom to top.

Limiting case: $a_{\min} \to 0$, $a_{\max} \to \infty$:

$$\hat{\eta} \to 1 - \sqrt{T_2/T_1}.$$

Uniform Prior

$$\pi(a_1) = \frac{1}{a_{\max}}$$

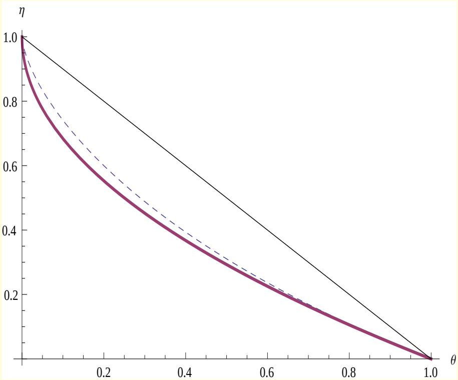
defined in the range $[0, a_{\max}]$.
The efficiency at maximum work in the limit, $a_{\max} \to \infty$ is

$$(1 - \eta^*)^3 - (1 + \eta^*)\theta^2 = 0,$$

whose real solution is

$$\eta^*_{\gamma=0} = 1 + \frac{\theta^{4/3}}{3\left(1 + \sqrt{1 + \frac{\theta^2}{27}}\right)^{1/3}} - \theta^{2/3}\left(1 + \sqrt{1 + \frac{\theta^2}{27}}\right)^{1/3}.$$

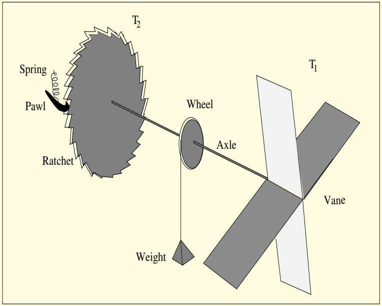
Efficiency at optimal expected work



Universal Efficiency at Optimal Work with Bayesian Statistics, Phys. Rev. E **82**, 061113 (2010).

Feynman's Ratchet and Pawl Model

Pawl and ratchet inside the cold bath at T_c.
Vane inside the hot bath at T_h.
ϵ_2: energy to raise the pawl.
$\epsilon_1 = \epsilon_2 + Z\delta$: energy to lift the weight.



The rates of forward/backward jumps for lifting the weight:

$$R_{\mathrm{F}} = r_0 e^{-\epsilon_1/T_1}, \quad R_{\mathrm{B}} = r_0 e^{-\epsilon_2/T_2}.$$

The rate of heat absorbed from the hot bath:

$$\dot{Q}_1 = r_0 \epsilon_1 \left(e^{-\epsilon_1/T_1} - e^{-\epsilon_2/T_2} \right),$$

The rate of heat rejected to the cold bath

$$\dot{Q}_2 = r_0 \epsilon_2 \left(e^{-\epsilon_1/T_1} - e^{-\epsilon_2/T_2} \right),$$

Power output:

$$P = r_0(\epsilon_1 - \epsilon_2) \left(e^{-\epsilon_1/T_1} - e^{-\epsilon_2/T_2} \right).$$

Efficiency:

$$\eta = \frac{P}{\dot{Q}_1} = 1 - \frac{\epsilon_2}{\epsilon_1}.$$

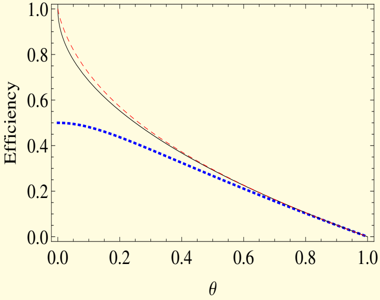
Maximum power: Optimization over ϵ_1 and ϵ_2.

$$\mathrm{EMP} \implies \tilde{\eta} = \frac{\eta_c^2}{\eta_c - (1 - \eta_c) \ln (1 - \eta_c)}.$$

EMP near equilibrium

$$\eta_{\mathrm{CA}} = \frac{\eta_{\mathrm{C}}}{2} + \frac{\eta_{\mathrm{C}}^2}{8} + \frac{6}{96}\eta_{\mathrm{C}}^3 + \cdots$$

$$\tilde{\eta} = \frac{\eta_{\mathrm{C}}}{2} + \frac{\eta_{\mathrm{C}}^2}{8} + \frac{7}{96}\eta_{\mathrm{C}}^3 + \cdots .$$



Power optimization with prior probability

For a given value of efficiency, consider ϵ_2 as the uncertain parameter.

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Prior distribution: $\Pi(\epsilon_2)$; $\epsilon_2 \in [\epsilon_{\min}, \epsilon_{\max}]$

$$
\begin{aligned}
P(\eta, \epsilon_2) &= \frac{r_0 \epsilon_2 \eta}{(1-\eta)} \left(e^{-\epsilon_2/(1-\eta)T_1} - e^{-\epsilon_2/T_2} \right), \\
\overline{P}(\eta) &= \int_{\epsilon_{\min}}^{\epsilon_{\max}} P(\eta, \epsilon_2) \Pi(\epsilon_2) d\epsilon_2. \\
\frac{\partial \overline{P}}{\partial \eta} &= 0.
\end{aligned}
$$

G. Thomas and RSJ, J. Phys. A: Math. Theor. **48** 335002 (2015).

$$
\begin{aligned}
\overline{P}(\eta) \;=\; & C\eta \left[T_1 \left(e^{-\epsilon_{\rm min}/(1-\eta)T_1} - e^{-\epsilon_{\rm max}/(1-\eta)T_1} \right) \right. \\
& \left. - \frac{T_2}{(1-\eta)} \left(e^{-\epsilon_{\rm min}/T_2} - e^{-\epsilon_{\rm max}/T_2} \right) \right].
\end{aligned}
$$

$$
C = r_0 \left[\ln \left(\frac{\epsilon_{\rm max}}{\epsilon_{\rm min}} \right) \right]^{-1}.
$$

$$
\begin{aligned}
\frac{\partial \overline{P}}{\partial \eta} \equiv \; & T_1 \left(e^{-\epsilon_{\min}/(1-\eta)T_1} - e^{-\epsilon_{\max}/(1-\eta)T_1} \right) \\
& - \frac{\eta}{(1-\eta)^2} \left(\epsilon_{\min} e^{-\epsilon_{\min}/(1-\eta)T_1} - \epsilon_{\max} e^{-\epsilon_{\max}/(1-\eta)T_1} \right) \\
& + \frac{T_2}{(1-\eta)^2} \left(e^{-\epsilon_{\max}/T_2} - e^{-\epsilon_{\min}/T_2} \right) = 0.
\end{aligned}
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$$\frac{\partial \overline{P}}{\partial \eta} \equiv T_1 \left(e^{-\epsilon_{\min}/(1-\eta)T_1} - e^{-\epsilon_{\max}/(1-\eta)T_1} \right)$$
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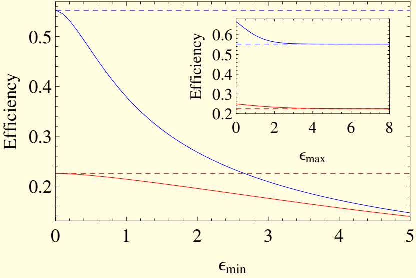

The EMP plotted versus $\epsilon_{\min}$, while $\epsilon_{\max} = 10$. The upper (lower) curve is for $\theta = 0.2$ ($\theta = 0.6$). The dashed lines represent CA values. Inset: The EMP plotted versus $\epsilon_{\max}$, with $\epsilon_{\min} = 0.01$.

Asymptotic limit

$$\boxed{\epsilon_{\min} << T_2 < T_1 << \epsilon_{\max}}$$

$$\eta \to 1 - \sqrt{\frac{T_2}{T_1}}.$$

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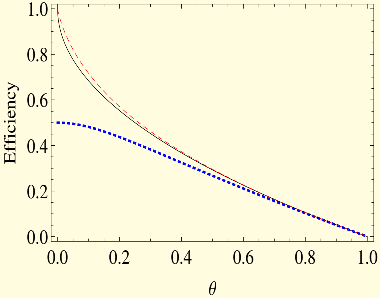

$$\eta_u = \frac{\eta_C}{2} + \frac{\eta_C^2}{16} + \frac{1}{64}\eta_C^3 + \cdots .$$

Conclusions

- Estimates of efficiency at optimal expected performance have been obtained with partial information.
- Jeffreys prior and uniform prior have been compared.
- It suggests that averaging over internal energy scales reproduces thermodynamic behavior.
- Exact optimization or tuning of internal parameters is not necessary to guess optimal behaviour like EMP.

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