

Catalytic enhancements in the performance of the microscopic two-stroke engine.

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LA-UR-24-25471

Motivation.

- 1) Understanding thermodynamics at the microscopic regime.

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- 2) Size vs efficiency trade-off.

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- 1) Understanding thermodynamics at the microscopic regime.
- 2) Size vs efficiency trade-off.
- 3) Quantum computing : Resetting of qubits.



Marcin Łobejko



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International Centre for Theory of Quantum Technologies (ICTQT)
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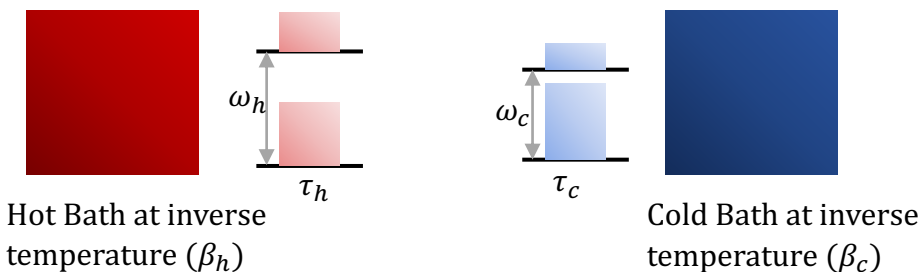
Outline of the talk.

- 1) Two-stroke heat engine in the microscopic regime.
 - A) Without Catalyst.
 - B) With Catalyst.
- 2) Thermodynamic framework.
- 3) Enhancements in the efficiency due to the catalyst.
- 4) Conclusion

Two-stroke heat engine in the microscopic regime.

Initial state

Without catalyst



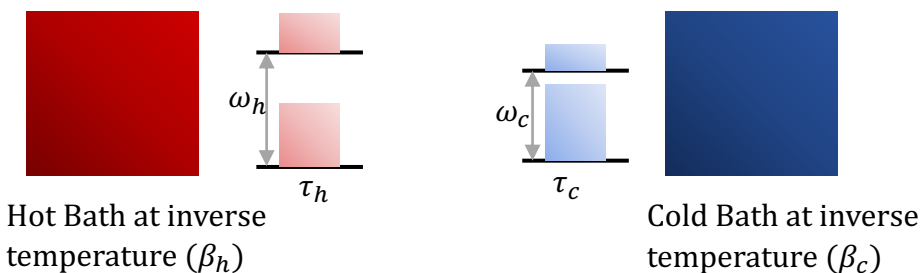
$$\tau_h \otimes \tau_c$$

$$\tau_h = \frac{1}{(1+e^{-\beta_h \omega_h})} \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta_h \omega_h} \end{pmatrix} ; \quad \tau_c = \frac{1}{(1+e^{-\beta_c \omega_c})} \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta_c \omega_c} \end{pmatrix}.$$

Two-stroke heat engine in the microscopic regime.

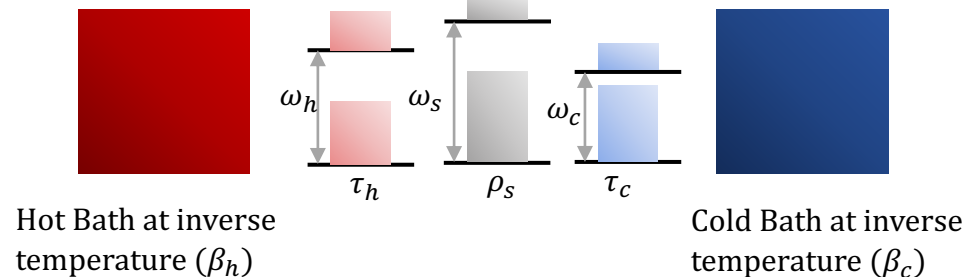
Initial state

Without catalyst



$$\tau_h \otimes \tau_c$$

With catalyst



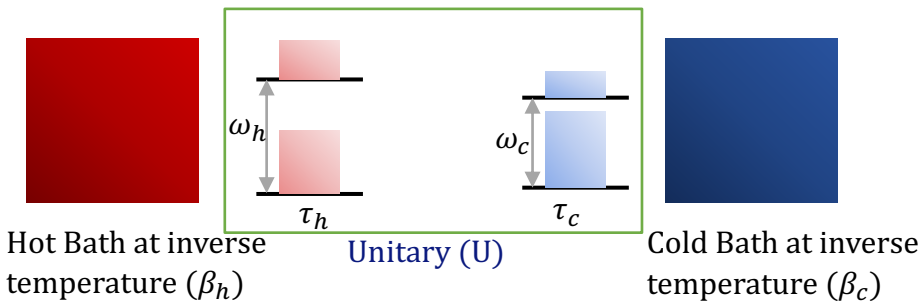
$$\rho_s \otimes \tau_h \otimes \tau_c$$

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Two-stroke heat engine in the microscopic regime.

Work Stroke

Without catalyst

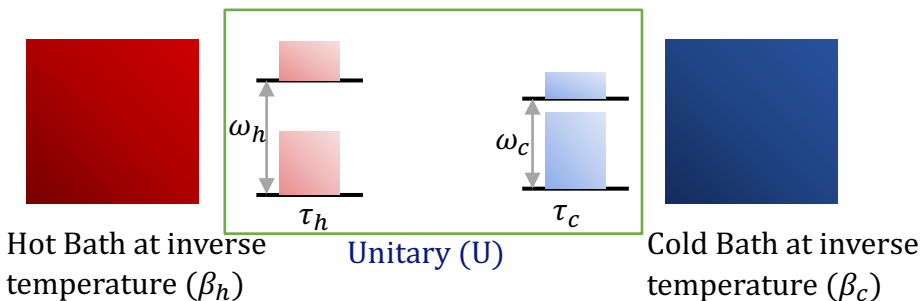


$$U(\tau_h \otimes \tau_c)U^\dagger$$

Two-stroke heat engine in the microscopic regime.

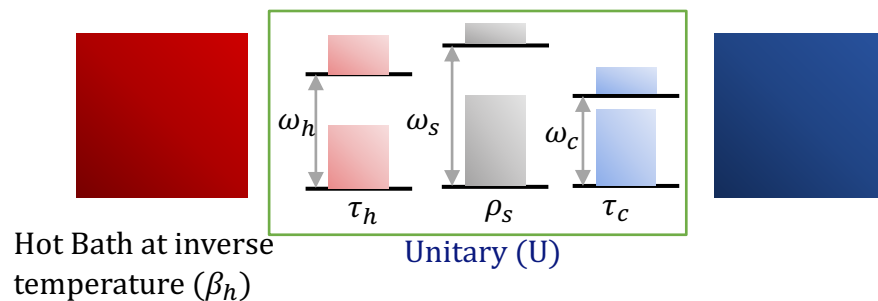
Work Stroke

Without catalyst



$$U(\tau_h \otimes \tau_c)U^\dagger$$

With catalyst



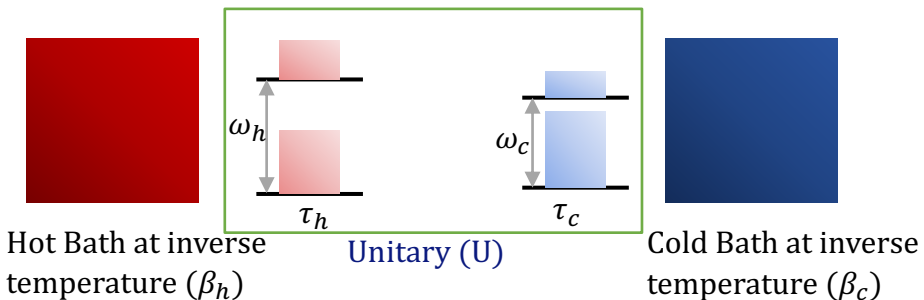
$$U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger$$

$$\text{Catalysis condition: } Tr_{h,c} U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger = \rho_s$$

Two-stroke heat engine in the microscopic regime.

Work Stroke

Without catalyst



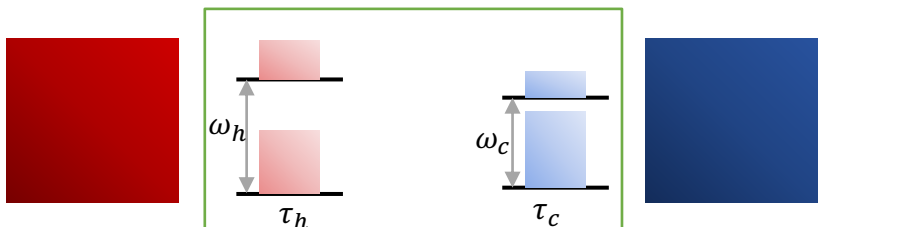
$$U(\tau_h \otimes \tau_c)U^\dagger$$

$$W = Tr[(H_h + H_c)(\tau_h \otimes \tau_c - U(\tau_h \otimes \tau_c)U^\dagger)]$$

Two-stroke heat engine in the microscopic regime.

Work Stroke

Without catalyst



Hot Bath at inverse temperature (β_h)

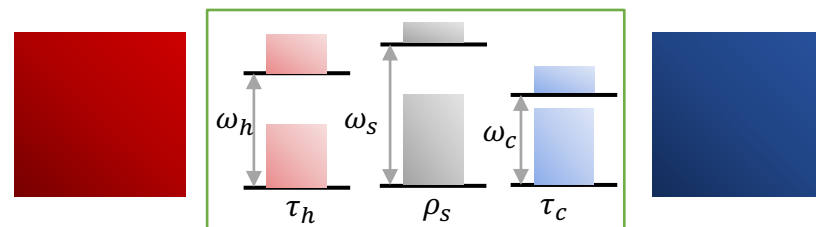
Unitary (U)

Cold Bath at inverse temperature (β_c)

$$U(\tau_h \otimes \tau_c)U^\dagger$$

$$W = \text{Tr}[(H_h + H_c)(\tau_h \otimes \tau_c - U(\tau_h \otimes \tau_c)U^\dagger)]$$

With catalyst



Hot Bath at inverse temperature (β_h)

Unitary (U)

$$U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger$$

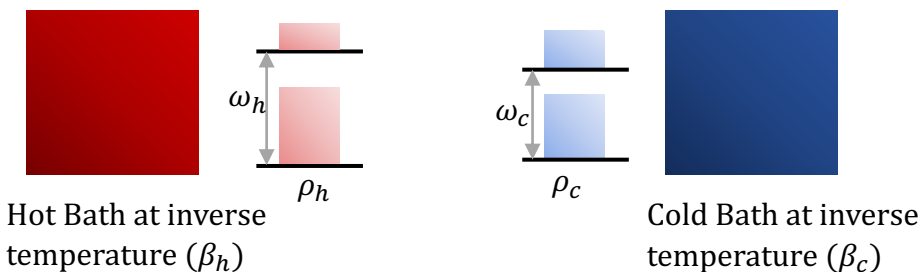
$$\text{Catalysis condition: } \text{Tr}_{h,c} U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger = \rho_s$$

$$W = \text{Tr}[(H_s + H_h + H_c)(\rho_s \otimes \tau_h \otimes \tau_c - U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger)]$$

Two-stroke heat engine in the microscopic regime.

Work Stroke

Without catalyst



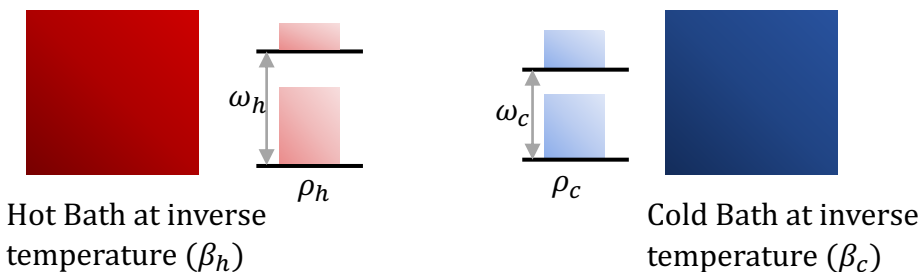
Final state of hot qubit $Tr_h(U(\tau_h \otimes \tau_c)U^\dagger) = \rho_h$

Final state of cold qubit $Tr_c(U(\tau_h \otimes \tau_c)U^\dagger) = \rho_c$

Two-stroke heat engine in the microscopic regime.

Work Stroke

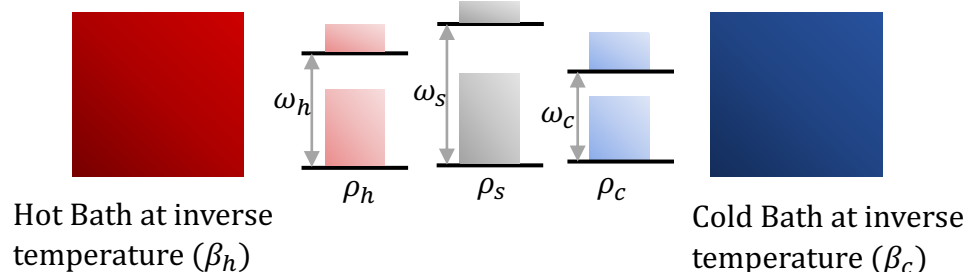
Without catalyst



Final state of hot qubit $Tr_h(U(\tau_h \otimes \tau_c)U^\dagger) = \rho_h$

Final state of cold qubit $Tr_c(U(\tau_h \otimes \tau_c)U^\dagger) = \rho_c$

With catalyst



Final state of hot qubit $Tr_{s,h}(U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger) = \rho_h$

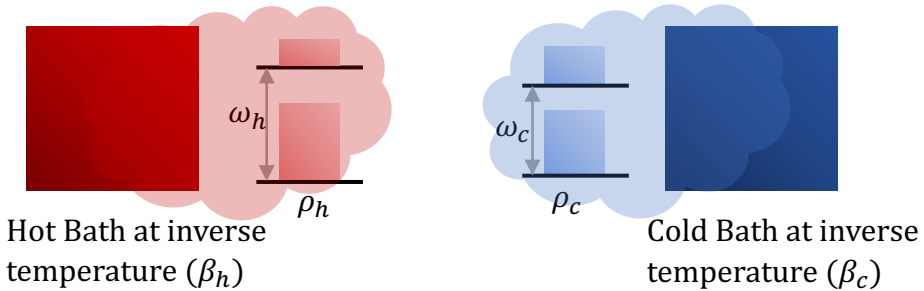
Final state of cold qubit $Tr_{s,c}(U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger) = \rho_c$

Final state of the catalyst $Tr_{h,c}(U(\rho_s \otimes \tau_h \otimes \tau_c)U^\dagger) = \rho_s$

Two-stroke heat engine in the microscopic regime.

Heat Stroke

Without catalyst

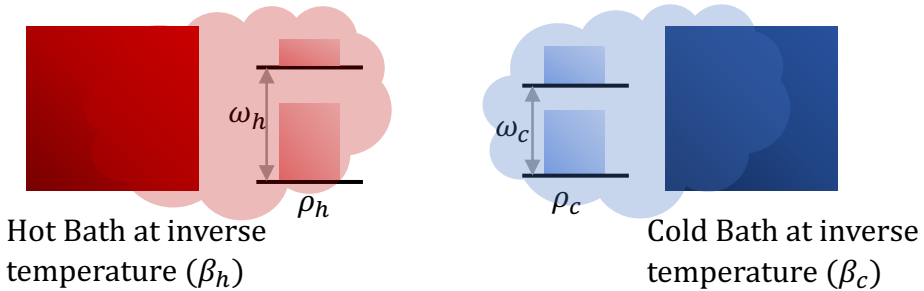


Rethermalization with respective baths

Two-stroke heat engine in the microscopic regime.

Heat Stroke

Without catalyst



Rethermalization with respective baths

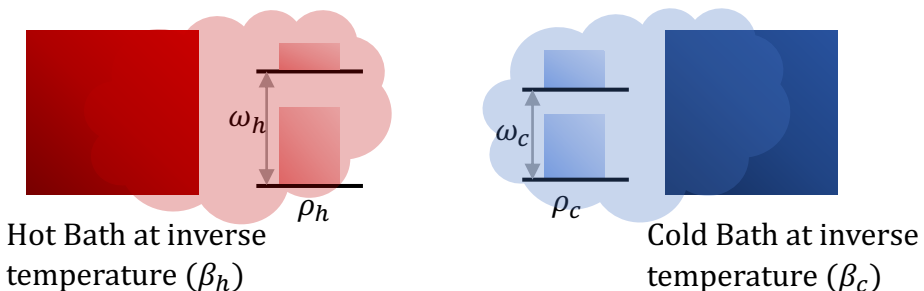
$$\text{Heat withdrawn from hot bath : } Q_h = \text{Tr}[H_h(\tau_h - \rho_h)]$$

$$\text{Heat discharged into cold bath : } Q_c = \text{Tr}[H_c(\tau_c - \rho_c)]$$

Two-stroke heat engine in the microscopic regime.

Heat Stroke

Without catalyst

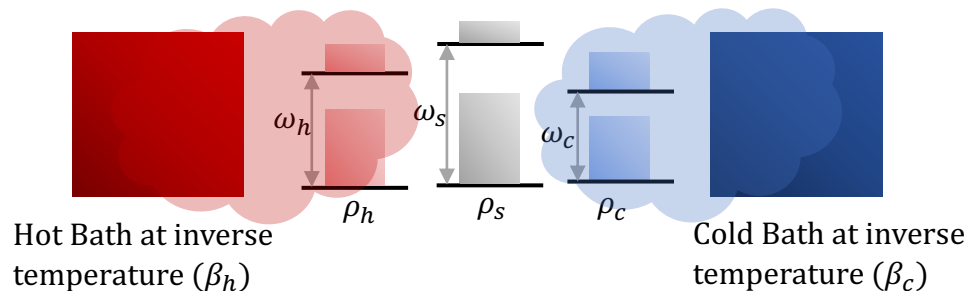


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With catalyst



Rethermalization with respective baths

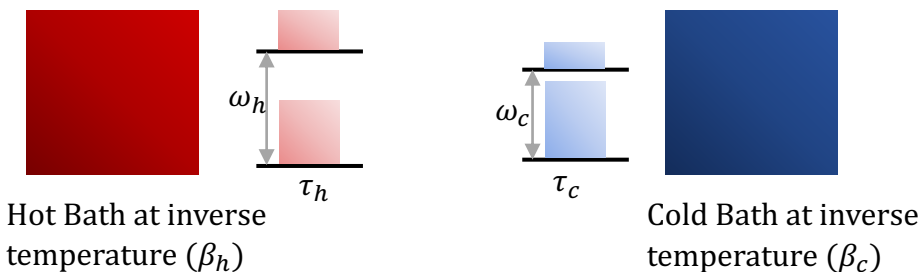
$$\text{Heat withdrawn from hot bath : } Q_h = Tr[H_h(\tau_h - \rho_h)]$$

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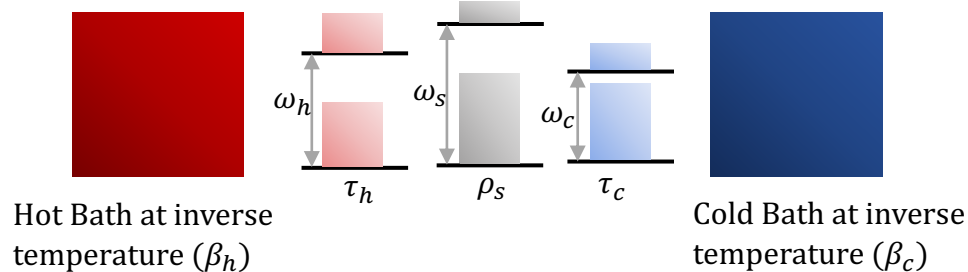
Two-stroke heat engine in the microscopic regime.

Closing the cycle

Without catalyst



With catalyst



Thermodynamic framework.

Manifestation of First Law:

Heat withdrawn from hot bath := Q_h

Heat discharged into cold bath := Q_c

Work produced by the engine := W

$$W = Q_h + Q_c$$

Thermodynamic framework.

Manifestation of First Law:

$$W = Q_h + Q_c$$

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Heat discharged into cold bath := Q_c

Work produced by the engine := W

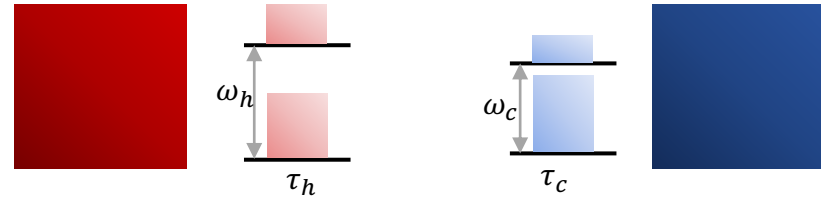
Manifestation of Second Law:

Efficiency := η

$$\eta := \frac{W}{Q_h} = 1 + \frac{Q_c}{Q_h} \leq 1 - \frac{\beta_h}{\beta_c} = \eta_{Carnot}$$

Optimal performance without catalyst.

For a fixed value of ω_h and ω_c



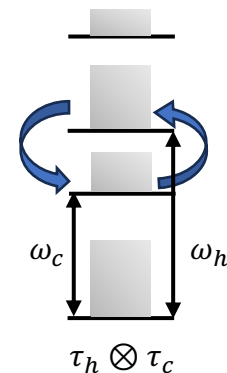
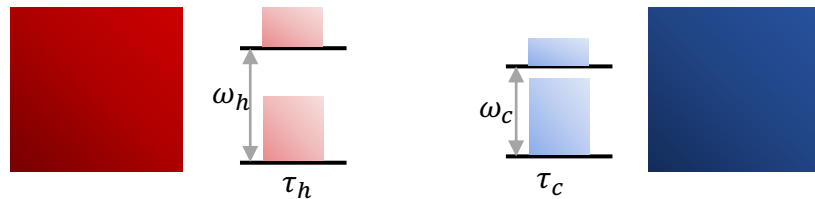
Optimal performance without catalyst.

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$$\text{Optimal Work} = \frac{1}{(1+a_h)(1+a_c)} (a_h - a_c)(\omega_h - \omega_c)$$

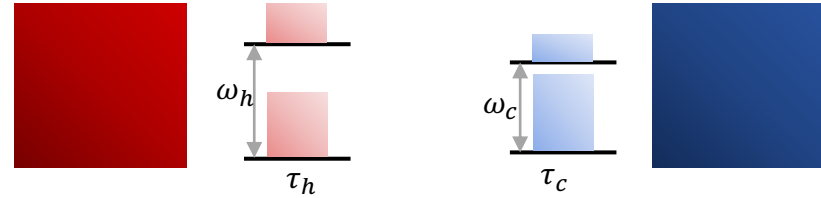
$$a_c = e^{-\beta_c \omega_c}$$

$$a_h = e^{-\beta_h \omega_h}$$



Optimal performance without catalyst.

For a fixed value of ω_h and ω_c

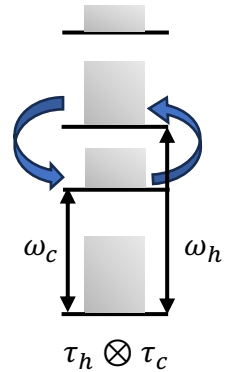


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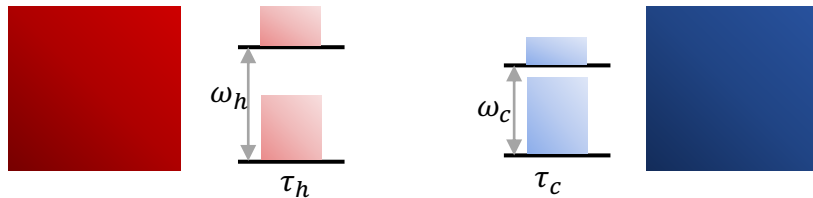
$$a_h = e^{-\beta_h \omega_h}$$

$$\text{Optimal Efficiency} = 1 - \frac{\omega_c}{\omega_h}. \text{ (Otto Efficiency)}$$



Optimal performance without catalyst.

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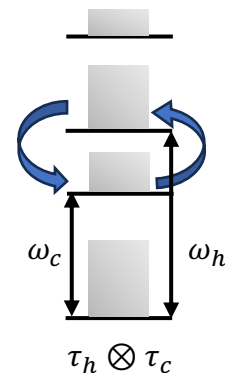
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When $\frac{\omega_c}{\omega_h} = \frac{\beta_h}{\beta_c}$ then $a_h = a_c$. This implies optimal work is 0



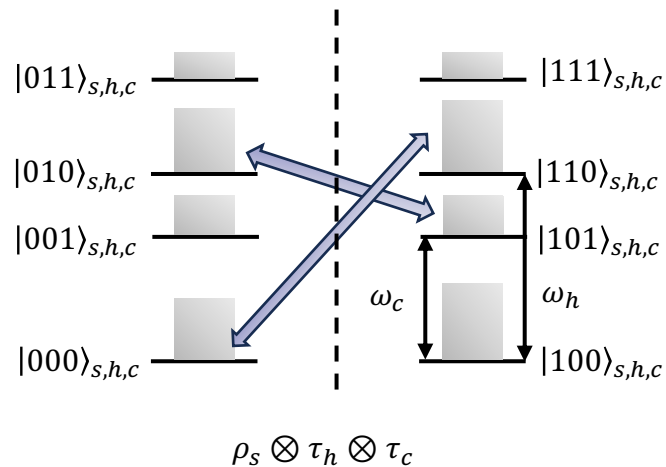
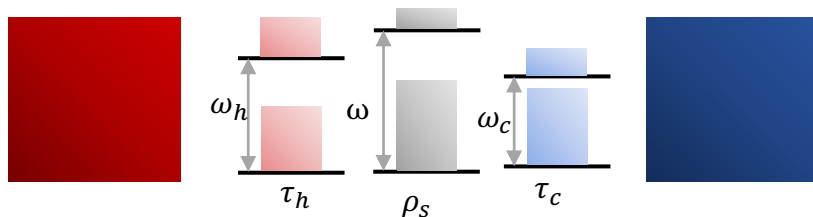
Catalytic enhancement

For a fixed value of ω_h and ω_c

$$\text{Efficiency: } \eta_2 = 1 - \frac{\omega_c}{2\omega_h} > 1 - \frac{\omega_c}{\omega_h}$$

= Optimal efficiency without catalyst

Catalysis condition: $Tr_{h,c} U(\rho_s \otimes \tau_h \otimes \tau_c) U^\dagger = \rho_s$

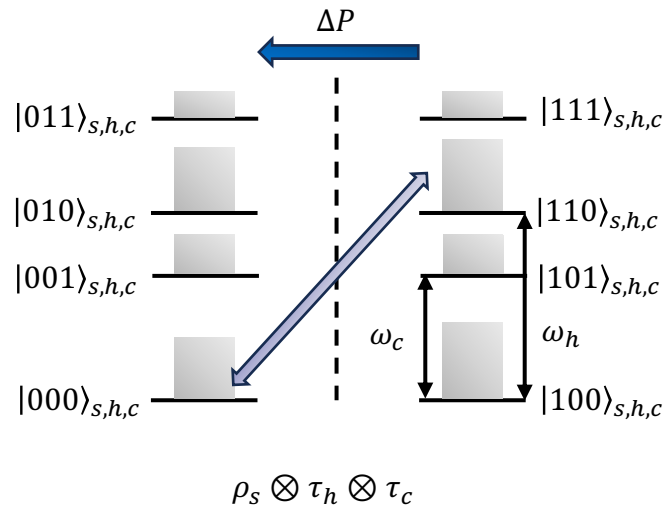
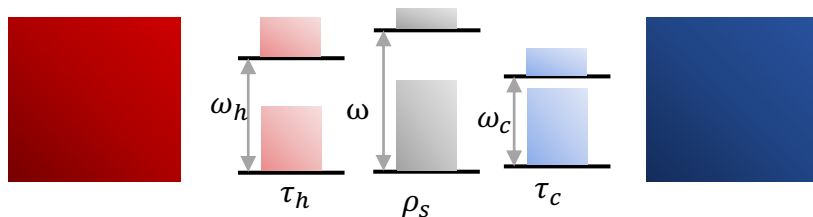


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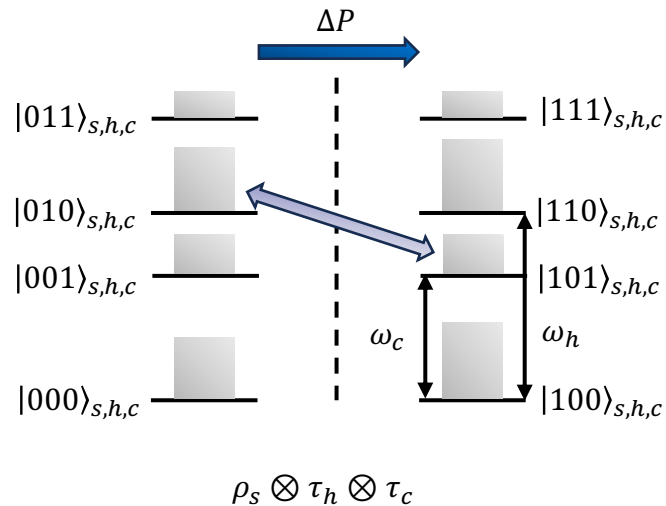
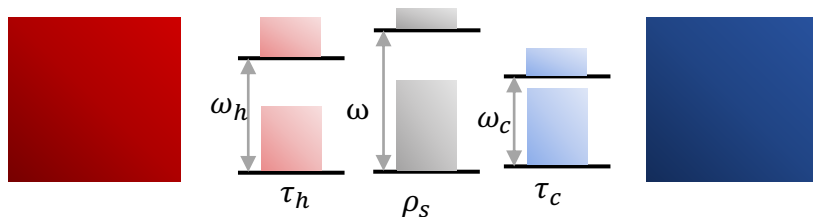


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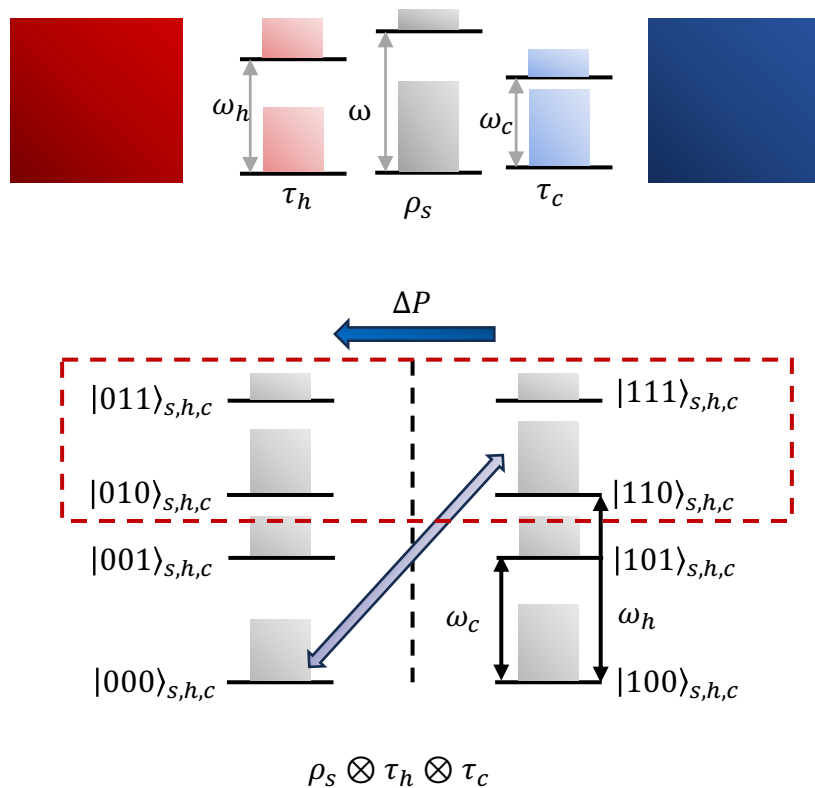
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$$Q_h = \text{Tr}[H_h(\tau_h - \rho_h)] = \Delta P \omega_h$$



Catalytic enhancement

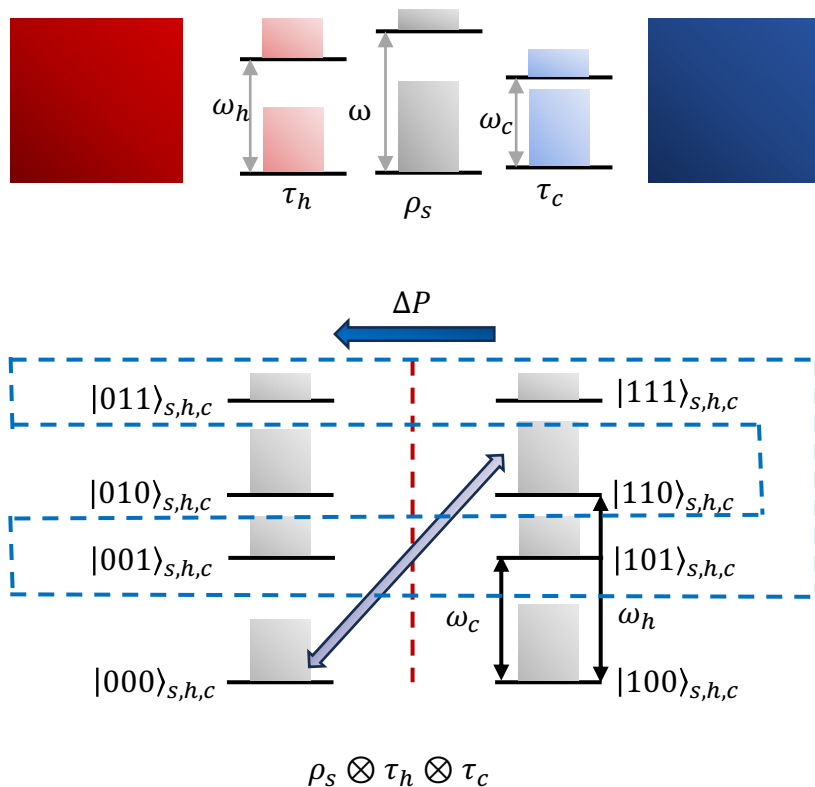
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$$Q_h = \text{Tr}[H_h(\tau_h - \rho_h)] = \Delta P \omega_h$$

$$Q_c = \text{Tr}[H_c(\tau_c - \rho_c)] = 0$$



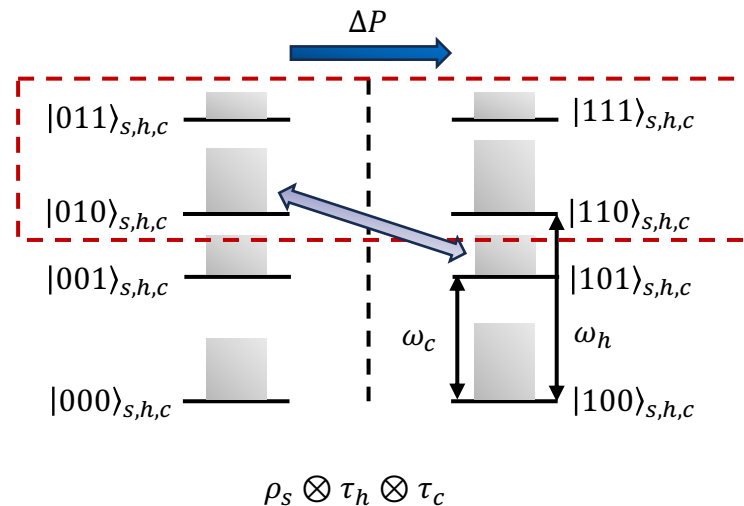
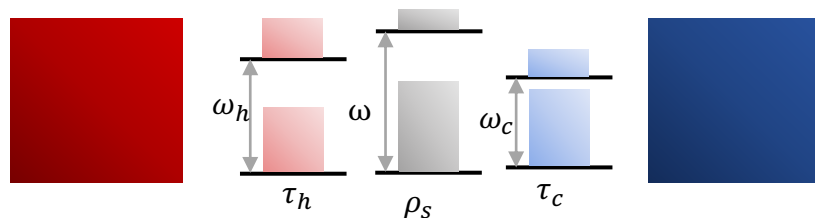
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Catalytic enhancement

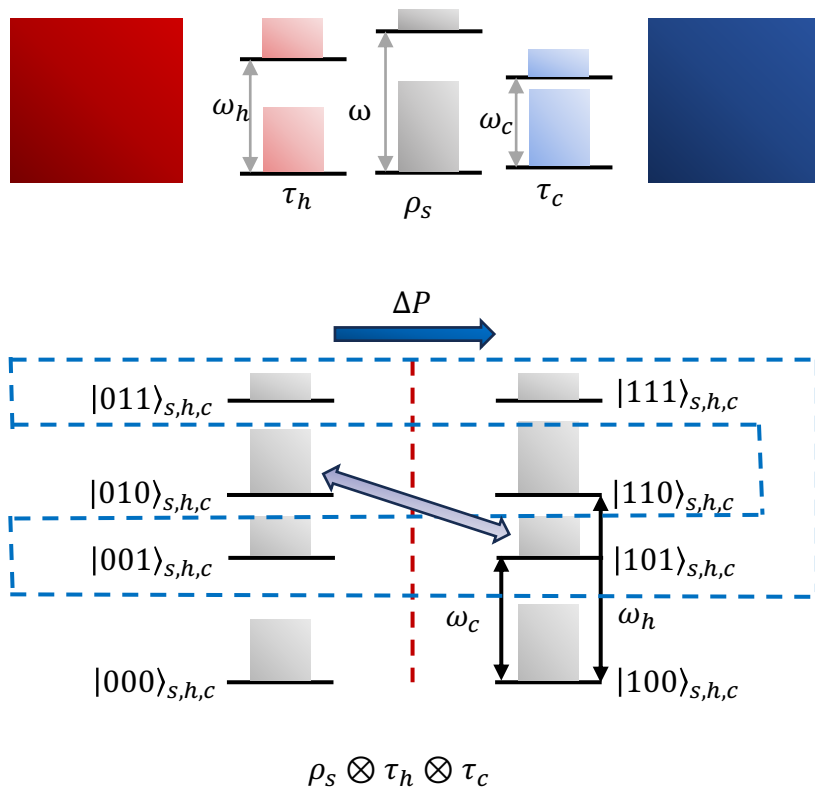
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$$Q_h = \text{Tr}[H_h(\tau_h - \rho_h)] = \Delta P \omega_h$$

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Catalytic enhancement

For a fixed value of ω_h and ω_c

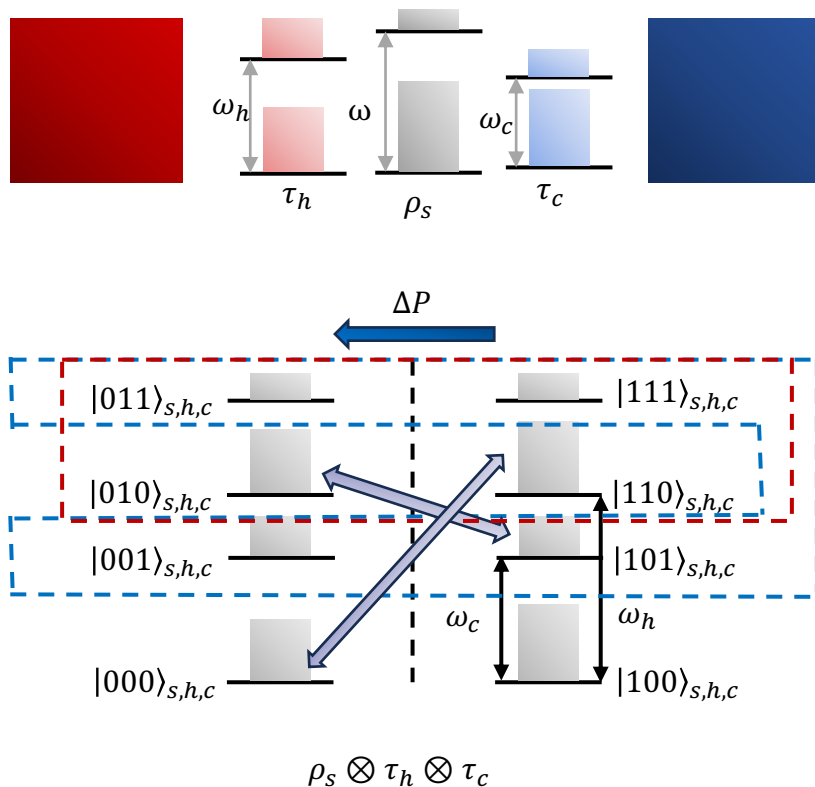
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= Optimal efficiency without catalyst

$$Q_h = \text{Tr}[H_h(\tau_h - \rho_h)] = 2\Delta P\omega_h$$

$$Q_c = \text{Tr}[H_c(\tau_c - \rho_c)] = -\Delta P\omega_c$$

$$\eta = 1 + \frac{Q_c}{Q_h} = 1 - \frac{\omega_c}{2\omega_h}$$



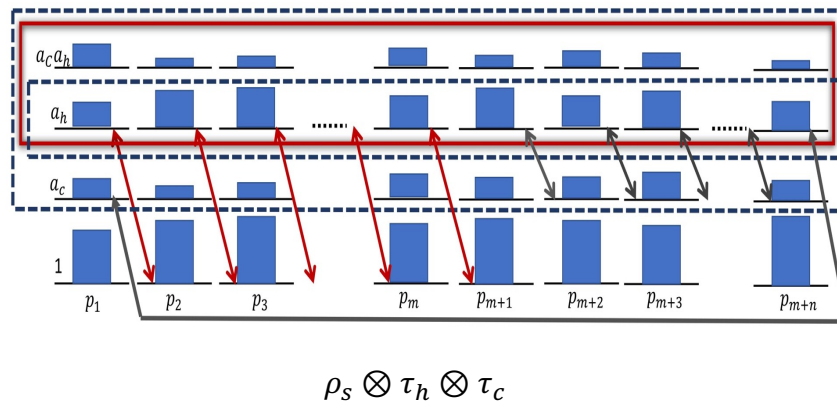
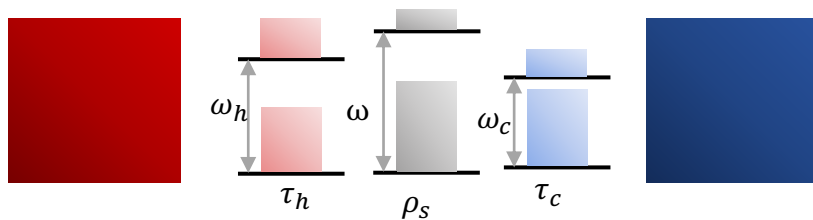
Catalytic enhancement

For a fixed value of ω_h and ω_c

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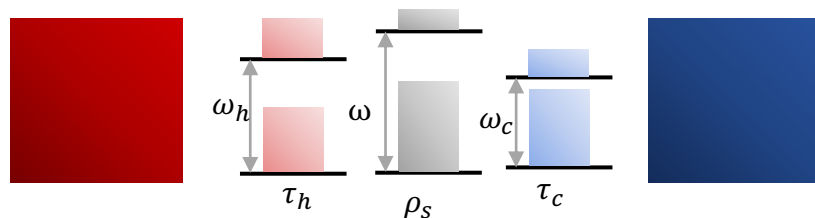
= Optimal efficiency without catalyst

$$\text{For a } d\text{-dimensional catalyst : } \eta_d = 1 - \frac{n\omega_c}{d\omega_h} \quad n \in \{1, \dots, d\}$$



Catalytic enhancement

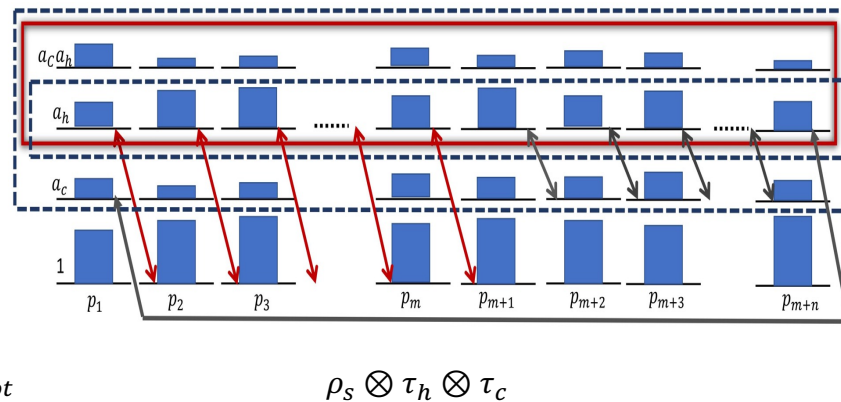
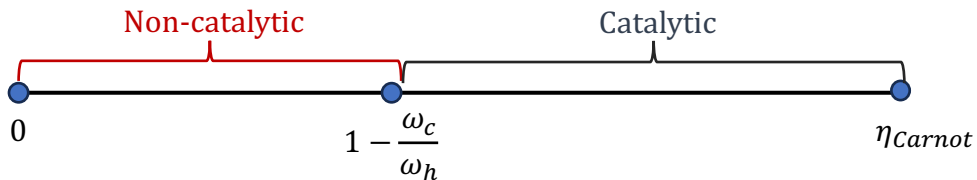
For a fixed value of ω_h and ω_c



Efficiency: $\eta_2 = 1 - \frac{\omega_c}{2\omega_h} > 1 - \frac{\omega_c}{\omega_h}$

= Optimal efficiency without catalyst

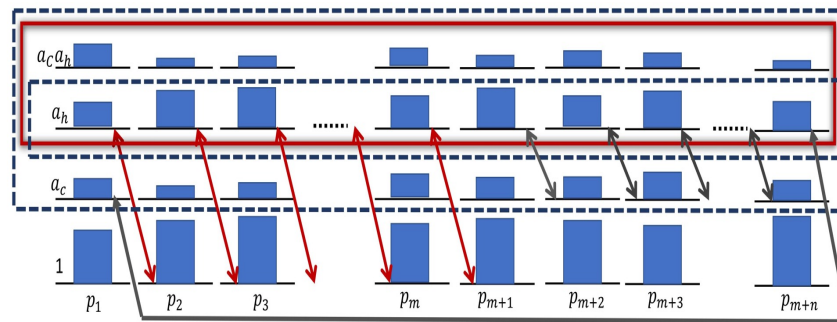
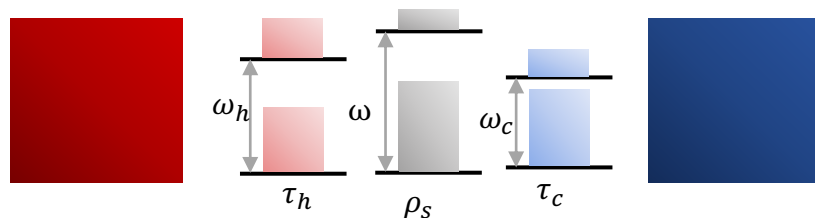
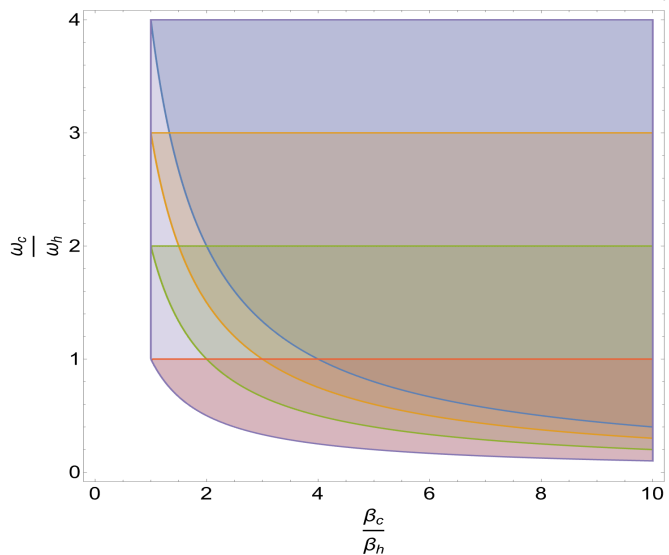
For a d -dimensional catalyst : $\eta_d = 1 - \frac{n\omega_c}{d\omega_h}$ $n \in \{1, \dots, d\}$



Catalytic enhancement

If $\omega_c > \omega_h$, then $1 - \frac{\omega_c}{\omega_h} < 0$;

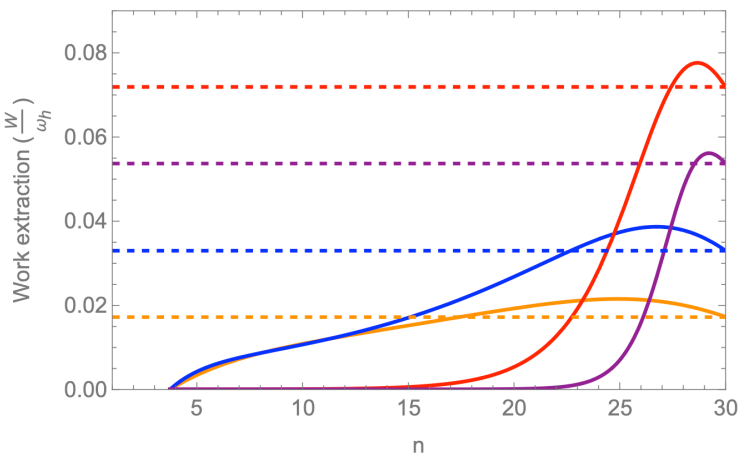
But efficiency in catalytic scenario can still be positive depending on n and d : $\eta = 1 - \frac{n\omega_c}{d\omega_h} > 0$



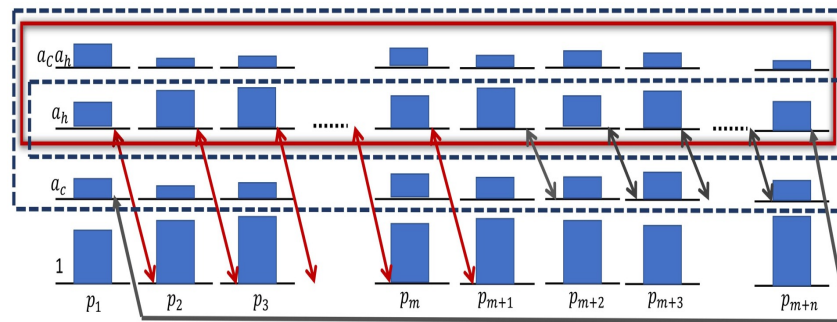
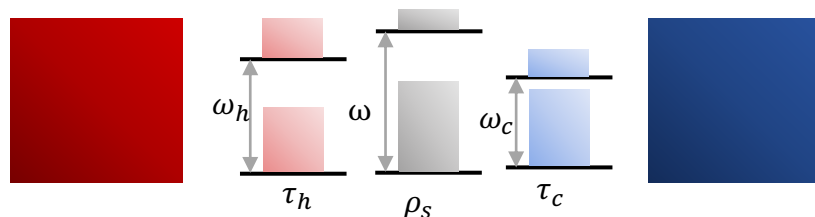
Catalytic enhancement

For a fixed value of ω_h and ω_c

$$W \propto (e^{-\beta_h \omega_h (m+n)} - e^{-n \beta_c \omega_c}) = (e^{-\beta_h \omega_h d} - e^{-n \beta_c \omega_c})$$



- $\beta_h \omega_h = 0.05, \beta_c \omega_c = 0.4$
- $\beta_h \omega_h = 0.1, \beta_c \omega_c = 0.8$
- $\beta_h \omega_h = 0.5, \beta_c \omega_c = 4$
- $\beta_h \omega_h = 1, \beta_c \omega_c = 8$



Conclusion and Outlooks.

- 1) Describing the catalyst assisted two-stroke engine.
- 2) We have shown the efficiency and work per cycle can be enhanced by incorporating a catalyst.
- 3) Exploring the roles of catalysis in cooling of qubits.
- 4) Bridging the gap between the catalyst assisted stroke-based and continuous thermal machines.