Quantum thermal engines: selected results and open problems

Giuliano Benenti
Center for Nonlinear and Complex Systems,
Univ. Insubria, Como, Italy
INFN, Milano, Italy

Thanks to collaborators:
Matteo Carrega, Fabio Cavaliere, Maura Sassetti (CNR, Genova)
Luca Razzoli (Como)

Acknowledgements: JSF Julian Schwinger Foundation

Outline (some selected questions)

A key question in (quantum) thermodynamics: What are the ultimate bounds to the performance of a heat engine?

Thermodynamics of precision: What is the relevance of thermal and quantum fluctuations?

Violating Thermodynamic Uncertainty Relations (TURs): is there a quantum advantage?

General consideration on thermal engines

Upper bound to efficiency given by the Carnot efficiency:

$$\eta = \frac{W}{Q_H} \leq \eta_C \doteq 1 - \frac{T_C}{T_H}$$

$$(T_H > T_C)$$

Carnot efficiency obtained for quasi-static transformation (zero extracted power)

The ideal Carnot engine is a reversible machine, since there is no dissipation (no entropy production)

Finite time thermodynamics

In an ideal Carnot engine conversion processes are quasi-static and the extracted power reduces to zero.

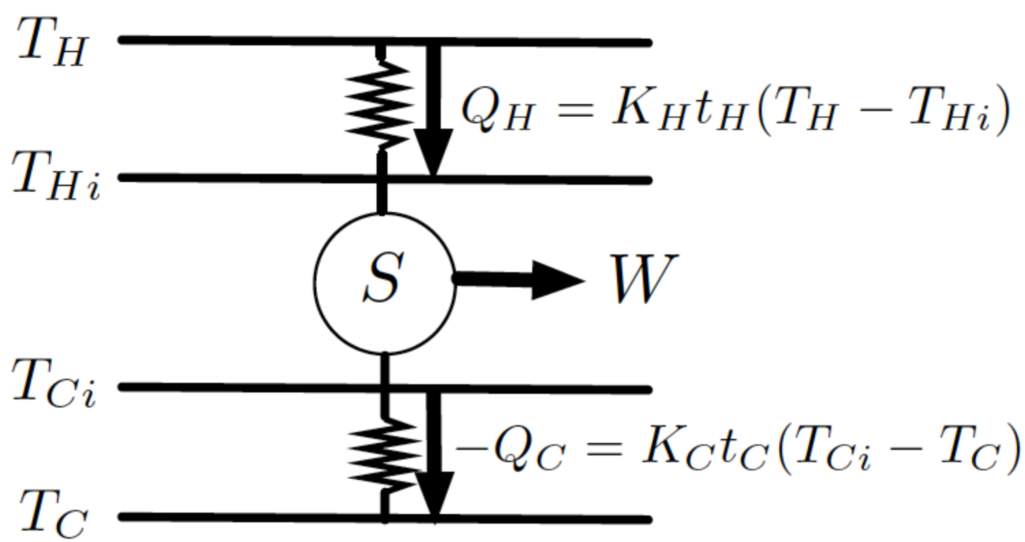
How much the efficiency deteriorates when heat to work conversion takes place in a finite time?

Finite time thermodynamics: finite-time steady-state conversion processes or thermodynamic cycles; the efficiency at the maximum output power is an important concept (more generally, power-efficiency trade-off)

[Andresen, Angew. Chem. Int. Ed. **50**, 2690 (2011),…]

Curzon-Ahlborn (endoreversible) engine

Dissipation is due to finite thermal conductances between heat reservoirs and the ideal heat engine



The efficiency at maximum power (Curzon-Ahlborn efficiency) is independent of the heat conductances:

$$\eta_{CA} = 1 - \sqrt{\frac{T_H}{T_C}} = 1 - \sqrt{1 - \eta_C}$$

[Curzon and Ahlborn, AJP **43**, 22 (1975)]

Schmiedl-Seifert (exoreversible) engine

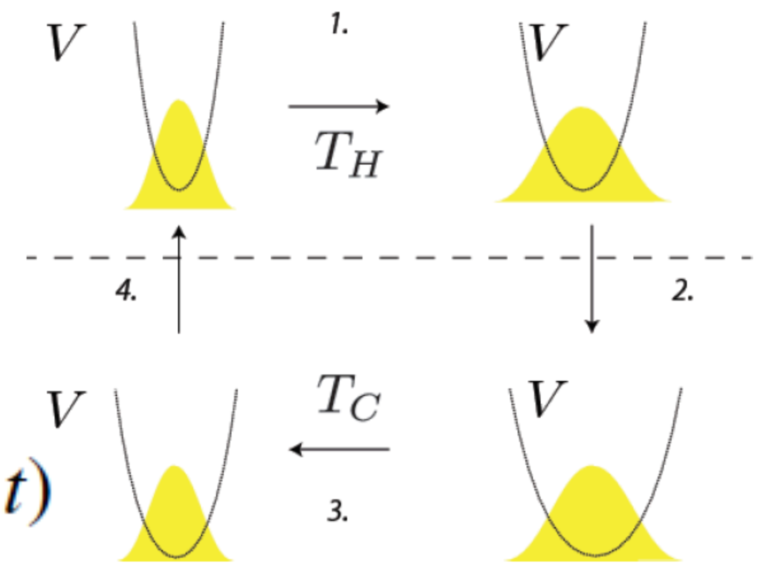
Irreversibility only arises due to internal dissipative processes

Stochastic thermodynamics

Trapping potential

$V(x, \lambda(t))$

Probability density $p(x,t)$



Schmiedl-Seifert efficiency at maximum power:

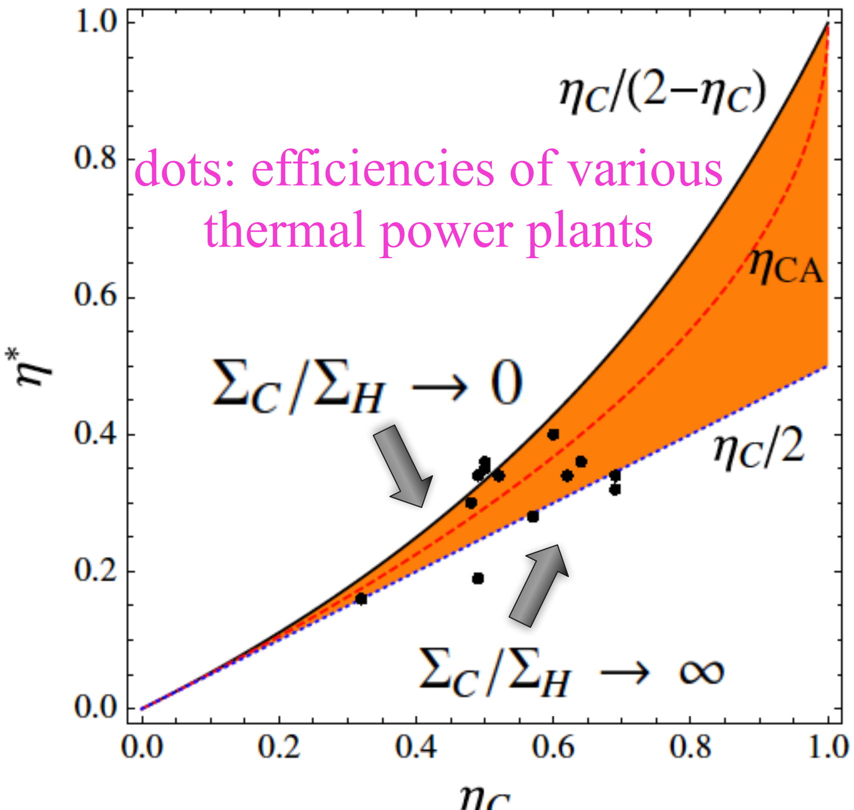
$$\eta_{SS} = \frac{\eta_C}{2 - \gamma\eta_C} \quad \gamma \in [0,1] \quad \gamma = 1/2.$$ for symmetric dissipation

[Schmiedl and Seifert, APL **81**, 2003 (2008)]

Low-dissipation engines

The entropy production vanishes in the limit of infinite-time cycles:

$$Q_H = T_H\left(\Delta\mathscr{S} - \frac{\Sigma_H}{t_H}\right), \quad Q_C = T_C\left(-\Delta\mathscr{S} - \frac{\Sigma_C}{t_C}\right)$$



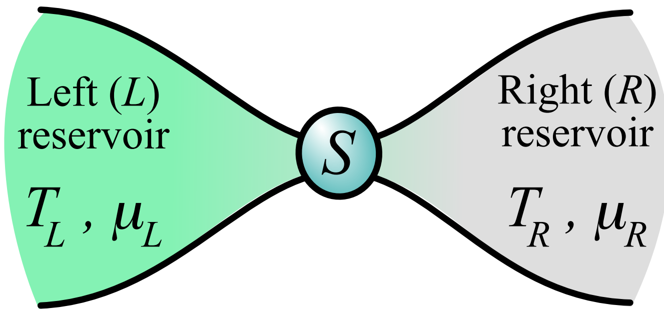
The CA limit is recovered for symmetric dissipation: $\Sigma_H = \Sigma_C$

TABLE I. Theoretical bounds and observed efficiency $\eta_{\rm obs}$ of thermal plants.

Plant	$T_h(K)$	$T_c(K)$	η_C	η_-	η_+	$\eta_{\rm obs}$
Doel 4 (Nuclear, Belgium) [6]	566	283	0.5	0.25	0.33	0.35
Almaraz II (Nuclear, Spain) [6]	600	290	0.52	0.26	0.35	0.34
Sizewell B (Nuclear, UK) [6]	581	288	0.5	0.25	0.34	0.36
Cofrentes (Nuclear, Spain) [6]	562	289	0.49	0.24	0.32	0.34
Heysham (Nuclear, UK) [6]	727	288	0.60	0.30	0.43	0.40
West Thurrock (Coal, UK) [1]	838	298	0.64	0.32	0.48	0.36
CANDU (Nuclear, Canada) [1]	573	298	0.48	0.24	0.32	0.30
Larderello (Geothermal, Italy)[1]	523	353	0.32	0.16	0.19	0.16
Calder Hall (Nuclear, UK) [6]	583	298	0.49	0.24	0.32	0.19
(Steam/Mercury,USA) [6]	783	298	0.62	0.31	0.45	0.34
(Steam, UK) [6]	698	298	0.57	0.29	0.40	0.28
(Gas Turbine, Switzerland) [6]	963	298	0.69	0.35	0.53	0.32
(Gas Turbine, France) [6]	953	298	0.69	0.34	0.52	0.34

[Esposito, Kawai, Lindenberg, Van den Broeck, PRL **105**, 150603 (2010)]

Carnot efficiency at finite power?



$$\mathcal{F}_e = \Delta V/T \quad (\Delta V = \Delta\mu/e)$$

$$\mathcal{F}_h = \Delta T/T^2$$

$$\Delta\mu = \mu_L - \mu_R$$

$$\Delta T = T_L - T_R$$

$$T_L > T_R, \quad \mu_L < \mu_R$$

$$\begin{cases} J_e = L_{ee}(\mathbf{B})\mathcal{F}_e + L_{eh}(\mathbf{B})\mathcal{F}_h \\ J_h = L_{he}(\mathbf{B})\mathcal{F}_e + L_{hh}(\mathbf{B})\mathcal{F}_h \end{cases}$$

B applied magnetic field or any parameter breaking time-reversibility such as the Coriolis force, etc.

$$P(\bar{\eta}_{\max}) = \frac{\bar{\eta}_{\max}}{4}\frac{|L_{eh}^2 - L_{he}^2|}{L_{ee}}\mathcal{F}_h$$

[G.B., K. Saito, G. Casati, PRL **106**, 230602 (2011)]

Onsager relations with broken time-reversal symmetry

$$H = \sum_i^N \frac{[\boldsymbol{p}_i - q_i \boldsymbol{A}(\boldsymbol{r}_i)]^2}{2m_i} + \frac{1}{2}\sum_{i \neq j} V(r_{ij})$$

Analytical result for $\boldsymbol{B} = B(x)\,\boldsymbol{k}$

Landau gauge: $A(x)\,\boldsymbol{j}$

$$\begin{cases} \dot{x}_i = \dfrac{p_i^x}{m_i}, \\ \dot{y}_i = \dfrac{1}{m_i}\,[p_i^y - q_i A(x_i)], \\ \dot{z}_i = \dfrac{p_i^z}{m_i}, \\ \dot{p}_i^x = F_i^x + \dfrac{q_i}{m_i}\,[p_i^y - q_i A(x_i)]\,B(x_i), \\ \dot{p}_i^y = F_i^y, \\ \dot{p}_i^z = F_i^z, \qquad F_i^\alpha = -\dfrac{\partial \sum_{j\neq i} V(r_{ij})}{\partial \alpha} \end{cases}$$

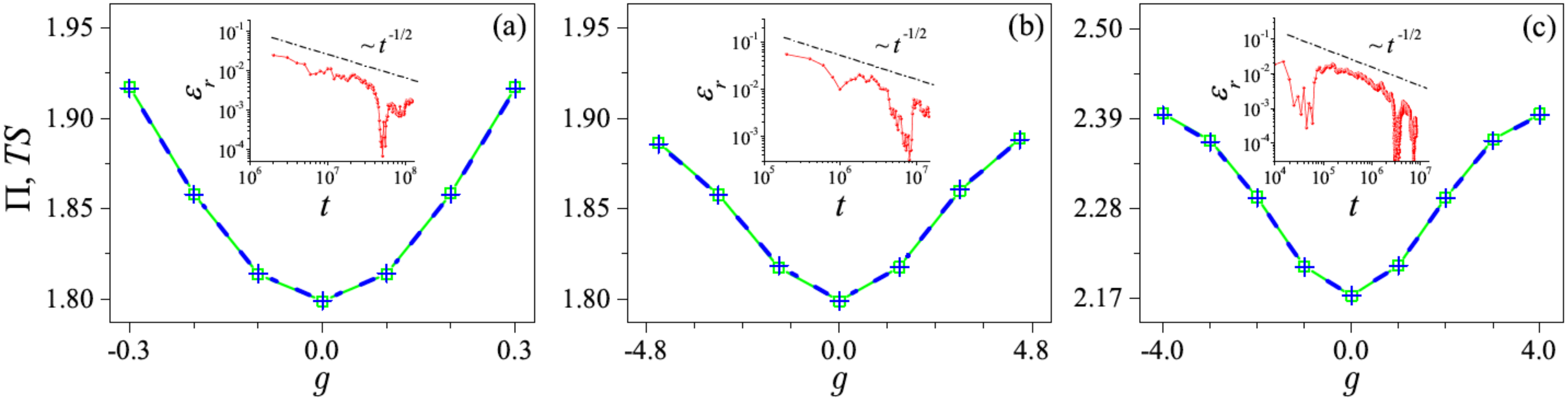
Equations of motion invariant under:

$$\mathcal{M}(x, y, z, p^x, p^y, p^z, t, \boldsymbol{B}) \equiv (x, -y, z, -p^x, p^y, -p^z, -t, \boldsymbol{B})$$

[for constant field see Bonella, Ciccotti, Rondoni, EPL **108**, 60004 (2014)]

[Luo, GB, Casati, Wang, Phys Rev Research **2**, 022009(R) (2020)]

Numerics for a generic magnetic field



$B(x) = gx$

generic 2D case:

$$B(x,y) = g\sin[\pi x/(2L)]\sin[\pi y/(2W)]$$

Theoretical argument: divide the system into small volumes dV_α

Time-reversal trajectories without reversing the field for $dV_\alpha \to 0$

generic 3D case:

$$\boldsymbol{B} = g(B_x, B_y, B_z),$$

$$B_x = f_y f_z,\ B_y = f_z f_x,\ B_z = f_x f_y,$$

$$f_x = \sin[\pi x/(2L)],\ f_y = \sin[\pi y/(2W)],$$

$$f_z = \sin[\pi z/(2H)]$$

[Luo, GB, Casati, Wang, Phys Rev Research **2**, 022009(R) (2020)]

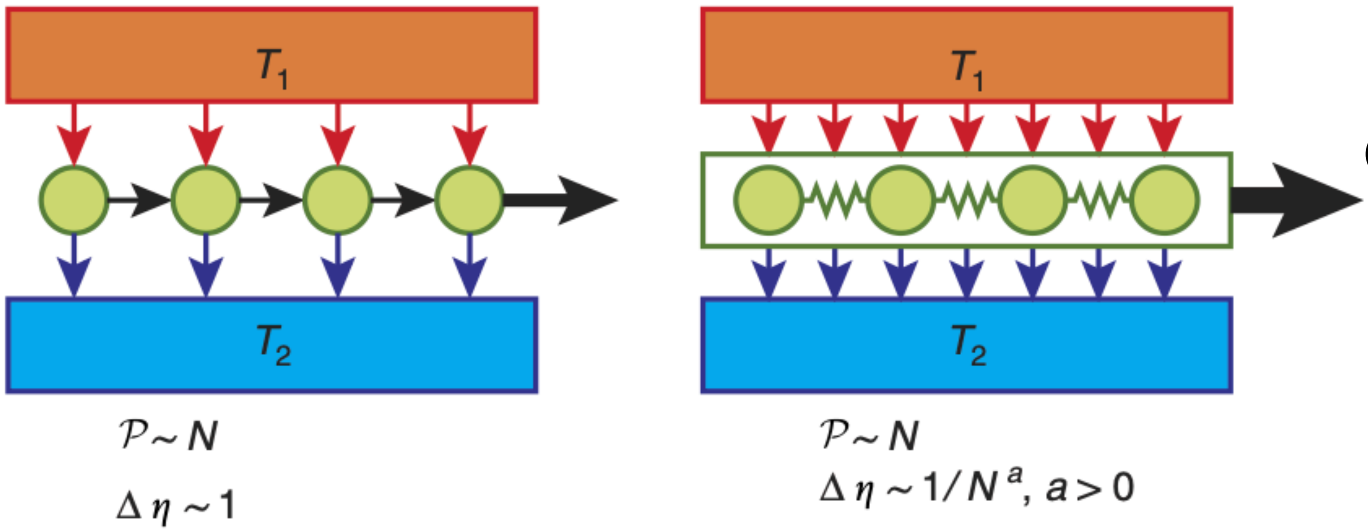
Power-efficiency trade-off

For heat engines described as Markov processes:

$$P \leq A(\eta_C - \eta)$$

[N. Shiraishi, K. Saito, H. Tasaki, PRL **117**, 190601 (2016)]

The prefactor A is system-dependent and may be arbitrarily large, for instance diverge close to a phase transition



Campisi and Fazio, Nature Comm. **7**, 11895 (2016)]

Diverging power fluctuations may, however, make such engines impractical

Thermodynamic uncertainty relations

Thermodynamic uncertainty relations (TURs), for steady-state stochastic heat engines (rate equations, overdamped Langevin dynamics)

First law: $j_w = j_h - j_c = P$

Fluctuations for each of the currents

$$\Delta_\alpha \equiv \lim_{t\to\infty} \langle (j_\alpha(t) - j_\alpha)^2 \rangle t \qquad \alpha = h,\ c,\ w$$

Entropy production rate

$$\dot{S} = j_c/T_c - j_h/T_h = j_w(\eta_C/\eta - 1)/T_c$$

TUR: $$\frac{j_\alpha^2}{\Delta_\alpha} \leq \frac{\dot{S}}{2k_B}$$

Power-efficiency-fluctuations trade-off

For the work current (power) $$\frac{P^2}{\Delta_P} \leq \frac{\dot{S}}{2k_B}$$

$$\Delta_P = \lim_{t\to\infty} [P(t) - P]^2 t$$

P(t) power delivered up to time t

Trade-off between the three desiderata of a heat engine:

$$\mathcal{Q} \equiv P \frac{\eta}{\eta_C - \eta} \frac{k_B T_c}{\Delta_P} \leq \frac{1}{2}.$$

[Pietzonka and Seifert, PRL **120**, 190602 (2018)]

Finite output power at Carnot efficiency only at the price at diverging fluctuations (no engine reliability)

TUR saturation within linear response

Within linear response charge current fluctuations related to conductance via the Johnson-Nyquist fluctuation-dissipation relation

$$\Delta_e = S_0 = 2k_{\rm B}TG,$$

S_0 equilibrium noise (voltage independent)

$$J_e = G\,\Delta V$$

$$\dot{S} = \mathcal{F}_e J_e = \Delta V\, J_e/T$$

$$\frac{J_e^2}{\Delta_e} = \frac{\dot{S}}{2k_{\rm B}}$$

Quantum coherent transport can lead to TUR violation

Expand charge noise and current in powers of the applied voltage

$$J_e = G_1(\Delta V) + \frac{1}{2!}G_2(\Delta V)^2 + \frac{1}{3!}G_3(\Delta V)^3 + \dots ,$$

$$\Delta_e = S_0 + S_1(\Delta V) + \frac{1}{2!}S_2(\Delta V)^2 + \frac{1}{3!}S_3(\Delta V)^3 + \dots$$

$$S_1 = k_B T G_2, \qquad G_1 \equiv G$$

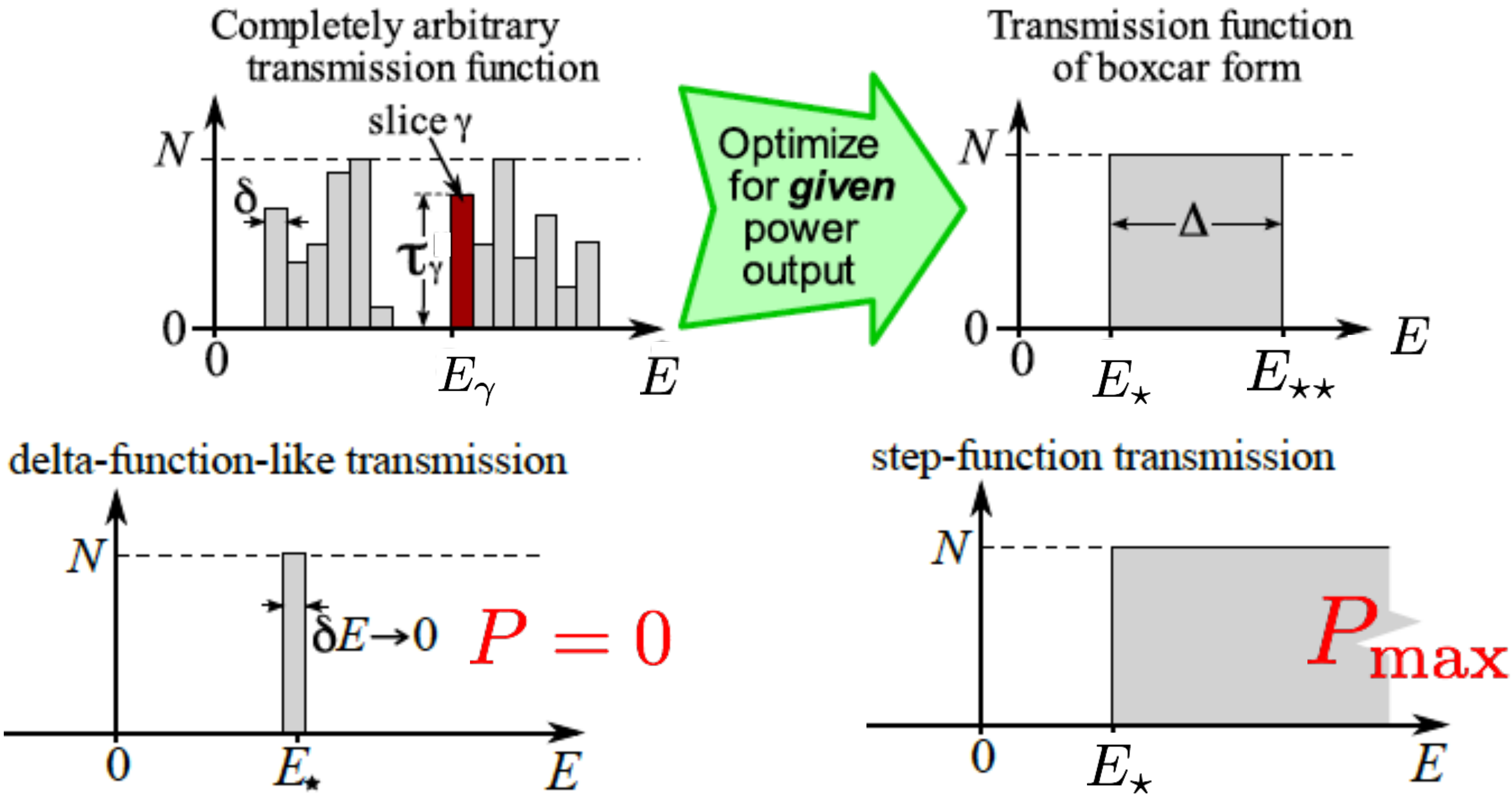
$$\frac{k_B J_e^2}{\dot{S}\Delta_e} = \frac{1}{2} + \frac{(\Delta V)^2}{24 k_B T G_1}(2k_B T G_3 - 3S_2) + O((\Delta V)^3)$$

Quantum coherent transport can lead to second-order correction violating TUR (quantum advantage in thermodynamics of precision)

[Agarwalla and Segal, PRB **98**, 155438 (2018); see also Ptaszyński Phys. Rev. B **98**, 085425 (2018), Rignon-Bret et al., PRE **103**, 012133 (2021), Kalee et al., PRE **104**, L012103 (2021),…]

TUR violation approaching Carnot efficiency?

Find the transmission function that optimizes the heat-engine efficiency for a given output power



[Whitney, PRL **112**, 130601 (2014); PRB **91**, 115425 (2015)]

Fluctuations (scattering theory)

Power fluctuations derived from the Levitov-Lesovik cumulant generating function

$$\Delta_P = (\Delta V)^2 \int_{-\infty}^{+\infty} d\epsilon (\mathcal{T}(\epsilon)\{f_L(\epsilon)[1 - f_L(\epsilon)]$$

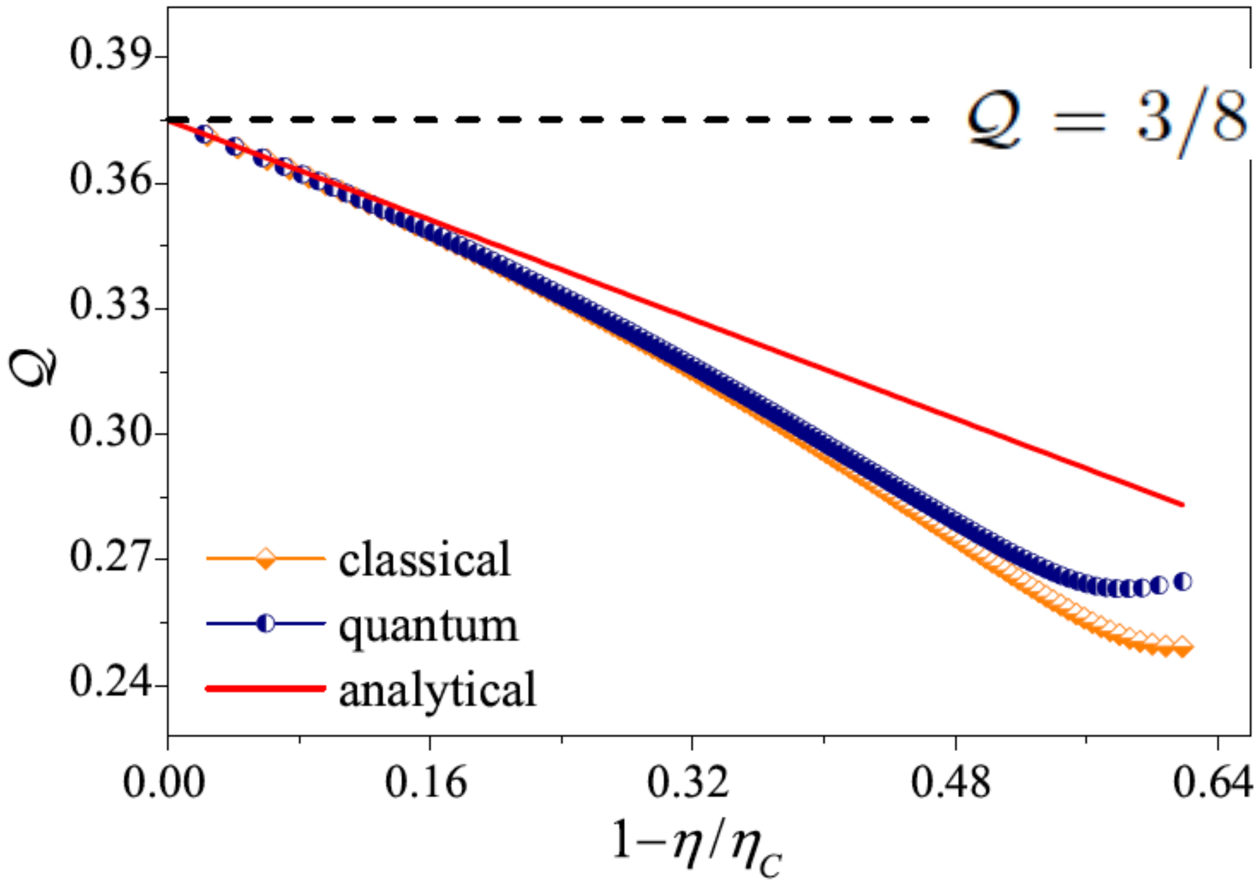
$$+ f_R(\epsilon)[1 - f_R(\epsilon)]\} + \mathcal{T}(\epsilon)[1 - \mathcal{T}(\epsilon)][f_L(\epsilon) - f_R(\epsilon)]^2)$$

For a boxcar transmission function:

$$\Delta_P = \frac{(\Delta\mu)^2}{h} \int_{\epsilon_0}^{\epsilon_1} d\epsilon \left[f_L(\epsilon) + f_R(\epsilon) - f_L^2(\epsilon) - f_R^2(\epsilon)\right]$$

Power-efficiency-fluctuations trade-off

More restrictive bound within Landauer approach

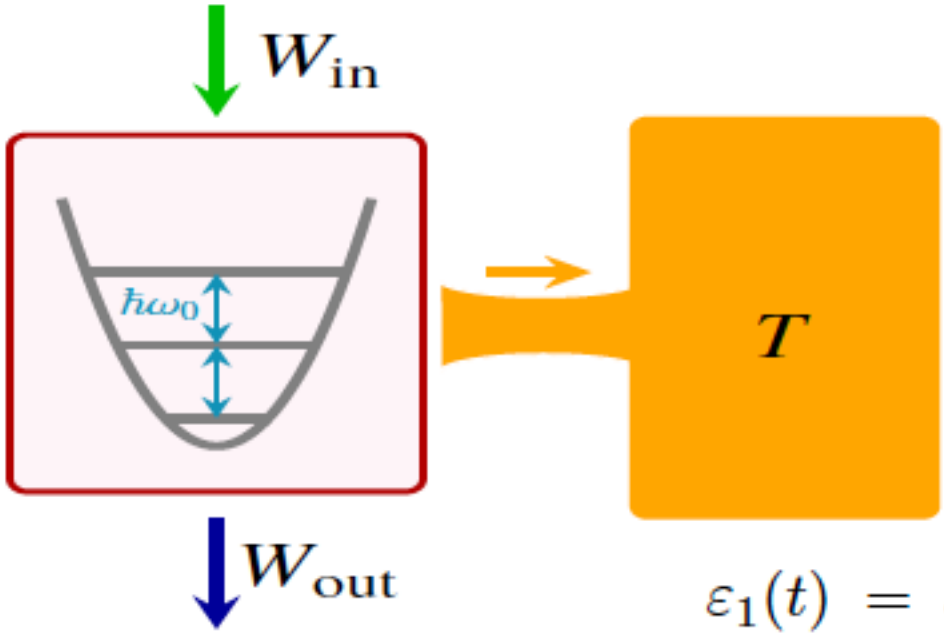


$$\mathcal{Q} = \frac{3}{8} - \frac{9}{128}\frac{T_L + T_R}{T_R}\left(1 - \frac{\eta}{\eta_C}\right) + \mathcal{O}\left[\left(1 - \frac{\eta}{\eta_C}\right)^2\right]$$

[GB, G. Casati, J. Wang; Phys Rev E **102**, 040103(R) (2020)]

Overcoming the bound: periodically driven systems

Isothermal heat engine



$$H(t) = H_{\rm S}(t) + H_{\rm R} + H_{\rm SR}$$

$$H_{\rm S}(t) = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2 - \varepsilon_1(t)x - \varepsilon_2(t)p$$

$$\varepsilon_i(t) = \varepsilon_i(t + \mathcal{T})$$

$$\varepsilon_1(t) \;=\; \varepsilon_1 \sin\omega t,\; \varepsilon_2(t) \;=\; \varepsilon_2 \cos(\omega t - \varphi)$$

$$H_{\rm R} + H_{\rm SR} = \sum_{k=1}^{\infty} \frac{P_k^2}{2m_k} + \frac{m_k\omega_k^2}{2}\left(X_k - \frac{c_k}{m_k\omega_k^2}x\right)^2$$

[L. M. Cangemi, M. Carrega, A. De Candia, V. Cataudella, G. De Filippis, M. Sassetti, GB, PRR **3**, 013237 (2021)]

Advantages of the model

It can be analytically solved, also in the far from equilibrium regime and for strong system-bath coupling, without resorting to overdamped limit, Markovian master equation or other approximations

Possible to break time reversibility

Address all driving regimes from the quasistatic to the antiadiabatic one

Non-Markovian effects can be addressed by engineering the bath spectral density

$$J(\omega) = m\gamma_s \bar{\omega}^{1-s} \frac{\omega^s}{1 + (\omega/\omega_c)^2}$$

Equations of motion

$$\langle \dot{x}(t) \rangle = \frac{\langle p(t) \rangle}{m} - \varepsilon_2(t),$$

$$\langle \ddot{x}(t) \rangle + \int_{-\infty}^{t} dt' \gamma(t-t') \langle \dot{x}(t') \rangle + \omega_0^2 \langle x(t) \rangle = \frac{\varepsilon_1(t)}{m} - \dot{\varepsilon}_2(t),$$

starting from a factorised initial state, with the bath at thermal equilibrium

$$\rho_{\rm tot}(t_0) = \rho_S(t_0) \otimes \rho_R(t_0) \qquad \rho_R(t_0) = \exp(-H_{\rm R}/T)/{\rm Tr}\{\exp(-H_{\rm R}/T)\}$$

with $t_0 \to -\infty$ the initial time

the memory kernel describes friction:

$$\gamma(t) = \tfrac{2}{\pi m} \theta(t) \int_0^{+\infty} d\omega J(\omega) \cos(\omega t)/\omega$$

Power and fluctuations

Power along the input/output channels

$$P_1(t) = -\dot{\varepsilon}_1(t)\langle x(t)\rangle, \quad P_2(t) = -\dot{\varepsilon}_2(t)\langle p(t)\rangle$$

Average powers $$P_i = \frac{1}{\mathcal{T}}\int_{\bar{t}}^{\mathcal{T}+\bar{t}} dt P_i(t)$$

Power fluctuations $$D_i(t) = \frac{1}{t-t_0}\int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_1 \langle \delta P_i(t_2)\delta P_i(t_1)\rangle,$$

$$\delta P_1(t) = -\dot{\varepsilon}_1(t)[x(t) - \langle x(t)\rangle],$$

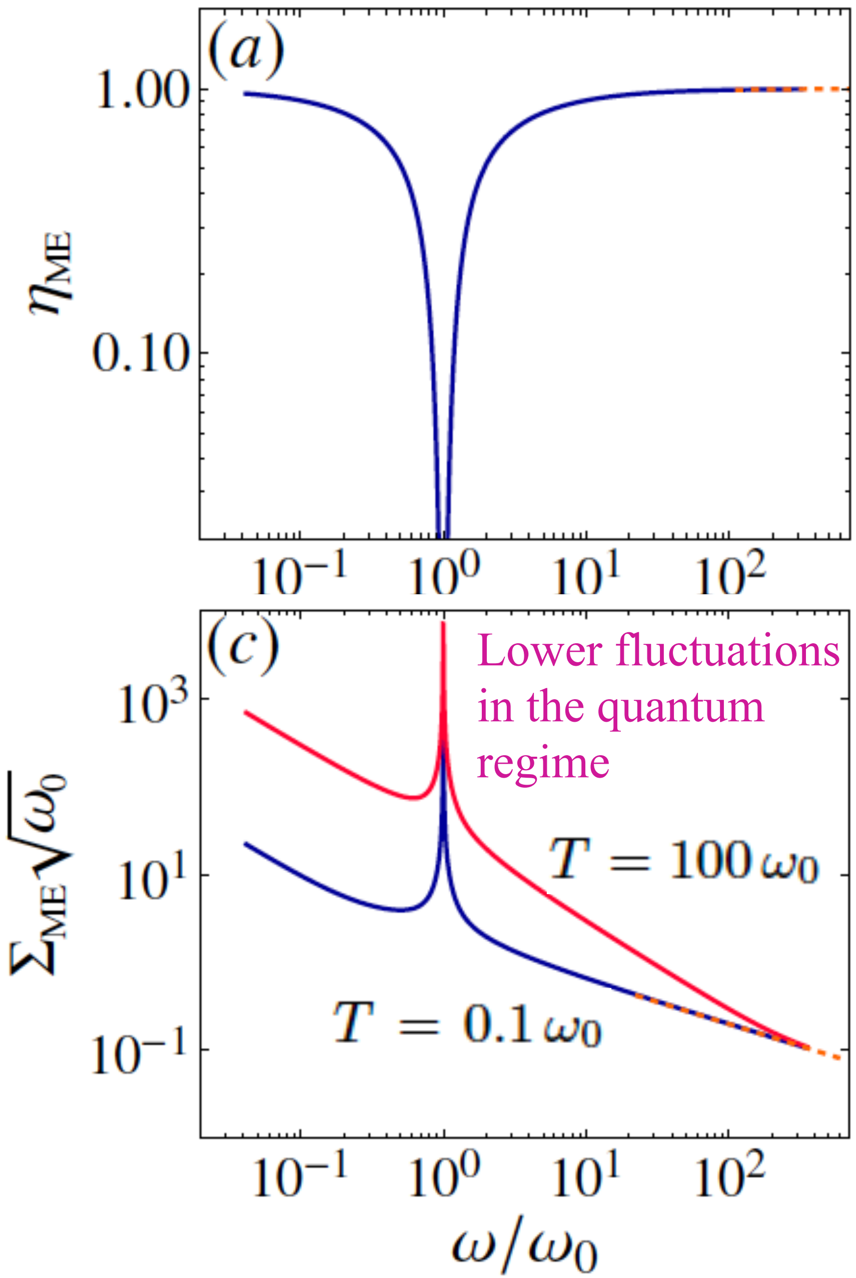
$$\delta P_2(t) = -\dot{\varepsilon}_2(t)[p(t) - \langle p(t)\rangle]$$

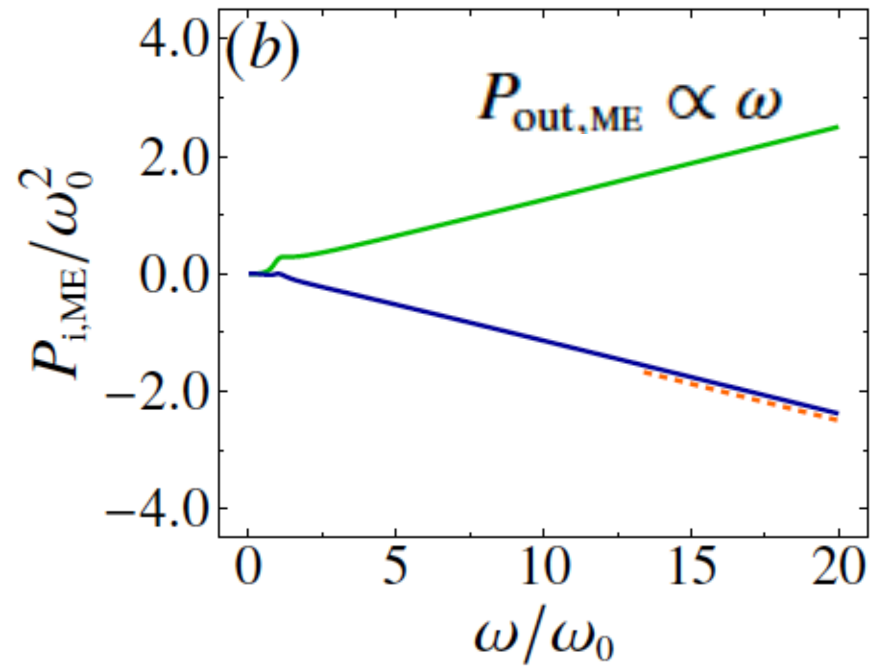
Heat $$P = P_1 + P_2 = \langle \dot{H}_R\rangle$$

Efficiency $$\eta \equiv \frac{P_{\text{out}}}{P_{\text{in}}} \qquad P_{\text{in}} = P_2 > 0 \qquad P_{\text{out}} = -P_1 \quad (P_1 < 0)$$

Anti-adiabatic regime: approaching Carnot at finite power and small fluctuations

Ohmic friction $s = 1$



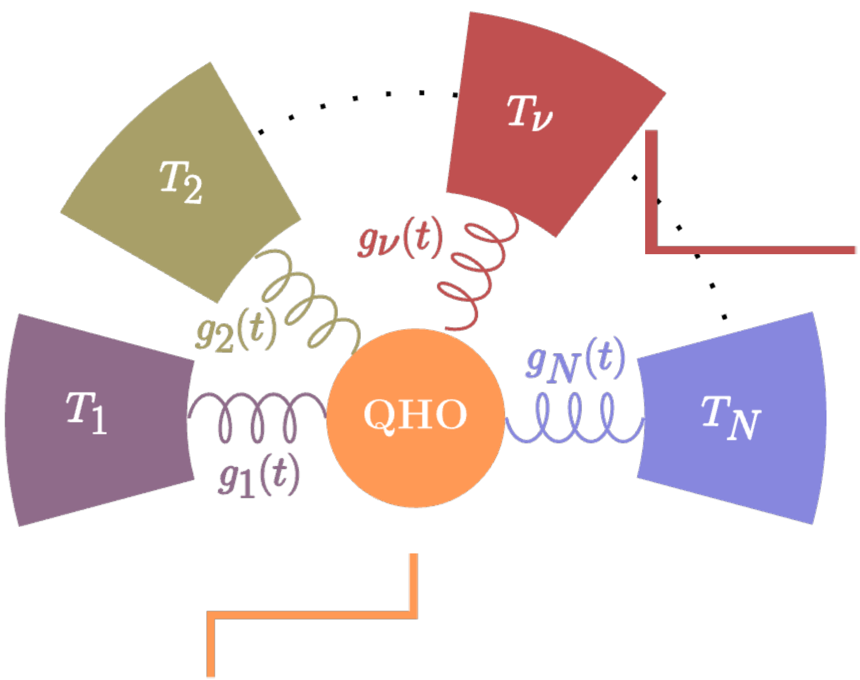


$$\Sigma_{\rm ME} = \sqrt{D_{\rm out,ME}/P^2_{\rm out,ME}}$$

Required ingredients:

- breaking time-reversal symmetry
- beyond the overdamped approximation

Generalization to two or more reservoirs (with periodically modulated system-baths couplings)



$$H^{(t)} = H_{\rm WM} + \sum_{\nu=1}^{N} \left[H_\nu + H^{(t)}_{{\rm int},\nu} \right]$$

Bath

Collection of harmonic oscillators (Caldeira-Leggett framework)

$$H_\nu = \sum_{k=1}^{\infty} \left[\frac{P^2_{k,\nu}}{2m_{k,\nu}} + \frac{1}{2} m_{k,\nu}\omega^2_{k,\nu} X^2_{k,\nu} \right]$$

Interaction WM-Bath

Driven periodic coupling

$$H^{(t)}_{{\rm int},\nu} = \sum_{k=1}^{\infty} \left\{ -x g_\nu(t) c_{k,\nu} X_{k,\nu} + x^2 g^2_\nu(t) \frac{c^2_{k,\nu}}{2m_{k,\nu}\omega^2_{k,\nu}} \right\}$$

$c_{k,\nu}$ coupling strength

g_ν (t) dimensionless function

$$g_\nu(t) = g_\nu(t+\mathcal{T}) = \sum_{n=-\infty}^{+\infty} g_{n,\nu} e^{-in\Omega t}, \quad \Omega = 2\pi/\mathcal{T}$$

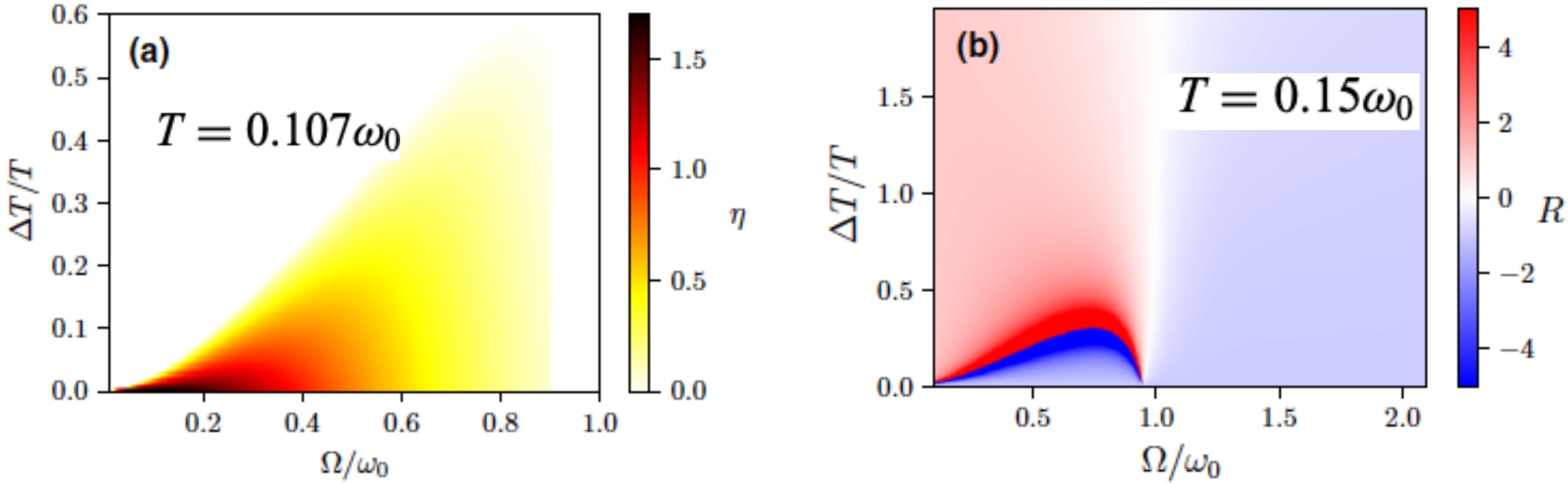
Working medium:

quantum harmonic oscillator

$$H_{\rm WM} = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2$$

[M. Carrega, L. M. Cangemi, G. De Filippis, V. Cataudella, GB, M. Sassetti, PRX Quantum **3**, 010323 (2022)]

The formalism is versatile and promising to investigate thermal engines and heat management in structured environments, also beyond weak coupling



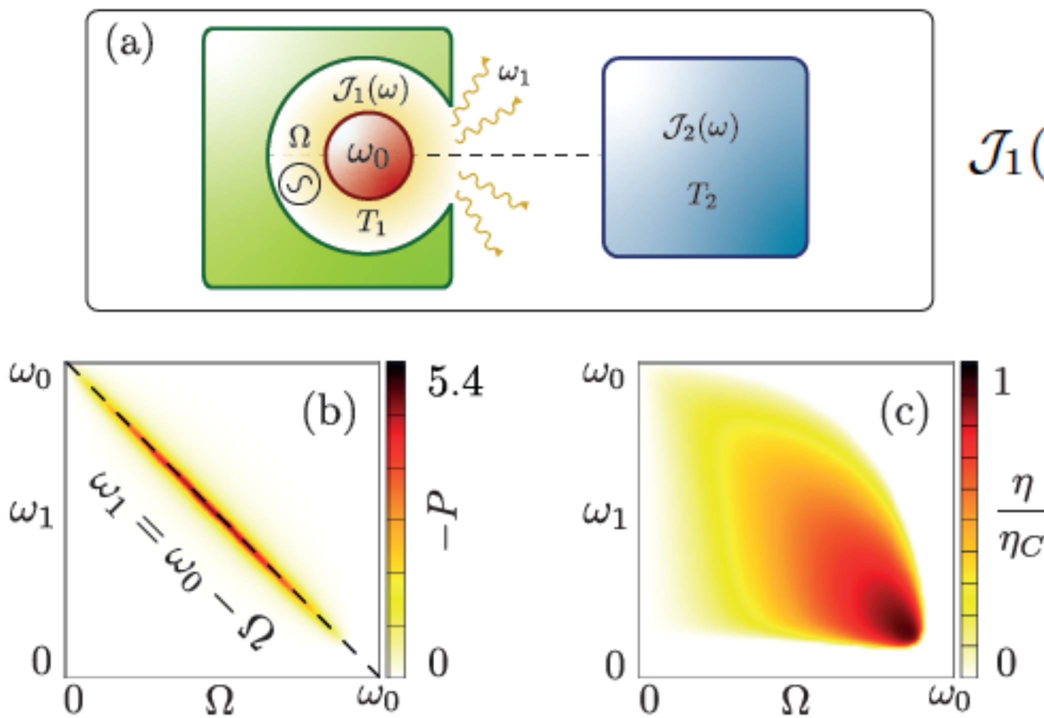
COP $J_1/|J_1 + J_2|$

Rectification factor $R \equiv -\frac{J_1^f(T, \Delta T)}{J_1^b(T, \Delta T)}$

[M. Carrega, L. M. Cangemi, G. De Filippis, V. Cataudella, GB, M. Sassetti, PRX Quantum **3**, 010323 (2022)]

Dynamical heat engines with non-Markovian environments

Non-Markovianity necessary but non sufficient condition to obtain a heat engine (with monochromatic driving of the coupling to one reservoir)



Lorentzian bath

$$\mathcal{J}_1(\omega) = \frac{d_1 m \gamma_1 \omega}{(\omega^2 - \omega_1^2)^2 + \gamma_1^2 \omega^2}$$

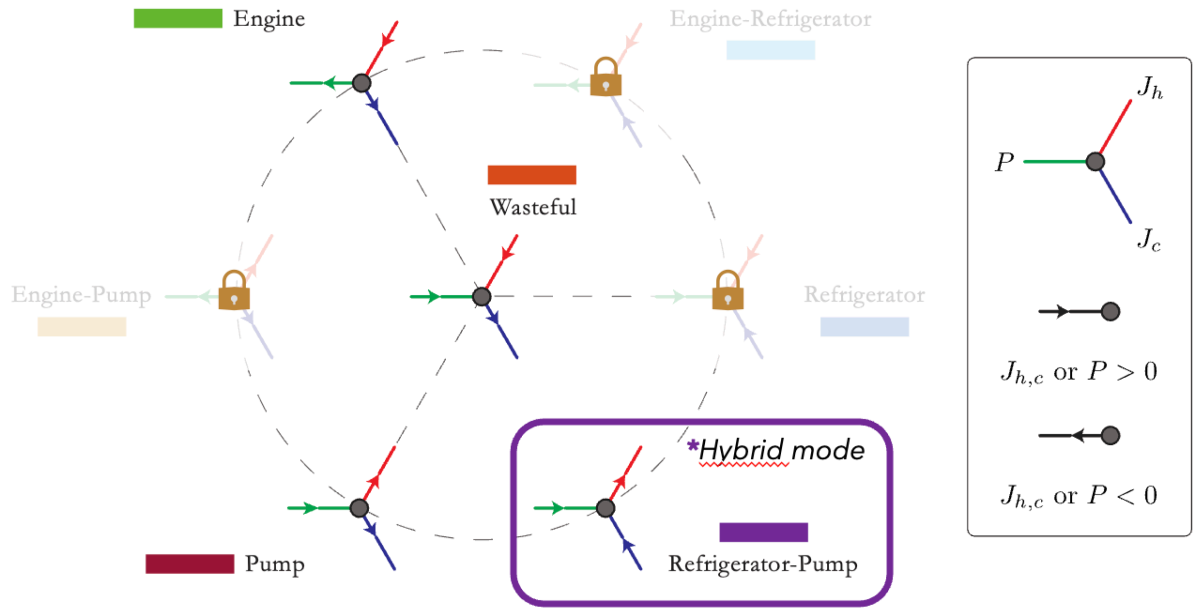
Paradigmatic example of **structured non-Markovian environment**

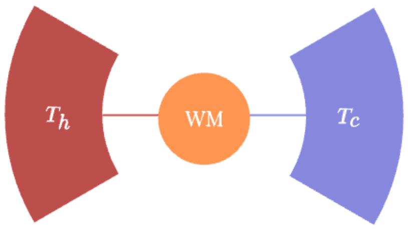
Ohmic bath

$J_2(\omega) = m\gamma_2\, \omega$

[F. Cavaliere, M. Carrega, G. De Filippis, V. Cataudella, GB, M. Sassetti, Phys. Rev. Res. **4**, 033233 (2022)]

Hybrid quantum thermal machines

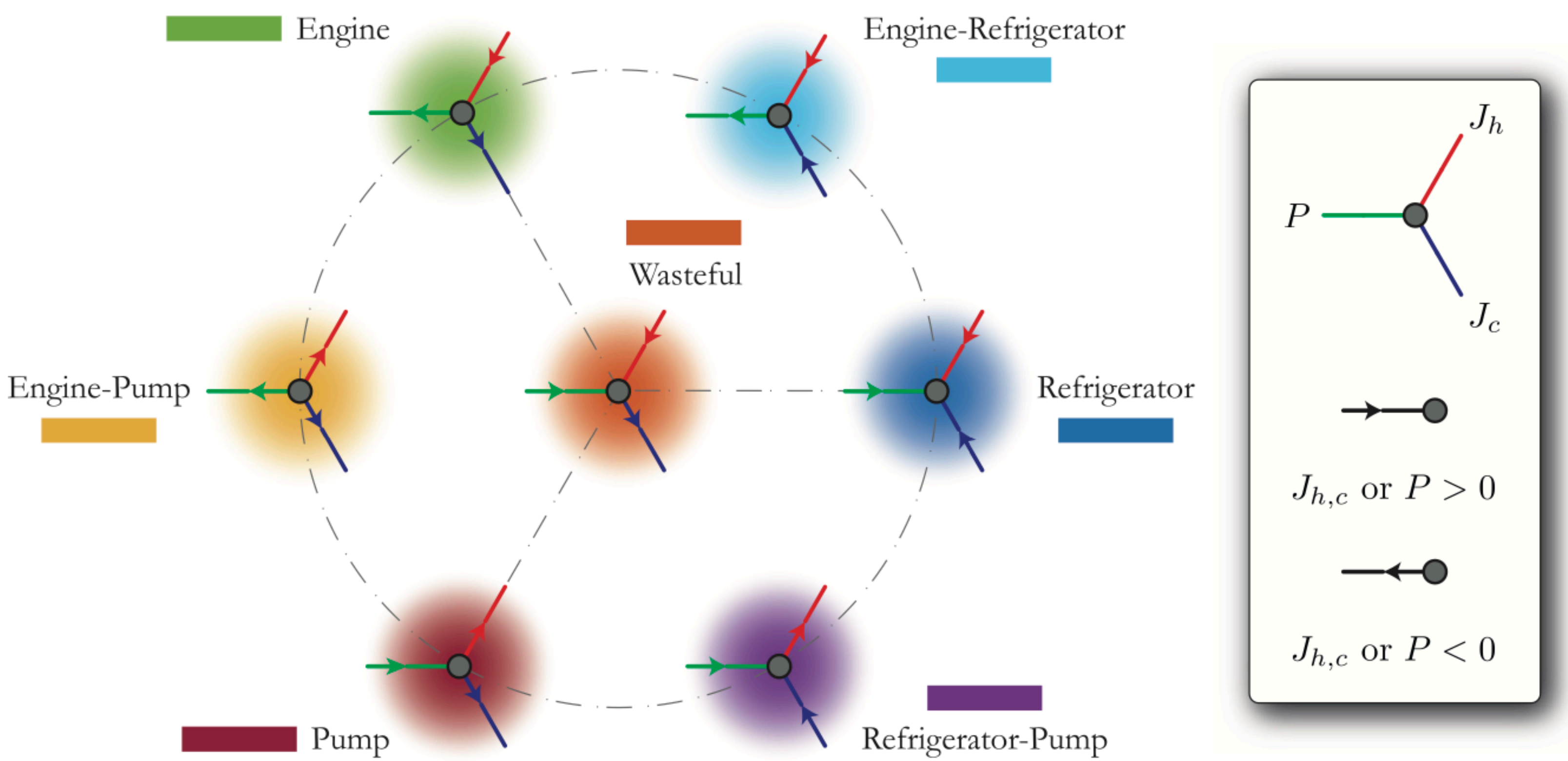


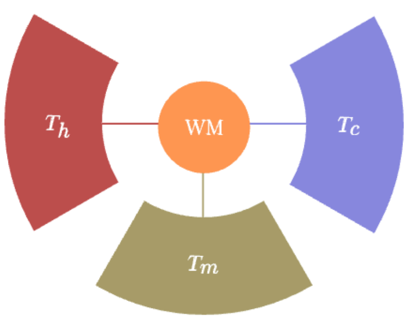


Two-terminal device

Standard thermal machines consists of a working medium connected to two heat baths, a cold reservoir and a hot one.

Thermodynamics laws allow only **three useful tasks** (heat engine, **refrigerator-pump***, and heat pump) and a **wasteful** one.





Three-terminal device

Multiterminal devices have the advantage of performing **more than one useful task simultaneously** (hybrid thermal machines).

In a three-terminal device we can explore **all** the three **pure modes** (engine, refrigerator, pump) and **all** the three **hybrid modes**.

[Entin-Wohlman et al.,Phys. Rev. B **91**, 054302 (2015); Manzano et al., Phys. Rev. Res. **2,** 043302 (2020); López et al., Phys. Rev. Research 5, 013038 (2023); Lu et al., Phys. Rev. B **107**, 075428 (2023), …]

Exergy efficiency (or second-law efficiency)

Entropy production rate $\dot{S} = -\sum_{\nu=1}^{N} \frac{J_\nu}{T_\nu} \geq 0$ (2nd Law of TD)

Split positive (+) from negative (−) contributions $\dot{S} = \dot{S}^{(+)} + \dot{S}^{(-)}$

The **exergy efficiency** is defined as the ratio of $\dot{S}^{(-)}$ (the useful inputs) to $\dot{S}^{(+)}$ (the wasteful outputs)

$$0 \leq \phi = -\frac{\dot{S}^{(-)}}{\dot{S}^{(+)}} \leq 1$$

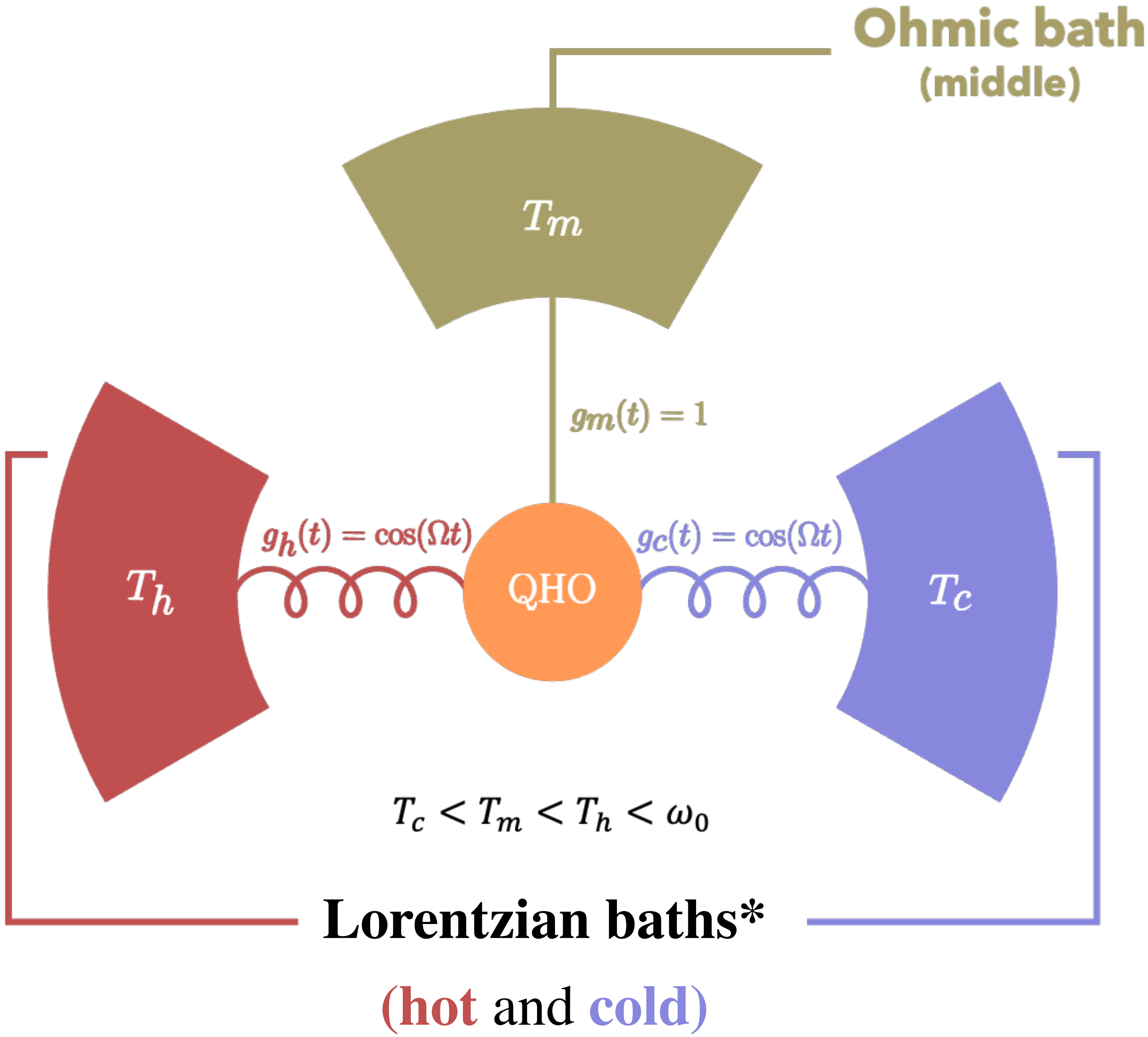
Bounds due to $\dot{S} = \dot{S}^{(+)} - |\dot{S}^{(-)}| \geq 0 \Rightarrow |\dot{S}^{(-)}| \leq \dot{S}^{(+)}$

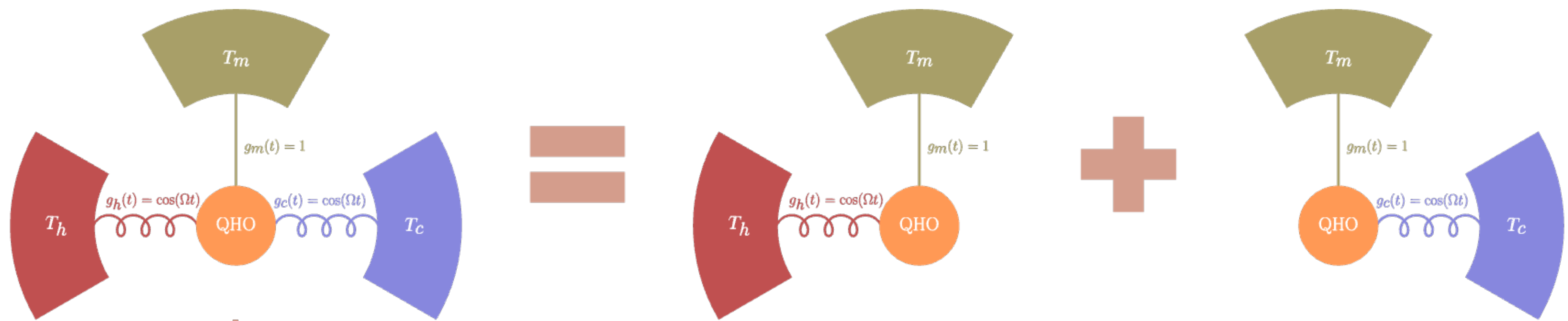
Model: *QHO coupled to three baths*

*Coupling **modulated** by a **monochromatic** driving

Spectral density, $\nu = h, c$

$$\mathcal{J}_\nu(\omega) = \frac{d_\nu m \gamma_\nu \omega}{\left(\omega^2 - \omega_\nu^2\right)^2 + \gamma_\nu^2 \omega_\nu^2}$$





$\gamma_m \ll \omega_0$

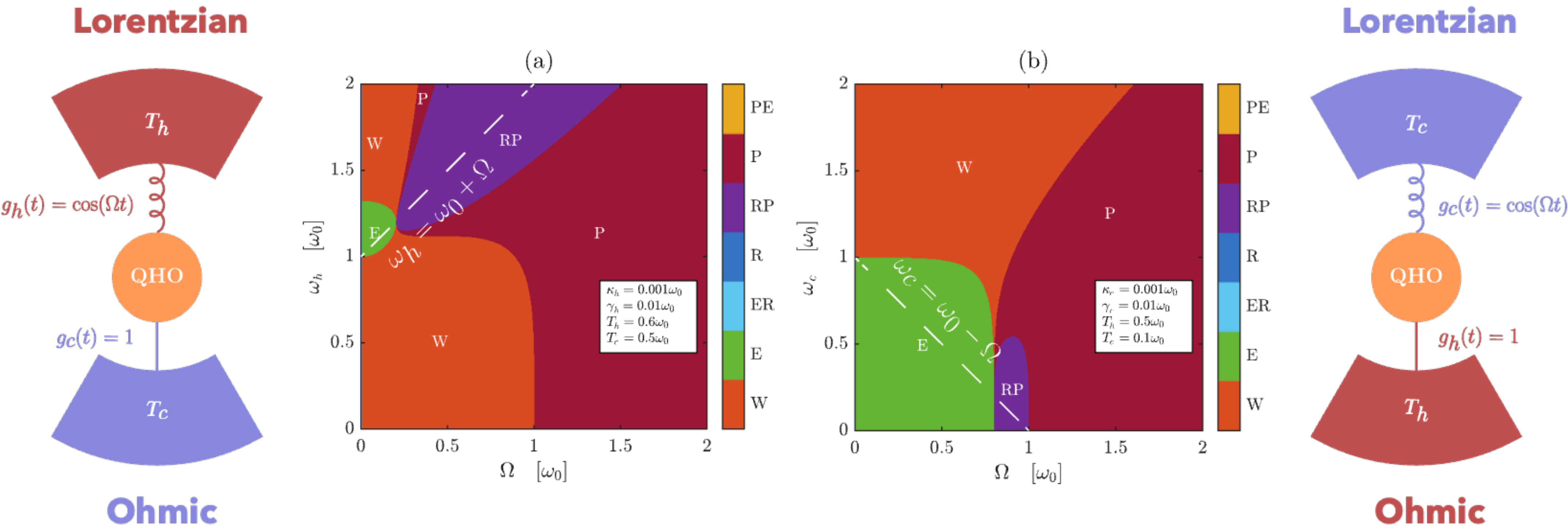
$$P = -\frac{\Omega}{8m\omega_0} \sum_{\nu=h,c} \sum_{p=\pm 1} p\mathcal{J}_\nu(\omega_0 + p\Omega) \left[\coth\left(\frac{\omega_0 + p\Omega}{T_\nu}\right) - \coth\left(\frac{\omega_0}{T_m}\right)\right]$$

$$J_\nu = \frac{1}{8m\omega_0} \sum_{p=\pm 1} (\omega_0 + p\Omega)\mathcal{J}_\nu(\omega_0 + p\Omega) \left[\coth\left(\frac{\omega_0 + p\Omega}{T_\nu}\right) - \coth\left(\frac{\omega_0}{T_m}\right)\right]$$

Weak-coupling with Lorentzian baths

In this regime the three-terminal device is equivalent to two two-terminal devices working together

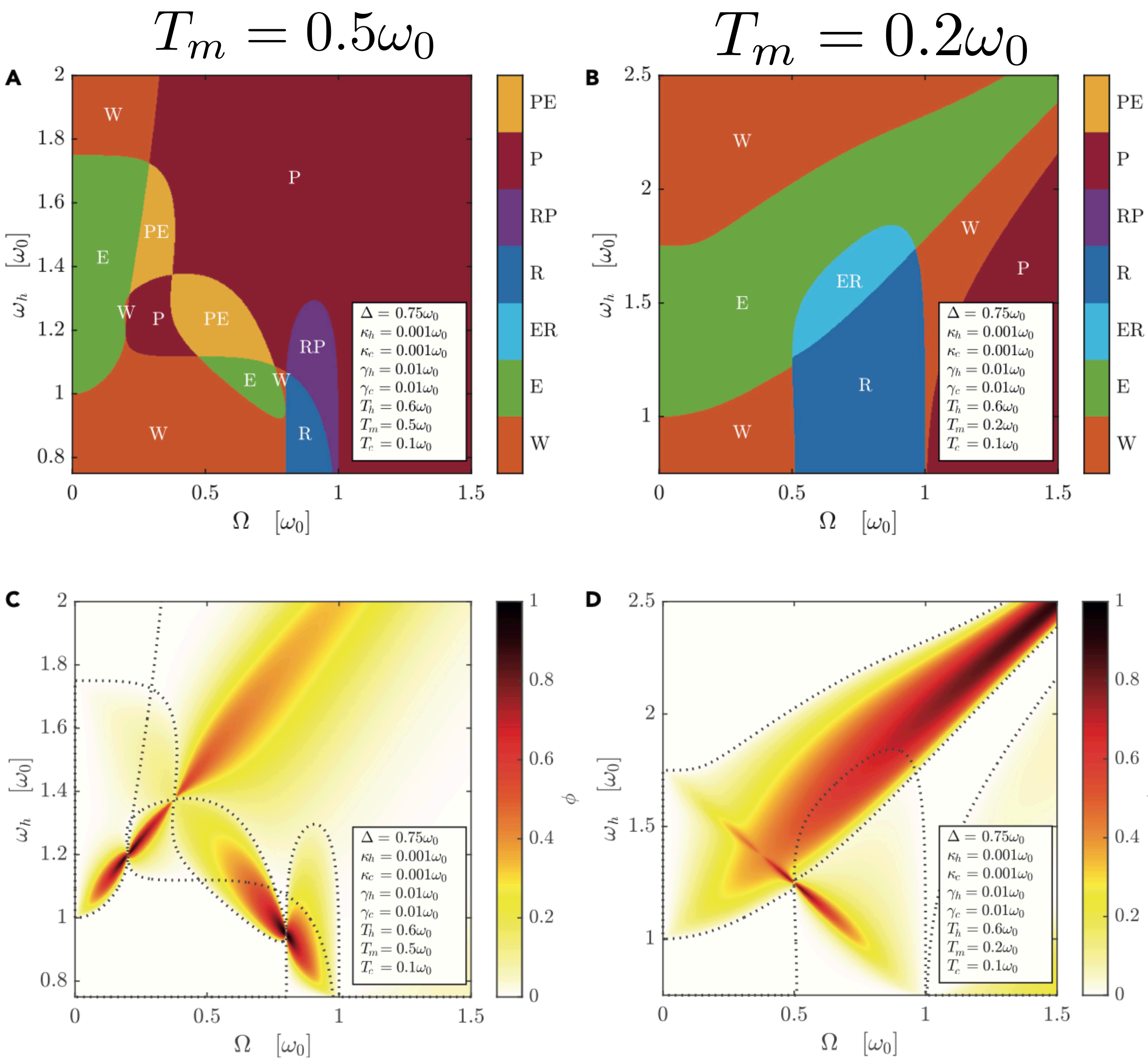
Operating modes in a two-terminal device



Introduce the **detuning parameter** $\Delta=\omega_c-\omega_h$, with ω_ν of the Lorentzian spectral density $J_\nu(\omega)$

Find Δ to obtain a suitable **mixing of the operating modes**

Hybrid operation of a three-terminal device



operating modes

exergy efficiency

[F. Cavaliere, L. Razzoli, M. Carrega, GB and M. Sassetti, iScience **26**, 106235 (2023)]

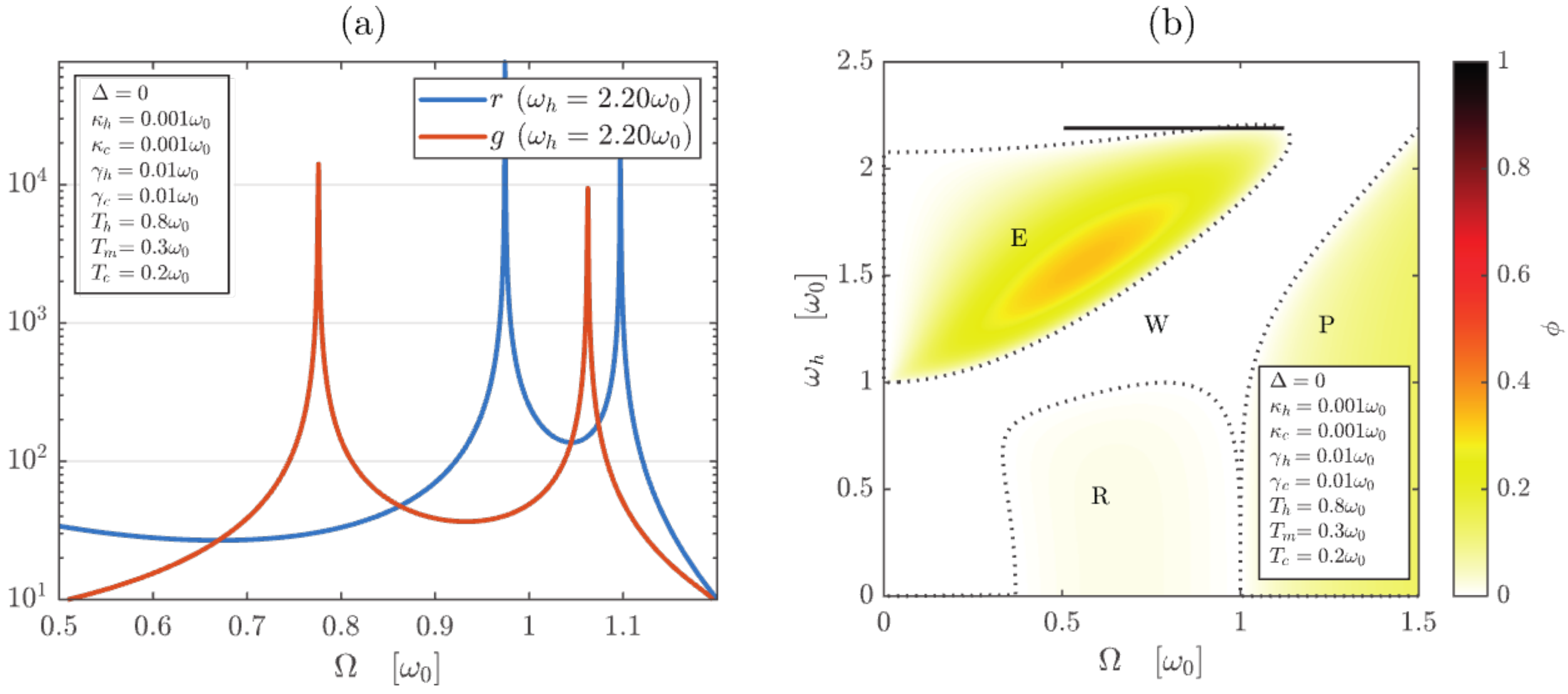
Three-terminal device as a thermal transistor

O/I ratio

$$r = \frac{J_h}{P}$$

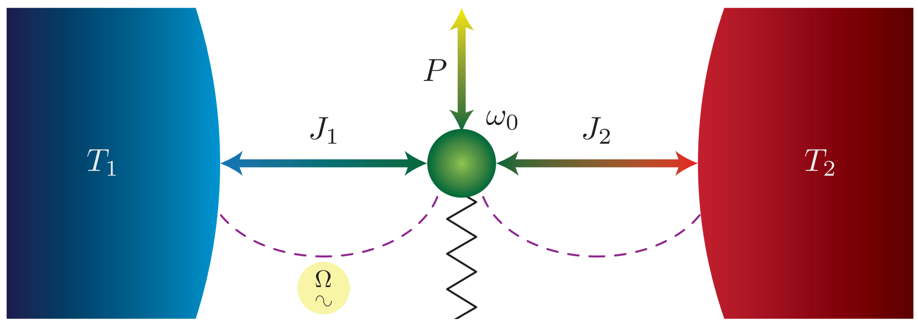
Differential gain

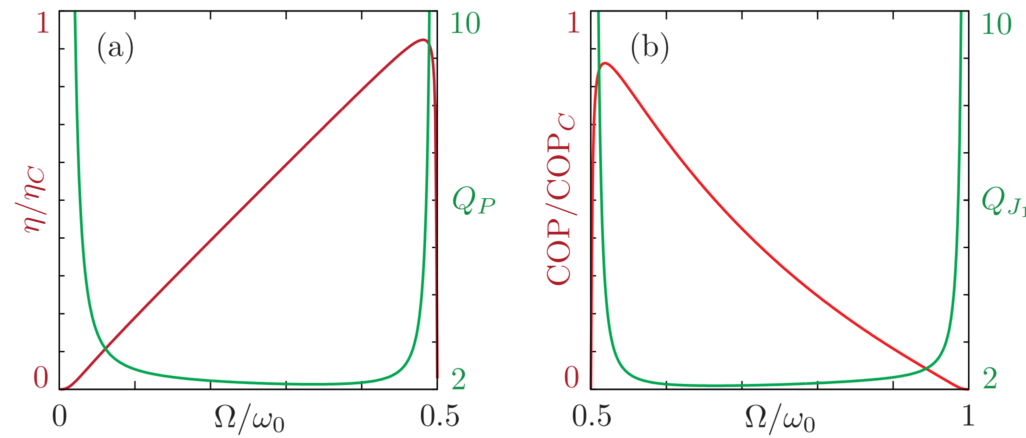
$$g = \left|\frac{\partial J_h}{\partial P}\right| = \left|\frac{\partial J_h/\partial \Omega}{\partial P/\partial \Omega}\right|$$



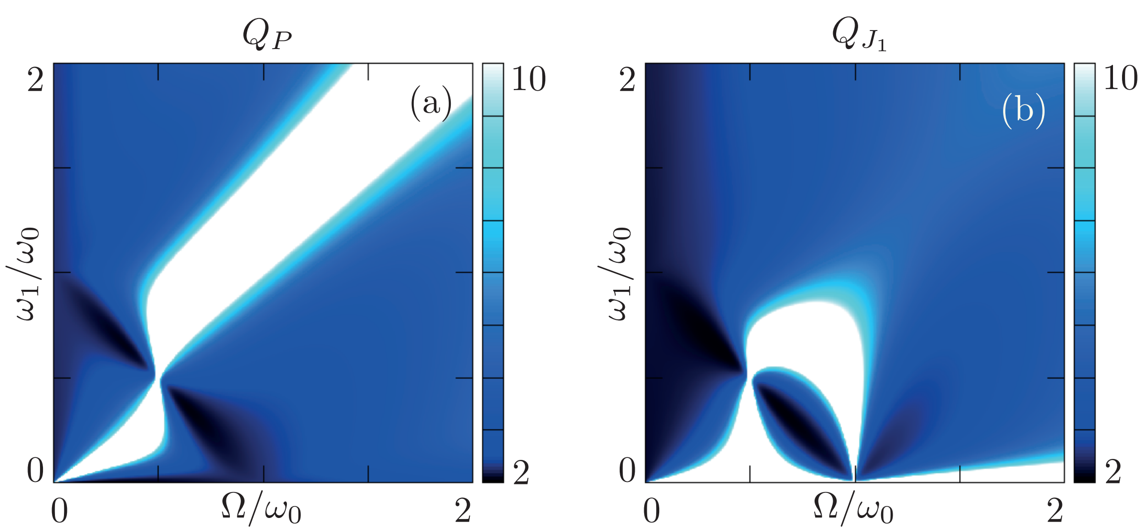
[F. Cavaliere, L. Razzoli, M. Carrega, GB and M. Sassetti, iScience **26**, 106235 (2023)]

No violation of TURs in this setup





$$\omega_1 = \omega_0 - \Omega$$



$$Q_P = \dot{S}\frac{D_P}{P^2} \geq 2 \quad Q_{J_1} = \dot{S}\frac{D_{J_1}}{J_1^2} \geq 2$$

[L. Razzoli, F. Cavaliere, M. Carrega, M. Sassetti and GB,
Eur. Phys. J. Spec. Top. (2023)]

Some open problems

Explore more complex architecture for the working medium: Violation of TURs possible?

Extend optimal control techniques to driven quantum heat engines, beyond Markovian master equations

Trade-off between precision and initialisation time for qubit preparation (cooling, third law of thermodynamics)

On a more general side, optimize the energetic consumption of future quantum technologies