Onsager relations, non equilibrium phase transitions and absolute negative mobility

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Outline

Coupled charge and heat flow: a dynamical system's perspective on a fundamental problem of statistical physics (with practical interest: thermoelectricity, ...)

Validity of Onsager reciprocal relations in the presence of a generic magnetic field: consequences for heat to work conversion

Power-efficiency-fluctuations trade-off: the role of interactions

Periodically driven heat engines in the anti-adiabatic regime

Inverse currents in coupled transport

General consideration on thermal engines

Upper bound to efficiency given by the Carnot efficiency:

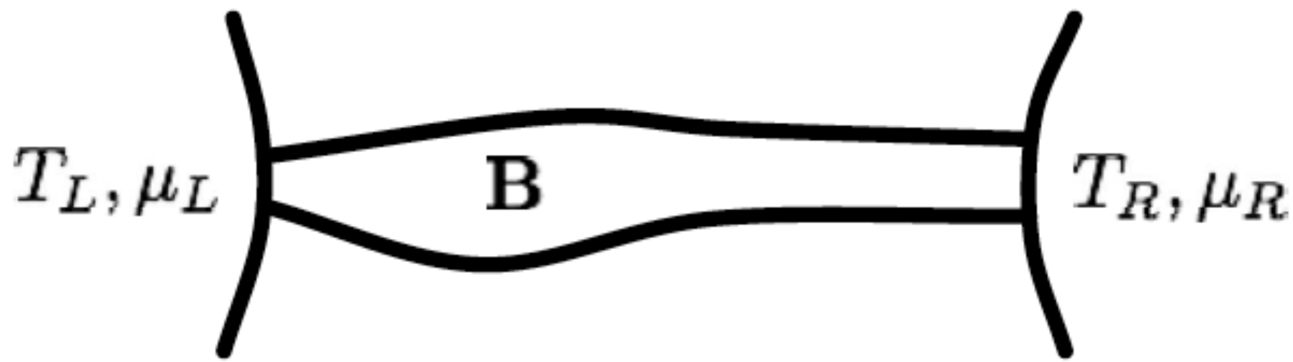
$$\eta = \frac{W}{Q_H} \leq \eta_C \doteq 1 - \frac{T_C}{T_H}$$

$$(T_H > T_C)$$

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)

Carnot efficiency at finite power with breaking Onsager symmetry?



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

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

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

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

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

$$\Delta T = T_L - T_R$$

(we assume $T_L > T_R, \;\; \mu_L < \mu_R$)

Constraints from thermodynamics

POSITIVITY OF THE ENTROPY PRODUCTION:

$$\dot{\mathcal{S}} = \mathfrak{F}_e J_e + \mathfrak{F}_h J_h \geq 0 \quad \Rightarrow \quad \begin{aligned} & L_{ee} \geq 0 \\ & L_{hh} \geq 0 \\ & L_{ee} L_{hh} - \frac{1}{4} (L_{eh} + L_{he})^2 \geq 0 \end{aligned}$$

ONSAGER-CASIMIR RELATIONS:

$$L_{ij}(\mathbf{B}) = L_{ji}(-\mathbf{B})$$

Breaking Onsager symmetry

Onsager reciprocal relations reflect at the macroscopic level the time-reversal symmetry of the microscopic dynamics, invariant under the transformation:

$$\mathcal{T}(\boldsymbol{r},\boldsymbol{p},t) \equiv (\boldsymbol{r},-\boldsymbol{p},-t) \quad \Rightarrow \quad L_{jk} = L_{kj}$$

Ex: the heat flow per unit voltage (related to Peltier coefficient) is equal to the charge flow per unit of temperature difference (related Seebeck coefficient)

With an applied magnetic field one instead obtains Onsager-Casimir relations:

$$\mathcal{T}_{\boldsymbol{B}}(\boldsymbol{r},\boldsymbol{p},t,\boldsymbol{B}) \equiv (\boldsymbol{r},-\boldsymbol{p},-t,-\boldsymbol{B}) \quad \Rightarrow \quad L_{jk}(\boldsymbol{B}) = L_{kj}(-\boldsymbol{B})$$

but in principle one could break the Onsager symmetry:

$$L_{jk}(\boldsymbol{B}) \neq L_{kj}(\boldsymbol{B})$$

Linear response: Maximum efficiency depends on two parameters

$$x = \frac{L_{eh}}{L_{he}} = \frac{S(\boldsymbol{B})}{S(-\boldsymbol{B})}$$

$$y = \frac{L_{eh}L_{he}}{\det \boldsymbol{L}} = \frac{G(\boldsymbol{B})S(\boldsymbol{B})S(-\boldsymbol{B})}{K(\boldsymbol{B})}T$$

$$\eta_{\max} = \eta_C \, x \, \frac{\sqrt{y+1}-1}{\sqrt{y+1}+1}$$

At $B = 0$ there is time-reversibility and:

asymmetry parameter $x = 1$

the efficiency only depends on $y(x = 1) = ZT$

Output power at maximum efficiency

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

When time-reversibility is broken, <u>within linear response</u> it is not forbidden from the second law to have simultaneously Carnot efficiency and non-zero power.

Terms of higher order in the entropy production, beyond linear response, will generally be non-zero. However, irrespective how close we are to the Carnot efficiency, we could in principle find small enough forces such that the linear theory holds.

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

Reversible part of the currents

$$J_i^{\text{rev}} = \sum_{j=e,h} \frac{L_{ij} - L_{ji}}{2} \mathcal{F}_j$$

$$J_i^{\text{irr}} = \sum_{j=e,h} \frac{L_{ij} + L_{ji}}{2} \mathcal{F}_j$$

The reversible part of the currents does not contribute to entropy production

$$\dot{\mathscr{S}} = \mathcal{F}_e J_e + \mathcal{F}_h J_h = J_e^{\text{irr}} \mathcal{F}_e + J_h^{\text{irr}} \mathcal{F}_h$$

Possibility of dissipationless transport?

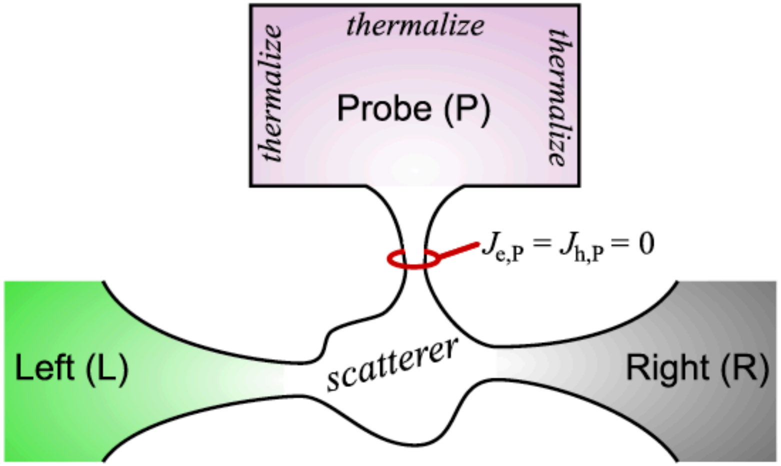
[K. Brandner, K. Saito, U. Seifert, PRL **110**, 070603 (2013)]

How to obtain asymmetry in the Seebeck coefficient?

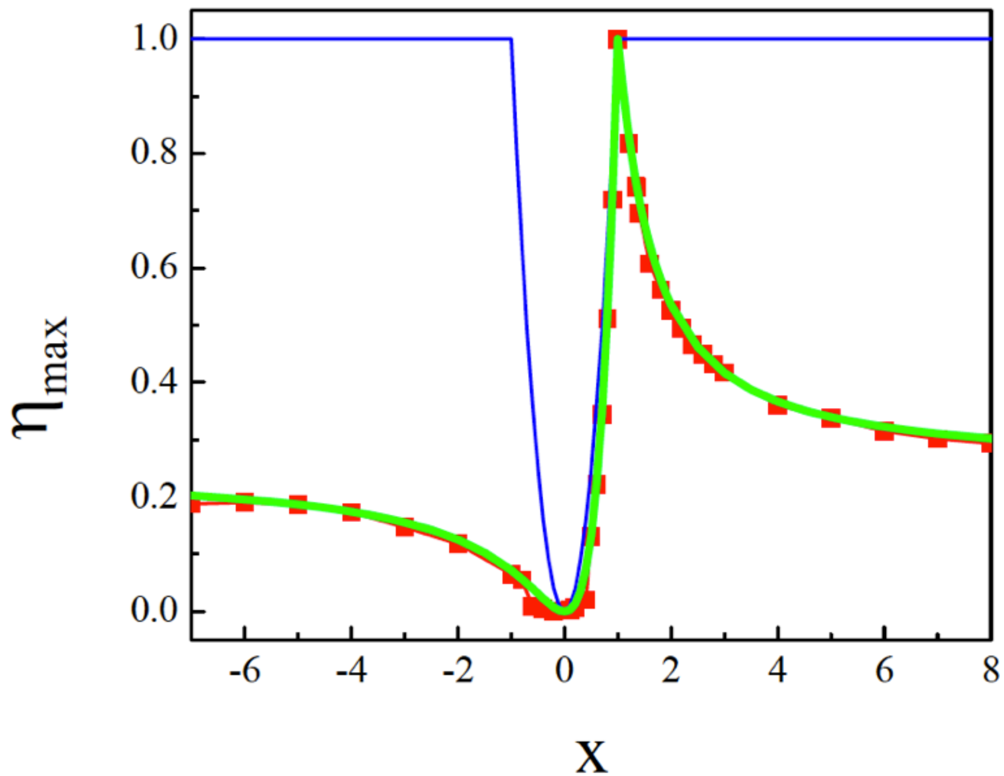
For non-interacting systems, due to the symmetry properties of the scattering matrix ⇒ $S(\mathbf{B}) = S(-\mathbf{B})$

This symmetry does not apply when electron-phonon and electron-electron interactions are taken into account

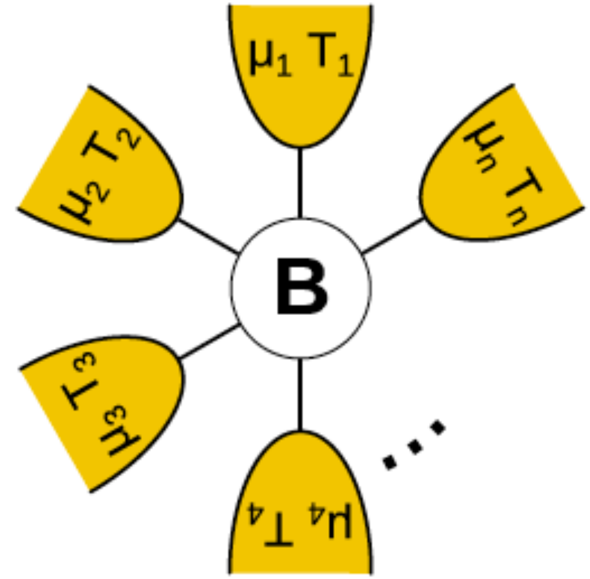
Let us consider the case of partially coherent transport, with inelastic processes simulated by **"conceptual probes"** mimicking inelastic scattering (Buttiker, 1988).

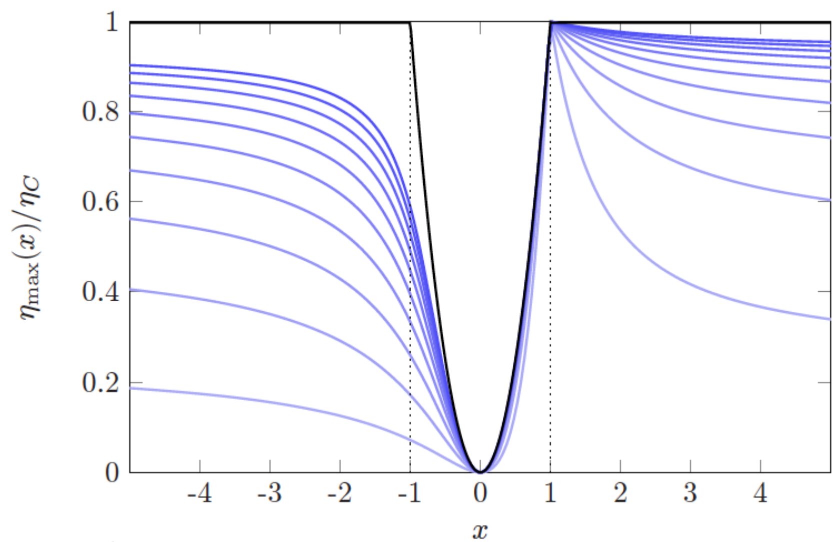


Non-interacting multi-terminal bound



[V.. Balachandran, G. B., G. Casati, PRB **87**, 165419 (2013)]



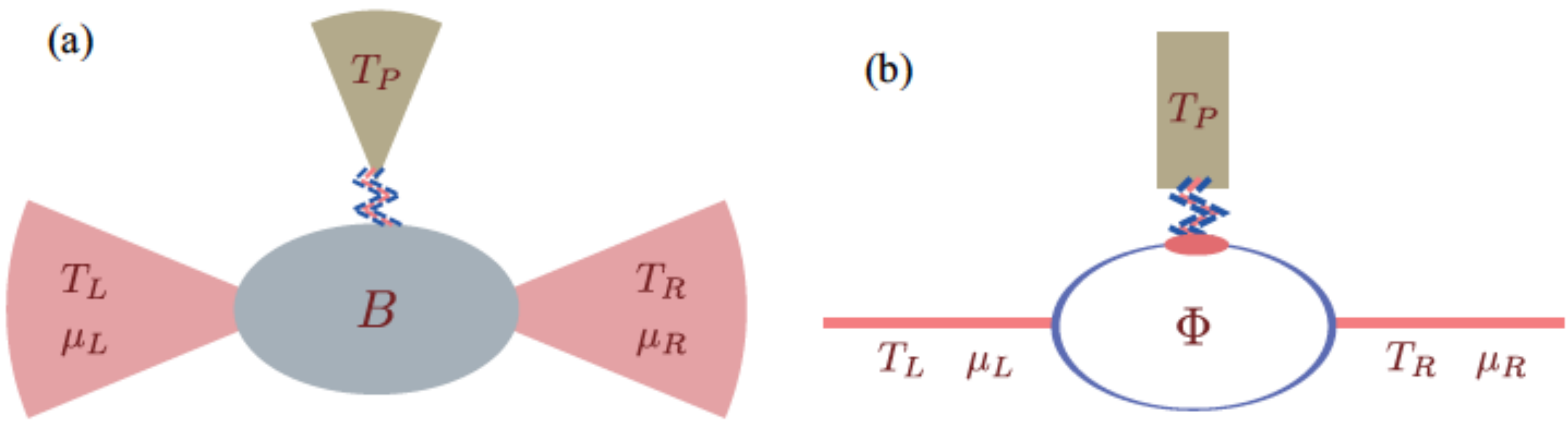


Bound obtained from the unitarity of the S-matrix

[K.. Brandner, K. Saito, U. Seifert, PRL **110**, 070603 (2013)]

[Brandner and Seifert, NJP **15**, 105003 (2013); PRE **91**, 012121 (2015)]

Bounds with electron-phonon scattering



Efficiency bounded by the non-negativity of the entropy production of the original three-terminal junction.

[Yamamoto, Entin-Wohlman, Aharony, Hatano; PRB **94**, 121402(R) (2015)]

Power-efficiency trade-off

For heat engines described as Markov processes:

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

[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

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

Moreover, the problem remains open for a generic purely Hamiltonian two-terminal system with interactions

Onsager relations with broken time-reversal symmetry

Onsager relations under an applied magnetic field remain valid:

1) for noninteracting systems

2) if the magnetic field is constant

[Bonella, Ciccotti, Rondoni, EPL **108**, 60004 (2014)]

What about for a generic, spatially dependent magnetic field?

Symmetry without magnetic field inversion

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

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

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

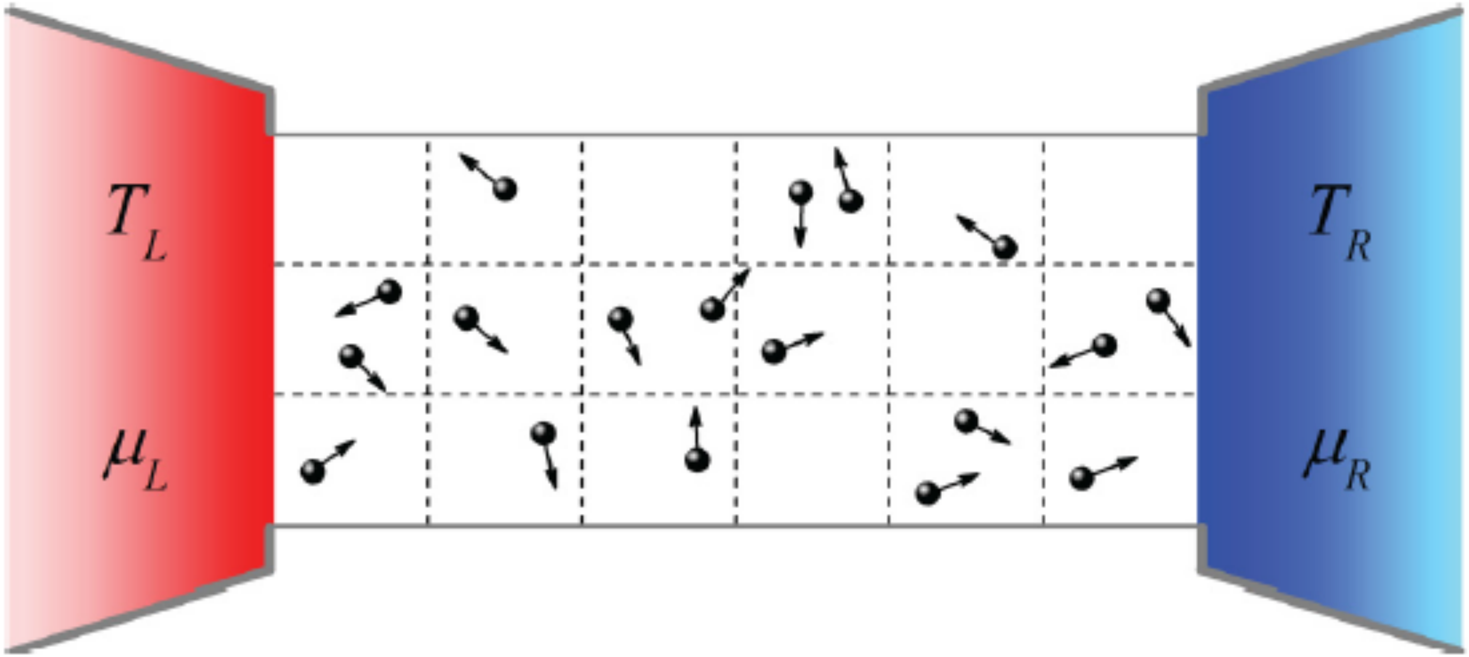
$$\begin{cases} \dot{x}_i = \dfrac{p_i^x}{m_i}, \\ \dot{y}_i = \dfrac{1}{m_i}\,[p_i^y - q_i A(x_i)], \\ \dot{z}_i = \dfrac{p_i^z}{m_i}, \\ \dot{p}_i^x = F_i^x + \dfrac{q_i}{m_i}\,[p_i^y - q_i A(x_i)]\,B(x_i), \\ \dot{p}_i^y = F_i^y, \\ \dot{p}_i^z = F_i^z, \end{cases}$$

$$F_i^\alpha = -\frac{\partial \sum_{j\neq i} V(r_{ij})}{\partial \alpha}$$

Equations of motion invariant under:

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

Numerics for a generic magnetic field



Use a stochastic model for the reservoirs

Dynamics described by the multi-particle collision method (Kapral method)

Multiparticle collision dynamics (Kapral model)

Streaming step: free propagation during a time τ

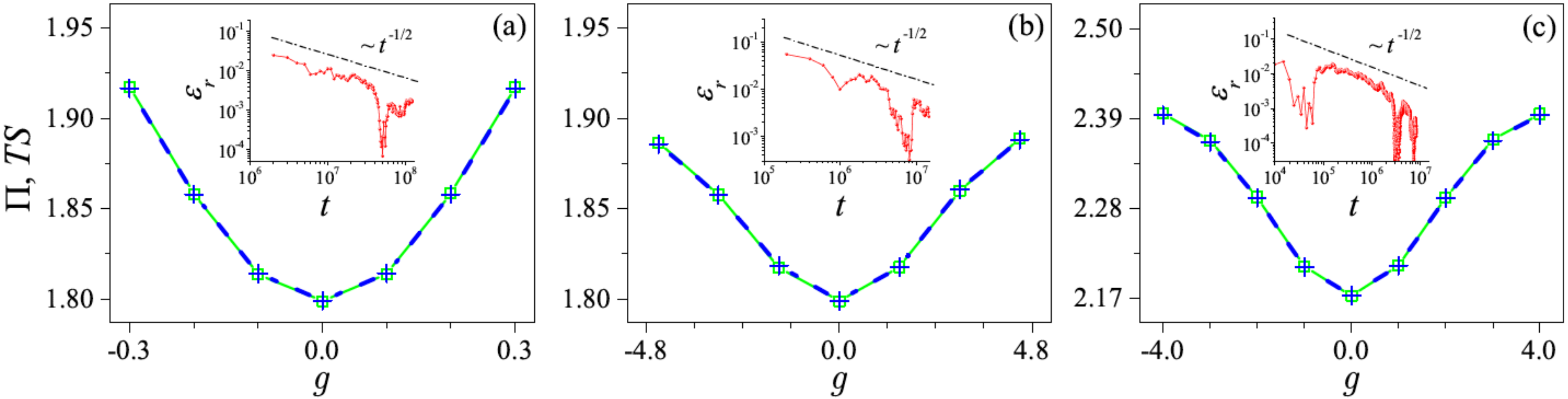
$$\vec{r}_i \longrightarrow \vec{r}_i + \vec{v}_i \tau$$

Collision step: random rotations of the velocities of the particles in cells of linear size a with respect to the center of mass velocity:

$$\vec{v}_i \longrightarrow \vec{V}_{\mathrm{CM}} + \hat{\mathcal{R}}^{\pm\alpha}\left(\vec{v}_i - \vec{V}_{\mathrm{CM}}\right)$$

Total energy and total momentum are conserved

Numerical results and theoretical argument



$$B(x) = gx$$

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)]

Consequences for heat engines

From the award ceremony speech, Nobel Prize for Chemistry 1968:

"…Onsager's reciprocal relations can be described as a universal natural law…It can be said that Onsager's reciprocal relations represent a further law making possible a thermodynamic study of irreversible processes…"

Onsager reciprocal relations much more general than expected so far.

No-go theorem for finite power at the Carnot efficiency on purely thermodynamic grounds?

Power-efficiency-fluctuations trade-off

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

For the work current (power) $$P^2 \leq \frac{1}{2}\sigma\Delta_P$$

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

P(t) mean power delivered up to time t

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

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

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

Scattering theory for thermoelectricity

Charge current $J_e = eJ_\rho = \frac{e}{h}\int_{-\infty}^{\infty} dE\tau(E)[f_L(E) - f_R(E)]$

Heat current from reservoirs:

$$J_{h,\alpha} = \frac{1}{h}\int_{-\infty}^{\infty} dE(E-\mu_\alpha)\tau(E)[f_L(E) - f_R(E)]$$

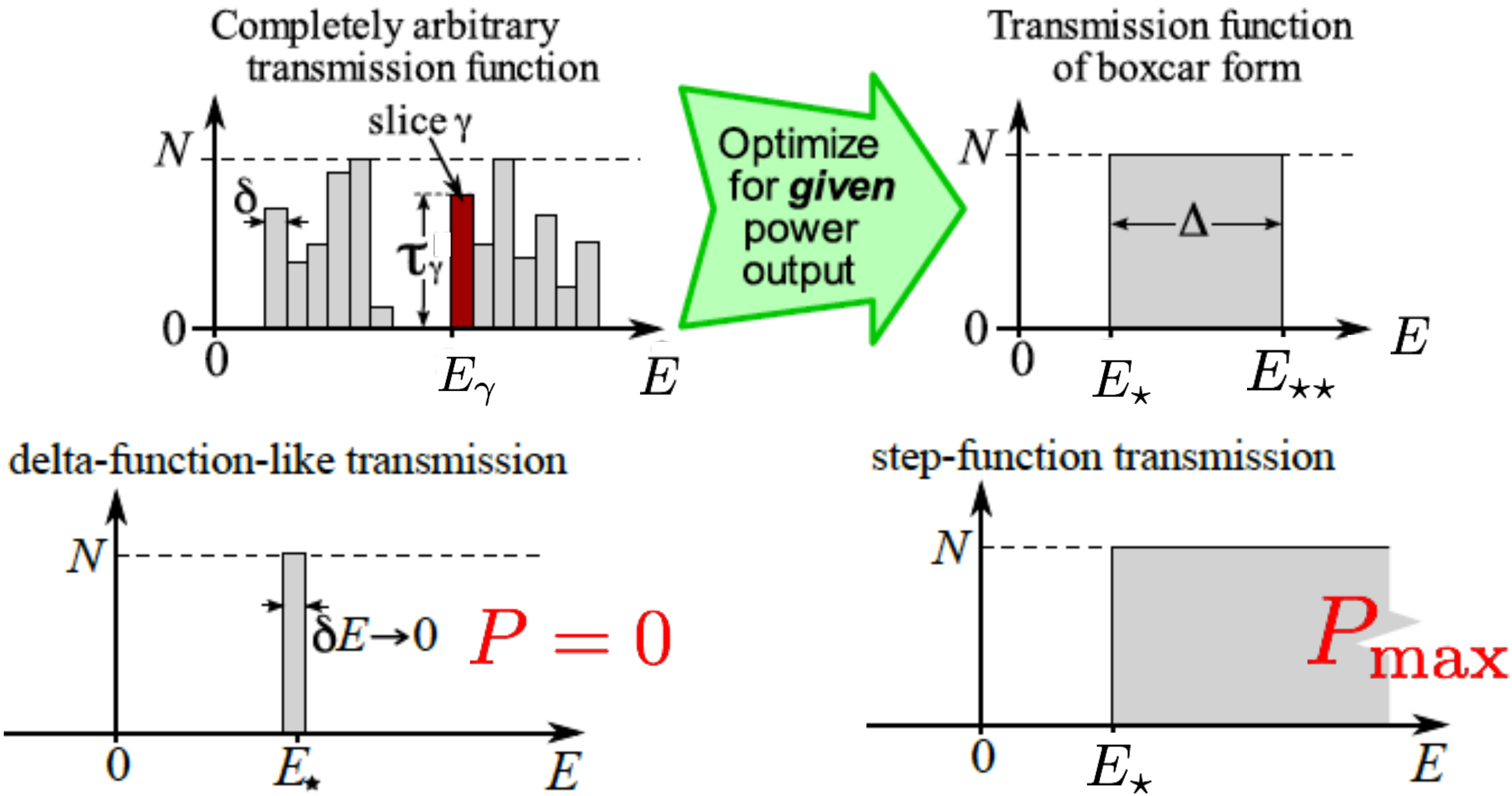
Efficiency:

$$\eta = \frac{P}{J_{h,L}} \quad (T_L > T_R)\ (\mu_R > \mu_L)\ \ P, J_{h,L} > 0$$

$$\eta = \frac{[(\mu_R - \mu_L)/e]J_e}{J_{\mathrm{h,L}}} = \frac{(\mu_R - \mu_L)\int_{-\infty}^{\infty} dE\tau(E)[f_L(E) - f_R(E)]}{\int_{-\infty}^{\infty} dE(E-\mu_L)\tau(E)[f_L(E) - f_R(E)]}$$

Efficiency optimization (at a given power)

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

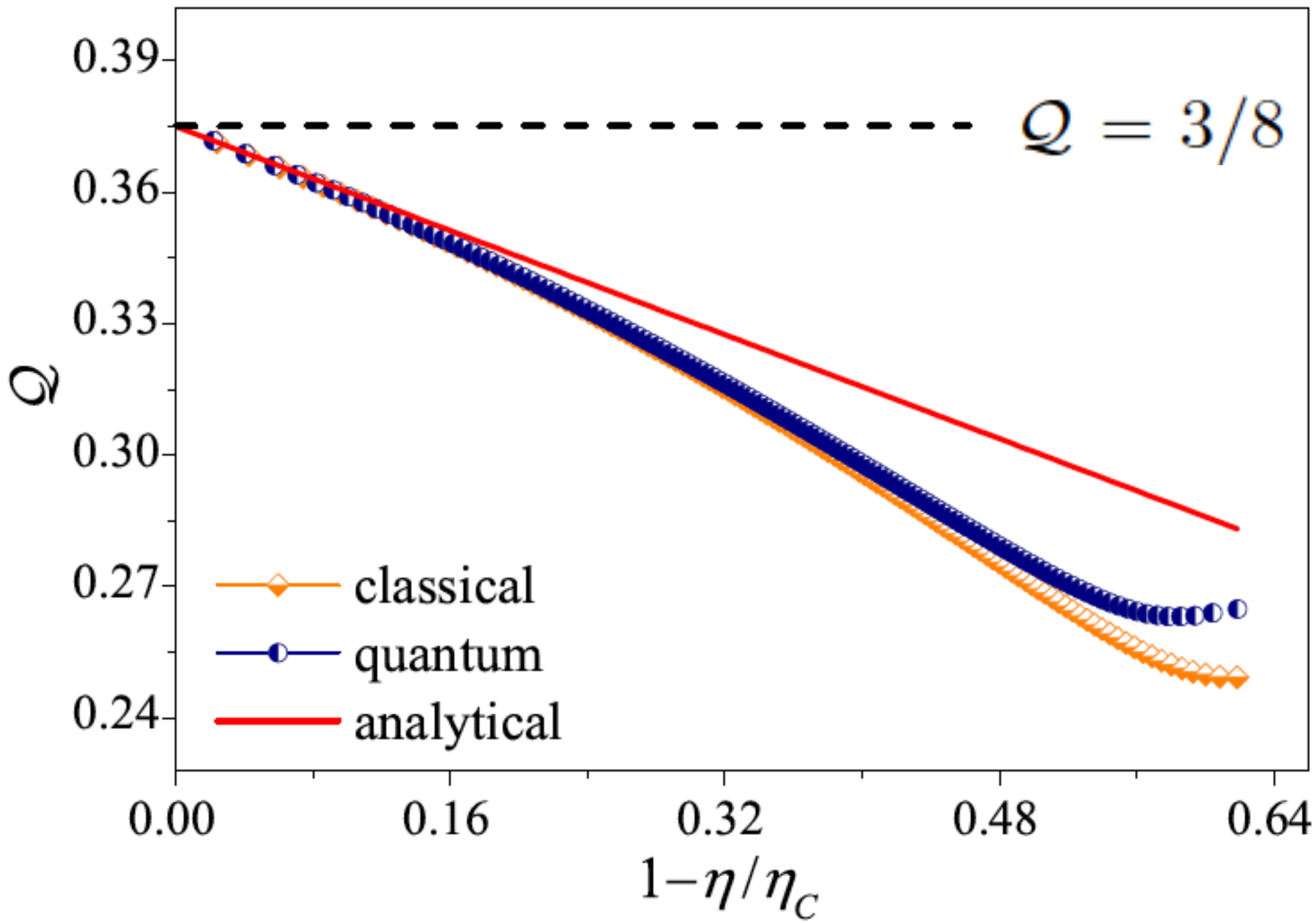
$$\Delta_P = (\Delta V)^2 \int_{-\infty}^{+\infty} d\epsilon (\mathcal{T}(\epsilon)\{f_L(\epsilon)[1 - f_L(\epsilon)]$$

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

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

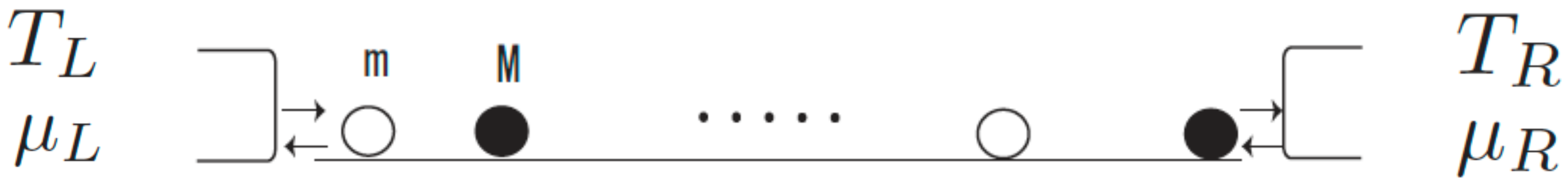


$$\mathcal{Q} = \frac{3}{8} - \frac{9}{128}\frac{T_L + T_R}{T_R}\left(1 - \frac{\eta}{\eta_C}\right) + \mathcal{O}\left[\left(1 - \frac{\eta}{\eta_C}\right)^2\right]$$

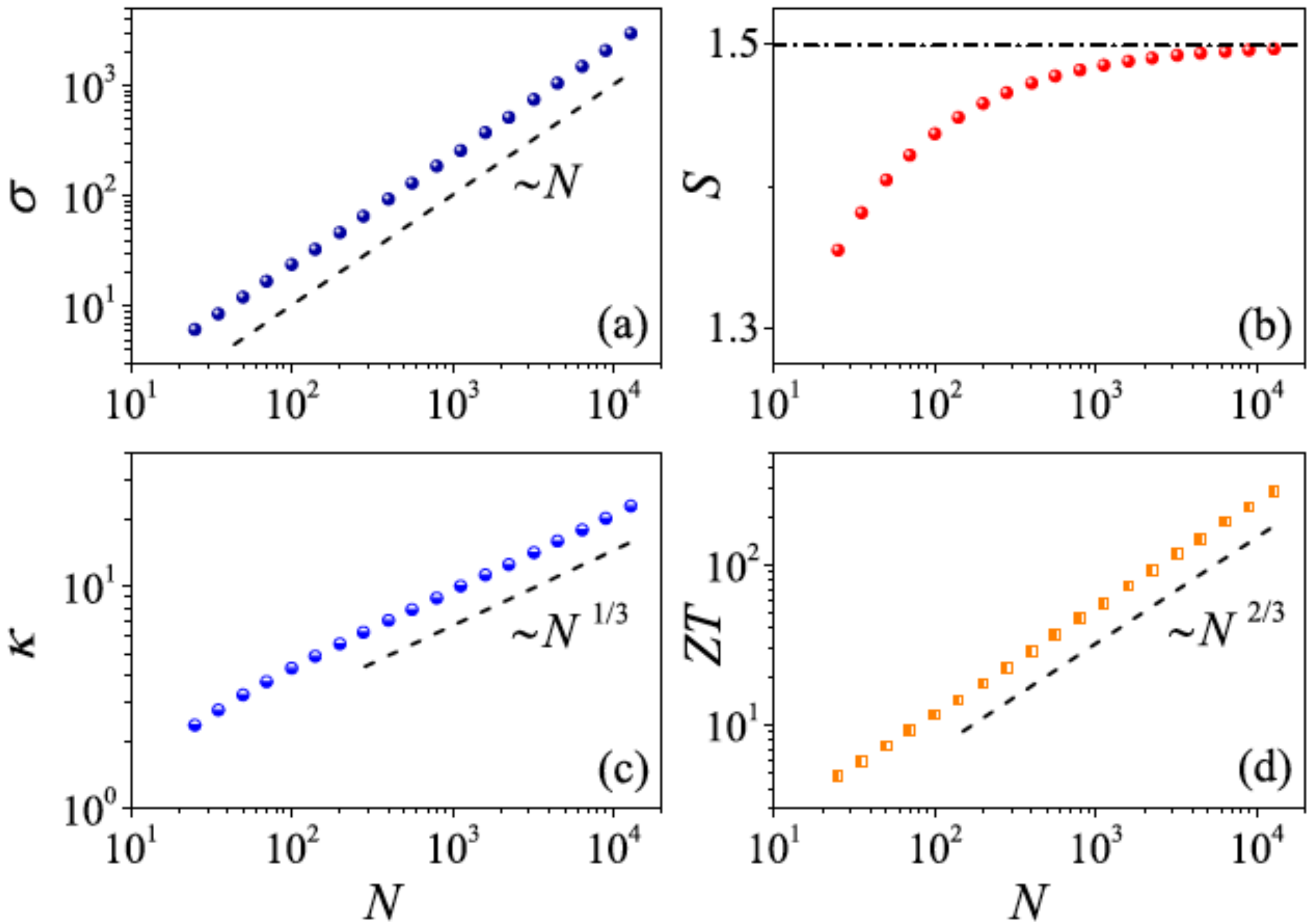
[GB, G. Casati, J. Wang; Phys Rev E **102**, 040103(R) (2020)]

Interacting, momentum-conserving systems

Example: one dimensional gas of elastically colliding particles with unequal masses: m, M



Carnot efficiency at the thermodynamic limit



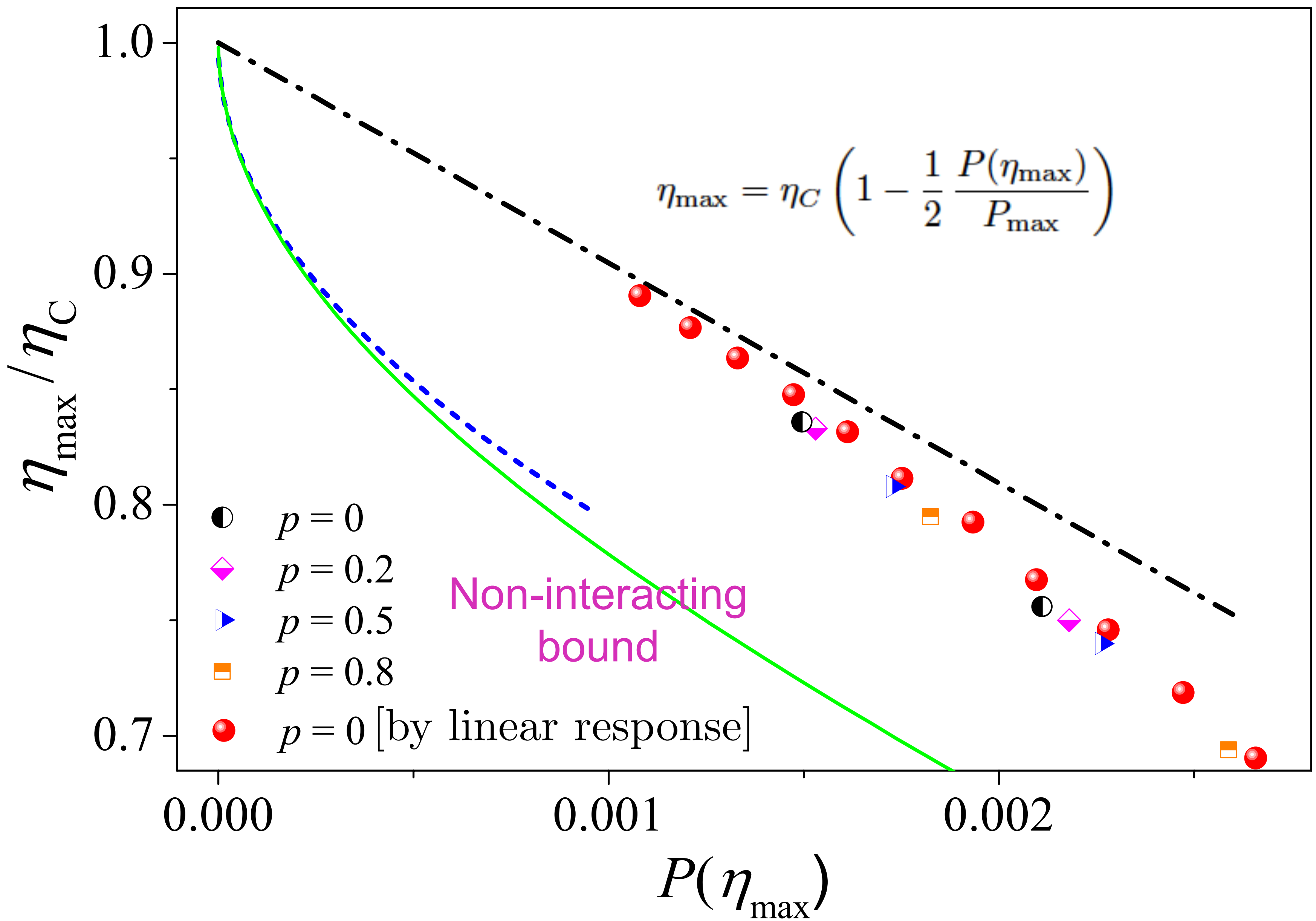
Anomalous thermal transport

$$ZT = \frac{\sigma S^2}{k} T$$

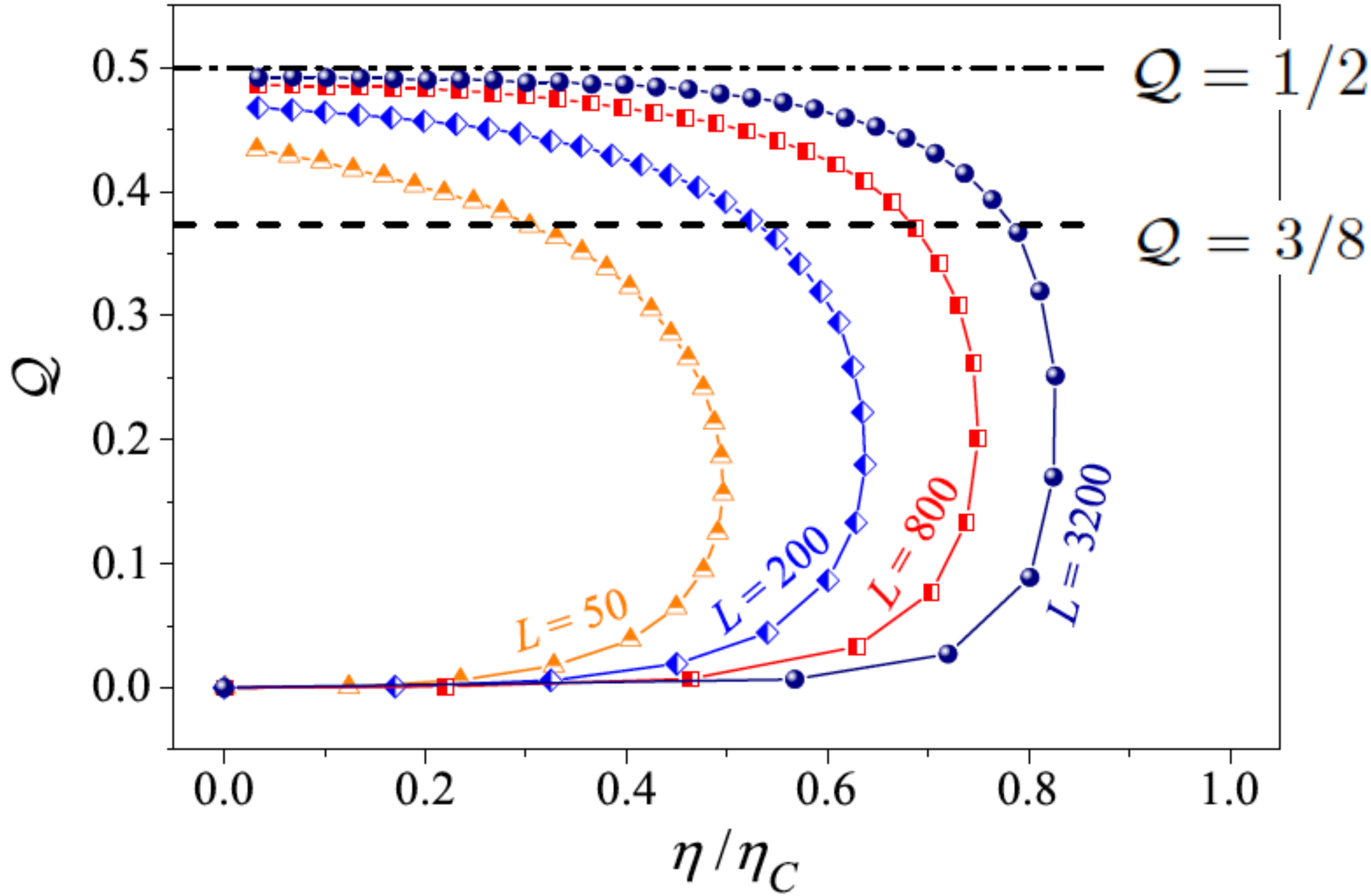
ZT diverges increasing the systems size

[R. Luo, G. B., G. Casati, J. Wang, PRL **121**, 080602 (2018)]

Power-efficiency trade-off: overcoming the noninteracting bound



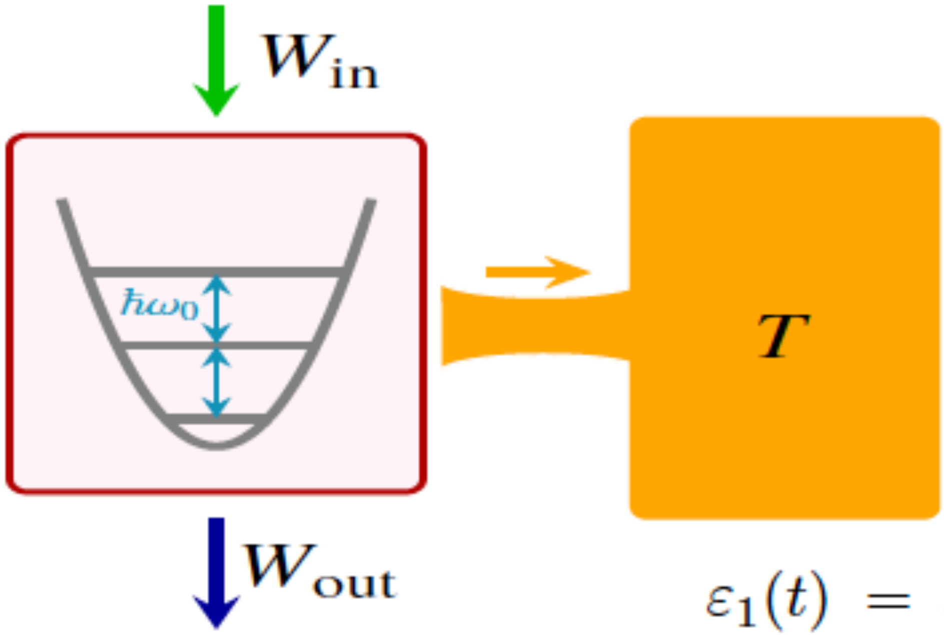
Power-efficiency-fluctuations trade-off: Achieving the upper bound



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

Overcoming the bound: periodically driven systems

Isothermal heat engine



$$H(t) = H_S(t) + H_R + H_{SR}$$

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

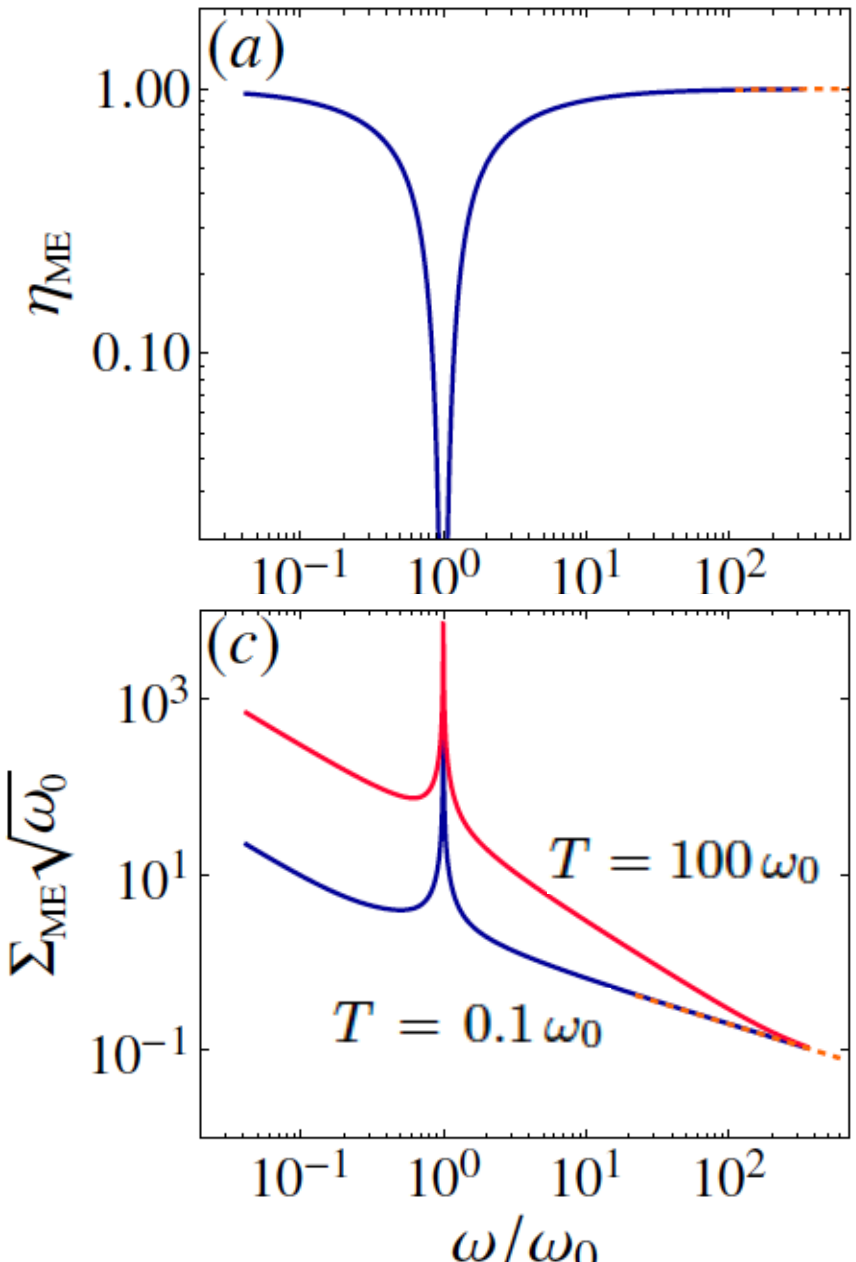
$$\varepsilon_{1/2}(t) = \varepsilon_{1/2}(t+\mathcal{T})$$

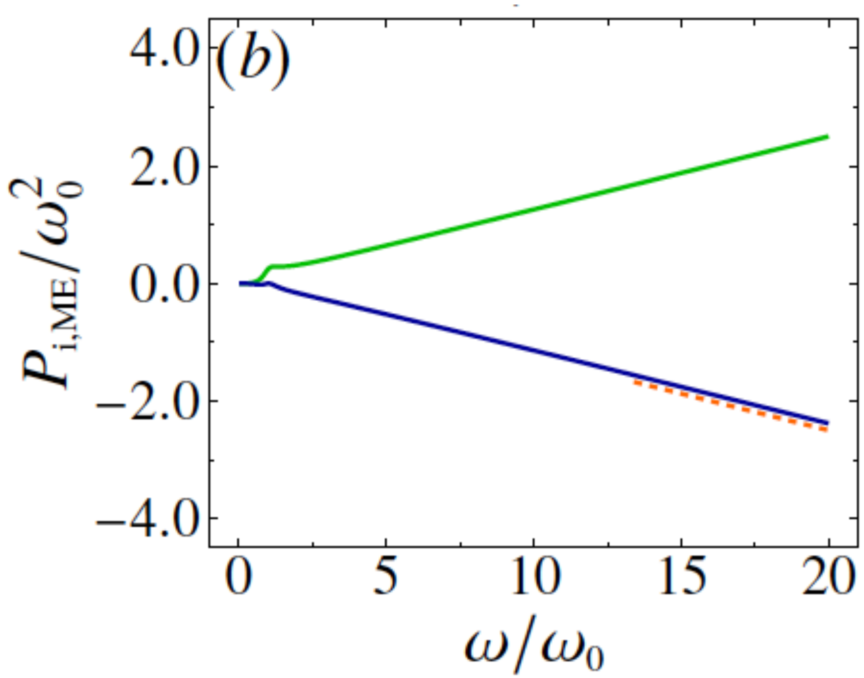
$$\varepsilon_1(t) = \varepsilon_1 \sin\omega t,\ \varepsilon_2(t) = \varepsilon_2\cos(\omega t - \varphi)$$

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

[L. M. Cangemi, M. Carrega, A. De Candia, V. Cataudella, G. De Filippis, M. Sassetti, G. B., arXiv:2009.10904]

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





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

Required ingredients:

- breaking time-reversal symmetry
- underdamped dynamics

Absolute negative mobility

ANM: permanent average motion against a static force, as illustrated by the donkey, moving in the direction opposite to the one which is required to it

Impossible at thermal equilibrium, a single heat bath would perform work against the force

Investigated in non-equilibrium setups

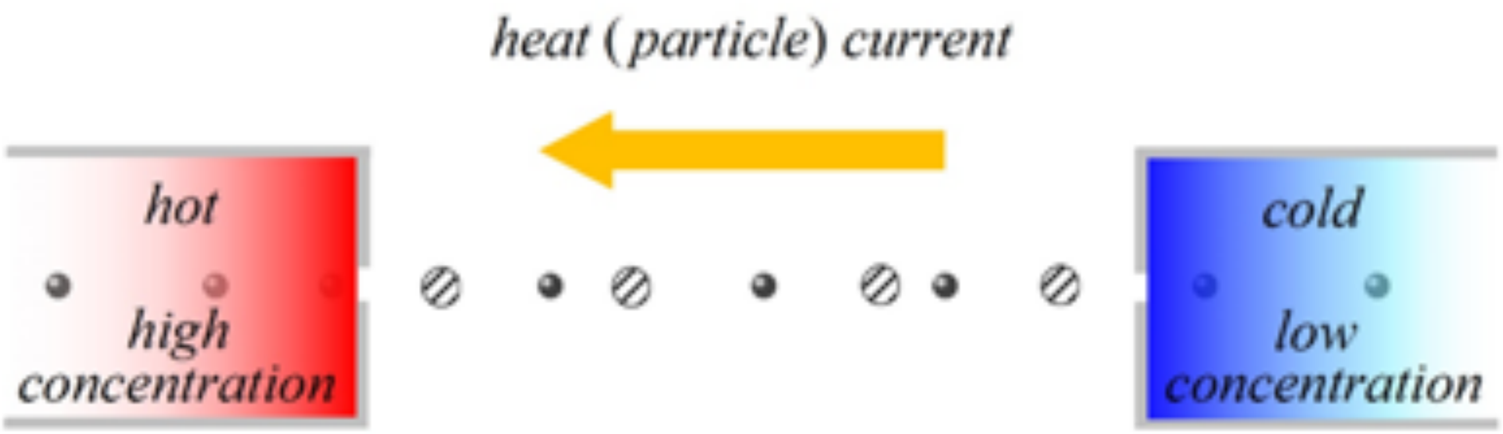
[Cleuren, Van den Broeck, EPL 54, 1 (2001); Eichorn, Reimann, Hanggi, PRL 88, 190601 (2002); Nagel et al., PRL 100, 217001 (2008),…]

ANM in equilibrium, for stochastic dynamics of a tracer particle subject to two driving forces

[Cividini, Mukamel, Posch, J. Phys. A **51**, 085001 (2018)]

Inverse Currents in Coupled transport (ICC) possible

For coupled flows it is allowed by thermodynamics to have a current opposite to both thermodynamic forces



Entropy production rate

$$\dot{S} = J_1 \mathcal{F}_1 + J_2 \mathcal{F}_2$$

$$\mathcal{F}_i > 0 \quad (i = 1,\ 2)$$

one current can be negative,
with overall positive entropy production

Classical version of Lieb-Liniger model

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} V(x_i - x_j)$$

$$V(x) = h \text{ for } x \leq |r|$$

$$V(x) = 0 \text{ otherwise}$$

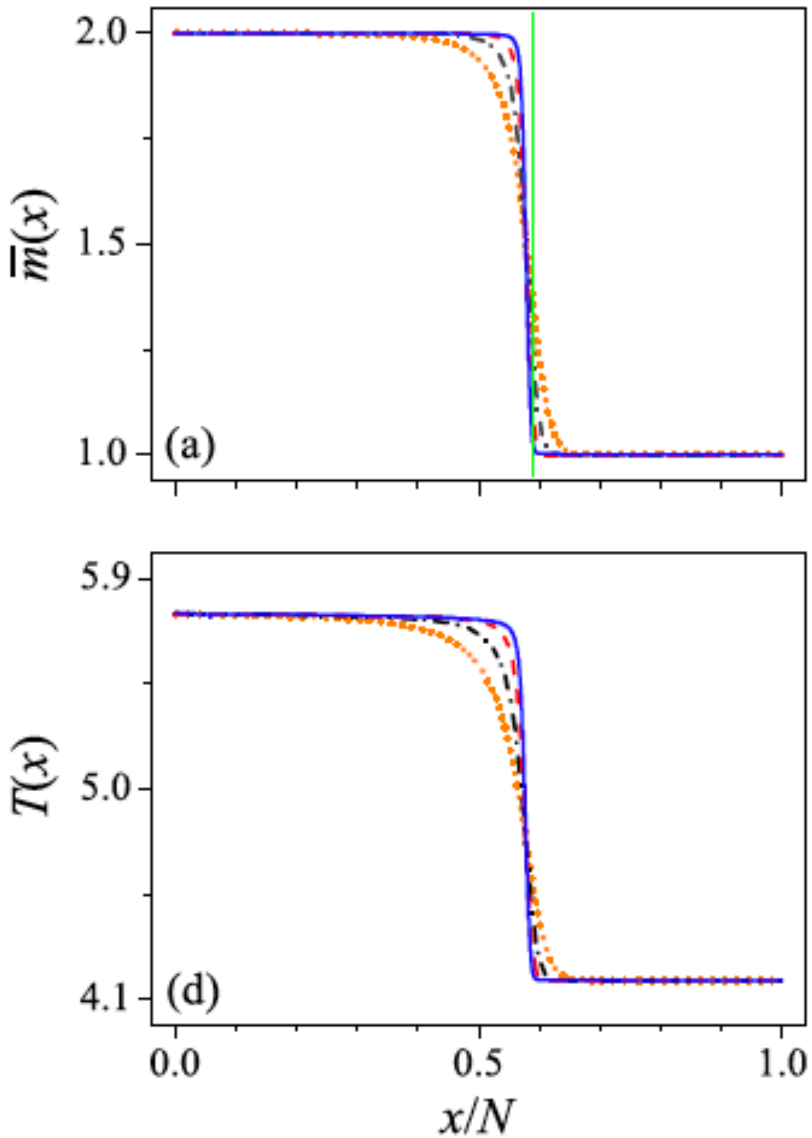
limit case $r \to 0$

Diatomic gas of particles $m_i \in \{\mathcal{M}_1, \mathcal{M}_2\}$

Easier for two colliding particle to overcome when the light particle come from the hot end (higher relative velocity)

Self-organisation (phase separation) in the far from equilibrium regime

(in a 1D Hamiltonian system)



Strong temperature difference between reservoirs

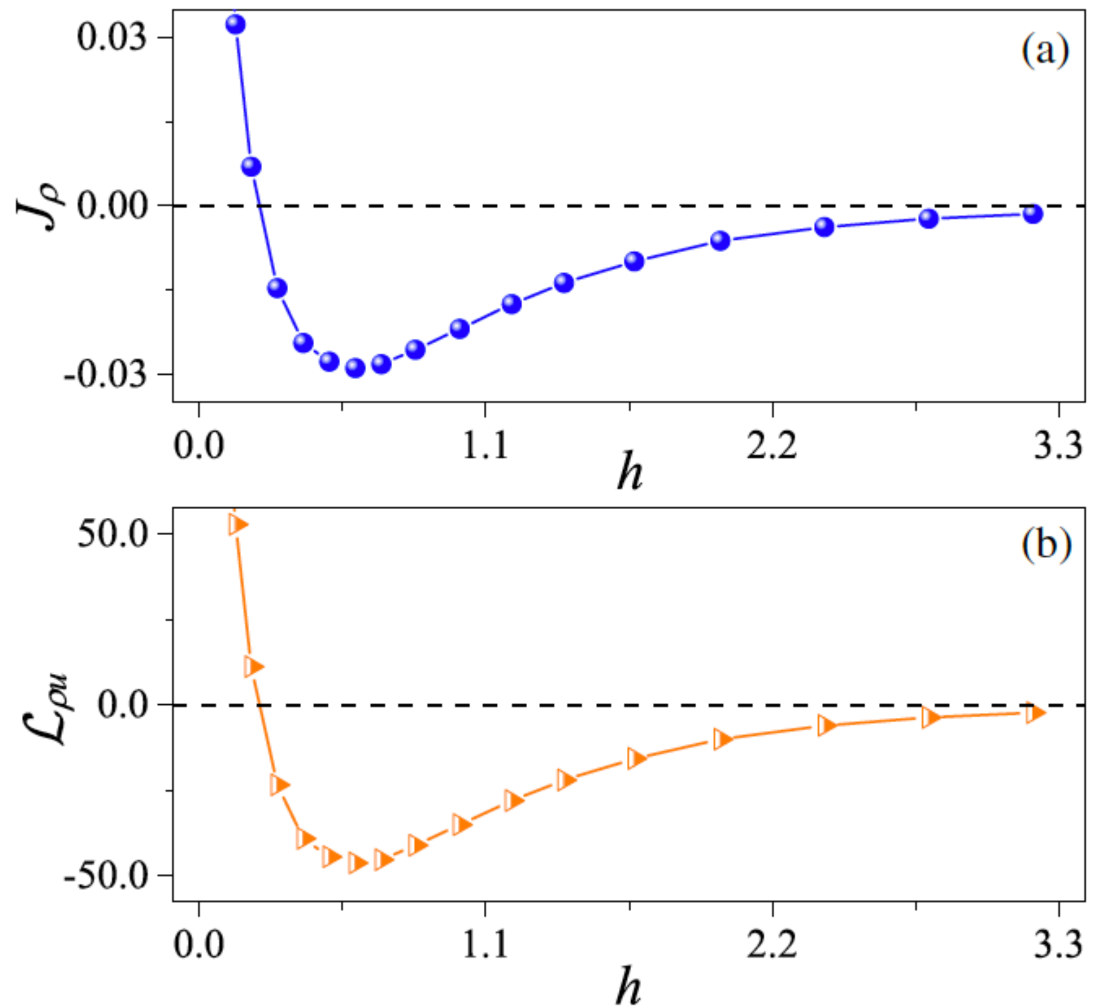
[J. Wang, G. Casati, PRL **118**, 040601 (2017)]

Negative cross-coefficient (Seebeck)

$$\begin{pmatrix} J_\rho \\ J_u \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{\rho\rho} & \mathcal{L}_{\rho u} \\ \mathcal{L}_{u\rho} & \mathcal{L}_{uu} \end{pmatrix} \begin{pmatrix} \mathcal{F}_\rho / L \\ \mathcal{F}_u / L \end{pmatrix}$$

$$\mathcal{F}_\rho = \mu_L \beta_L - \mu_R \beta_R$$

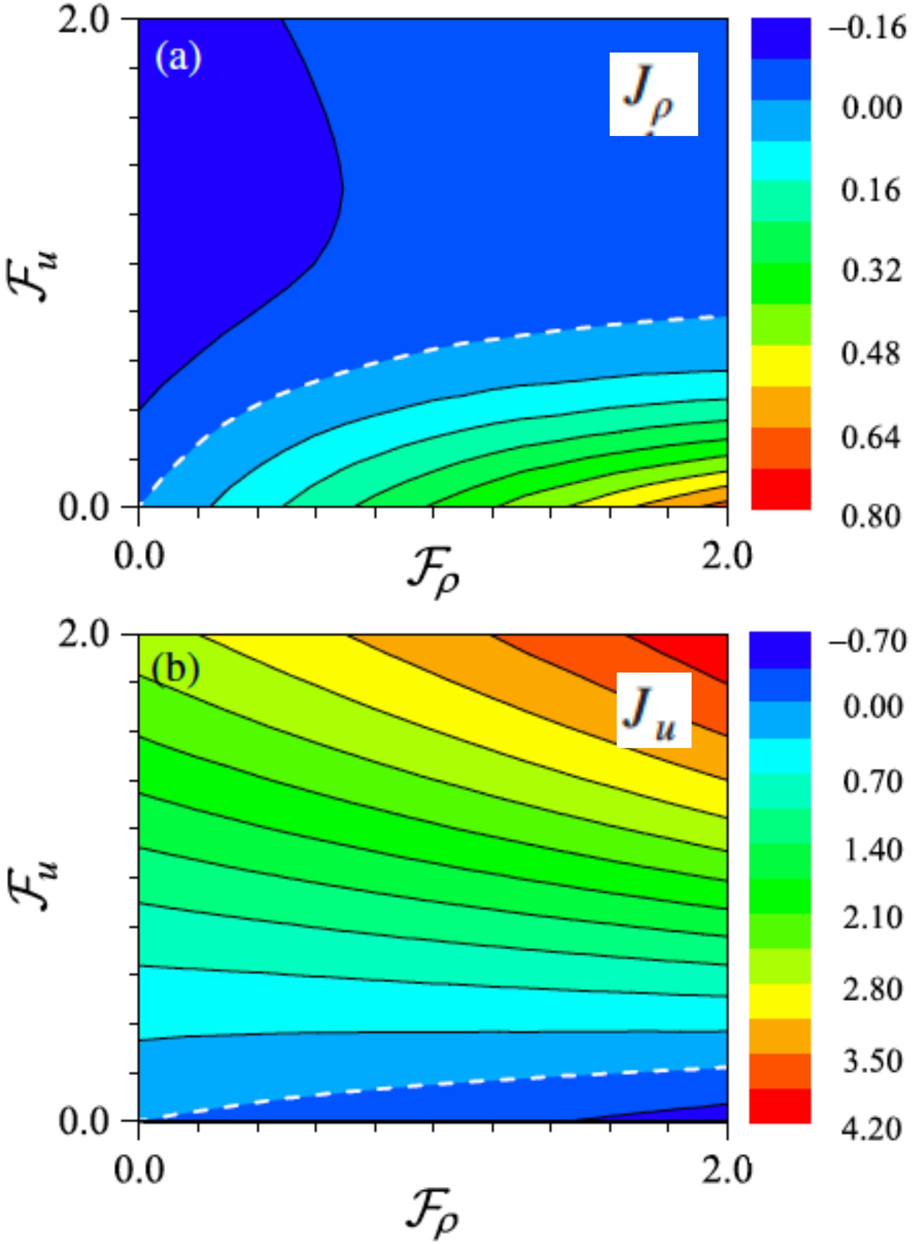
$$\mathcal{F}_u = \beta_R - \beta_L$$



[J. Wang, G. Casati, GB, PRL **124**, 110607 (2020)]

$\mathcal{F}_\rho = 0$ and $\mathcal{F}_u = 0.1$

Inverse currents in coupled transport (ICC)



ICC already exists in the linear response regime and is enhanced in the far-from-equilibrium regime with phase separation

Final remarks

Onsager reciprocal relations much more general than expected so far: No-go theorem for finite power at the Carnot efficiency on purely thermodynamic grounds?

Interactions are in principle useful to improve performance of a steady-state (thermoelectric) engine

Periodically driven heat engines can overcome the steady-state bound and allow to achieve all three desiderata of a heat engine: efficiency close to the ideal one, finite power and small fluctuations.

Possible to build thermoelectric circuits exploiting ICC?

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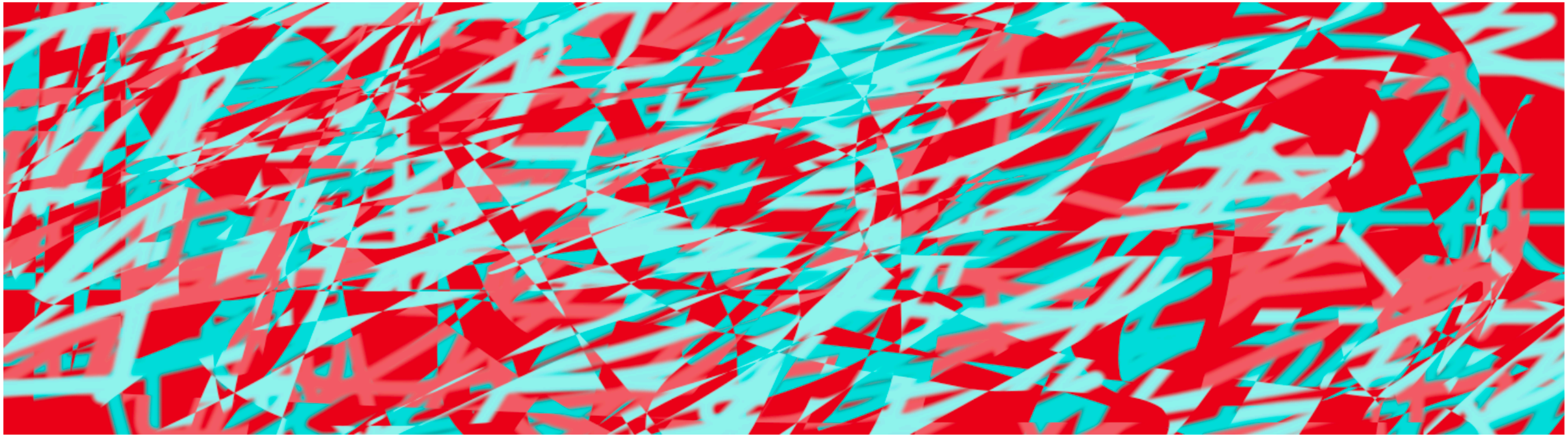

A network of scientists dedicated to understanding the thermodynamics of quantum systems and quantum transport.

Quantum computation and information is a rapidly developing interdisciplinary field. It is not easy to understand its fundamental concepts and central results without facing numerous technical details. This book provides the reader with a useful guide. In particular, the initial chapters offer a simple and self-contained introduction; no previous knowledge of quantum mechanics or classical computation is required.

Various important aspects of quantum computation and information are covered in depth, starting from the foundations (the basic concepts of computational complexity, energy, entropy, and information, quantum superposition and entanglement, elementary quantum gates, the main quantum algorithms, quantum teleportation, and quantum cryptography) up to advanced topics (like entanglement measures, quantum discord, quantum noise, quantum channels, quantum error correction, quantum simulators, and tensor networks).

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Principles of Quantum Computation and Information
A Comprehensive Textbook

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