Power-efficiency trade-off in thermoelectricity: From scattering theory to interacting systems

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General motivation

Carnot efficiency can be obtained only for infinitely slow heat engines, so the extracted power vanishes

What is the maximum allowed efficiency at a given power output?

For steady-state (thermoelectric) quantum systems modeled by the Landauer-Büttiker scattering theory a (rather restrictive) upper bound exists

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

Is it possible to overcome this bound for **interacting systems**, thus allowing *a better power-efficiency trade-off*?

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

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

Cyclic thermal machines

The upper bound to efficiency is given by the Carnot efficiency:

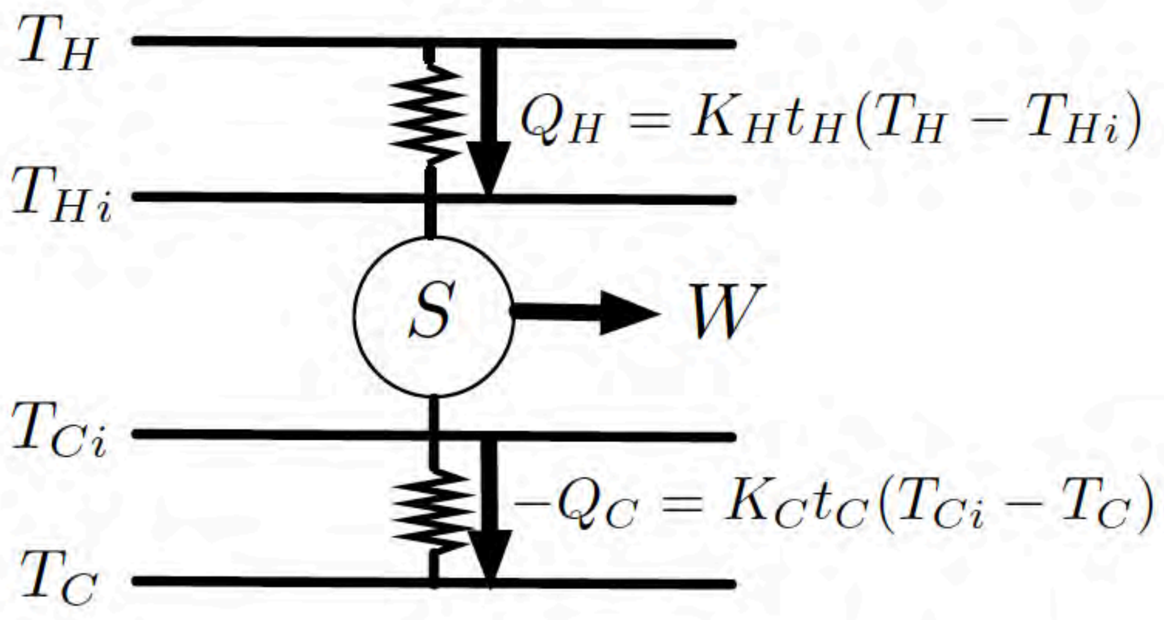
$$\eta = \frac{W}{Q_H} \leq \eta_C = 1 - \frac{T_C}{T_H} \qquad (T_H > T_C)$$

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 I: endoreversible cyclic engines

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



S is considered as a Carnot engine operating between the internal temperatures T_{Hi} and T_{Ci} ($T_H > T_{Hi} > T_{Ci} > T_C$)

$$1 - T_{Ci}/T_{Hi} = 1 + Q_C/Q_H$$

Output power:

$$P = \frac{W}{t} = \frac{Q_H + Q_C}{t} = \frac{K_H K_C \alpha\beta(T_H - T_C - \alpha - \beta)}{K_H \alpha T_C + K_C \beta T_H + \alpha\beta(K_H - K_C)}$$

Optimize power with respect to

$$\begin{aligned} \alpha &= T_H - T_{Hi} \\ \beta &= T_{Ci} - T_C \end{aligned}$$

$$T_{Hi} = c\sqrt{T_H}, \quad T_{Ci} = c\sqrt{T_C}, \qquad c \equiv \frac{\sqrt{K_H T_H} + \sqrt{K_C T_C}}{\sqrt{K_H} + \sqrt{K_C}}$$

$$P_{\max} = K_H K_C \left(\frac{\sqrt{T_H} - \sqrt{T_C}}{\sqrt{K_H} + \sqrt{K_C}} \right)^2$$

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

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

[Yvon, 1955; Chambadal, 1957; Novikov, 1958; Curzon and Ahlborn, Am. J. Phys. 43, 22 (1975)]

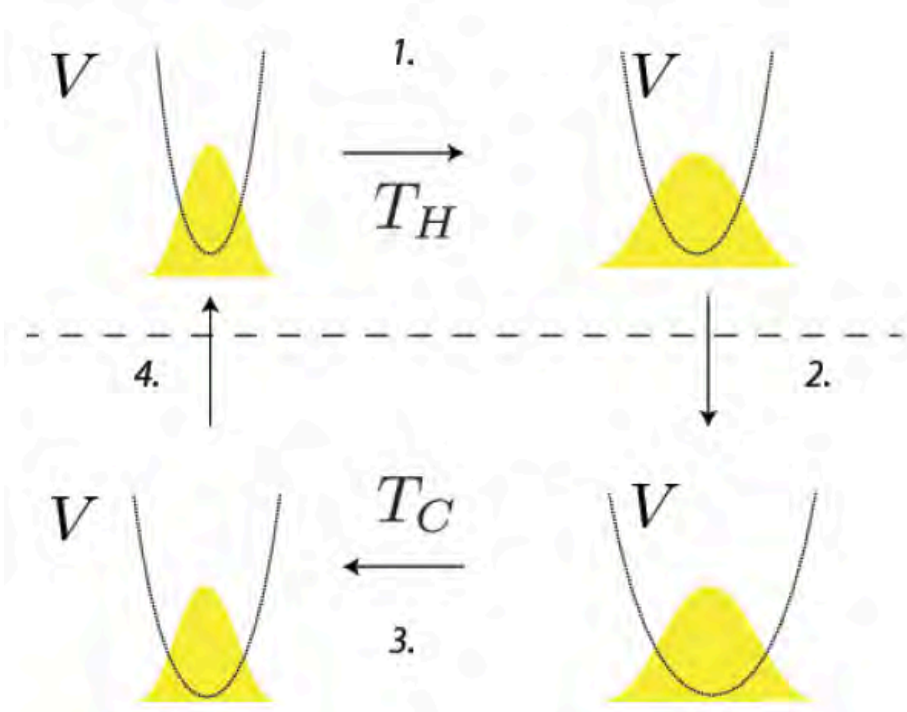
Within linear response: $\eta_{CA} = \dfrac{\eta_C}{2}$

Finite-time thermodynamics II: exoreversible cyclic engines

Irreversibility only arises due to internal dissipative processes

Stochastic thermodynamics

[Seifert, Rep. Prog. Phys. 75, 126001 (2012)]



Time-dependent trapping potential $V(x, \lambda(t))$

Time-dependent probability density $p(x, t)$

Fokker-Planck equation:

$$\frac{\partial}{\partial t}p(x,t) = \mu\left(\lambda(t)\frac{\partial}{\partial x}x + T\frac{\partial^2}{\partial x^2}\right)p(x,t)$$

μ is the mobility

Gaussian distribution $p(x,t)$

Exactly solvable model

Schmiedl-Seifert efficiency at maximum power:

$$\eta_{SS} = \frac{\eta_C}{2 - \gamma \eta_C}$$

$\gamma \in [0, 1]$ related to the ratio of entropy production during the hot and cold isothermal steps of the cycle

$\gamma = 1/2$ for the symmetric case

[Schmiedl and Seifert, EPL 81, 20003 (2008)]

Within linear response: $\eta_{CA} = \dfrac{\eta_C}{2}$

Low-dissipation engines

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

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

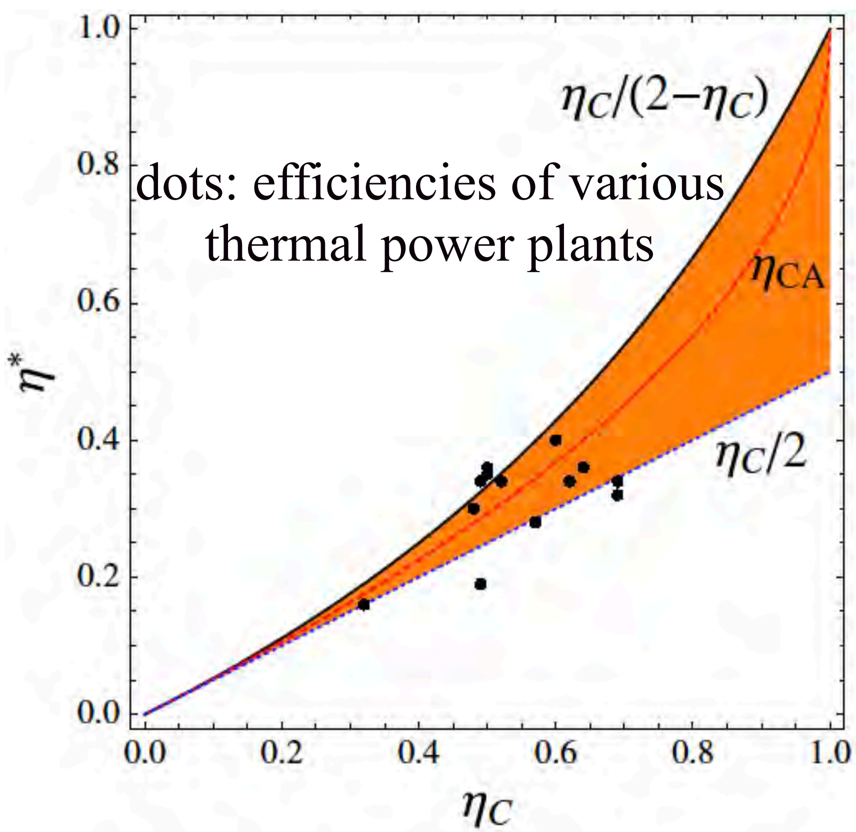
$$P = \frac{Q_H + Q_C}{t_H + t_C} = \frac{(T_H - T_C)\Delta\mathcal{S} - T_H\Sigma_H/t_H - T_C\Sigma_C/t_C}{t_H + t_C}$$

$$\eta(P_{\max}) = \frac{\eta_C\left(1 + \sqrt{\frac{T_C\Sigma_C}{T_H\Sigma_H}}\right)}{\left(1 + \sqrt{\frac{T_C\Sigma_C}{T_H\Sigma_H}}\right)^2 + \frac{T_C}{T_H}\left(1 - \frac{\Sigma_C}{\Sigma_H}\right)}$$

$$\eta_- = \frac{\eta_C}{2} \leq \eta(P_{\max}) \leq \eta_+ = \frac{\eta_C}{2 - \eta_C}$$

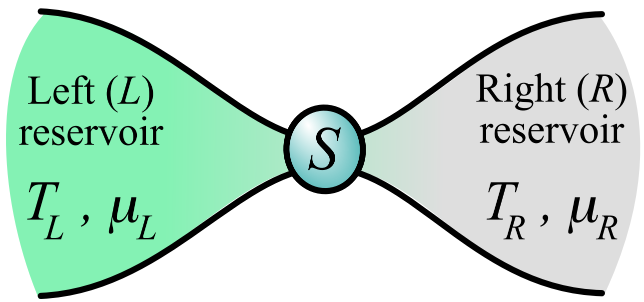
$\Sigma_C / \Sigma_H \to \infty$ $\qquad\qquad$ $\Sigma_C / \Sigma_H \to 0$

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



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

Steady-state (thermoelectric) power production



$$\eta = \frac{P}{J_{h,L}}$$

$$P = [(\mu_R - \mu_L)/e] J_e$$

$$(T_L > T_R,\ \mu_L < \mu_R) \qquad P, J_{h,L} > 0$$

The upper bound to efficiency is given by the Carnot efficiency:

$$\eta_C = 1 - \frac{T_R}{T_L}$$

Proc. Natl. Acad. Sci. USA
Vol. 93, pp. 7436–7439, July 1996
Applied Physical Sciences

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The best thermoelectric

G. D. MAHAN*† AND J. O. SOFO‡

ABSTRACT What electronic structure provides the largest figure of merit for thermoelectric materials? To answer that question, we write the electrical conductivity, thermopower, and thermal conductivity as integrals of a single function, the transport distribution. Then we derive the mathematical function for the transport distribution, which gives the largest figure of merit. A delta-shaped transport distribution is found to maximize the thermoelectric properties. This result indicates that a narrow distribution of the energy of the electrons participating in the transport process is needed for maximum thermoelectric efficiency. Some possible realizations of this idea are discussed.

Landauer formalism 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:

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

$\tau(E)$ transmission probability for a particle with energy E

$0 \le \tau(E) \le \mathcal{N}$, $\quad \mathcal{N}$ number of transverse modes

$f_\alpha(E)$ Fermi distribution of the particles injected from reservoir α

$$f_\alpha(E) = \{1 + \exp[(E - \mu_\alpha)/(k_B T_\alpha)]\}^{-1}$$

Thermoelectric efficiency (power production)

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

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

$$(\mu_R > \mu_L)$$

Delta-energy filtering and Carnot efficiency

If transmission is possible only inside a tiny energy window around E=$E_\star$ then

$$\eta = \frac{\mu_L - \mu_R}{E_\star - \mu_L}$$

In the limit $J_\rho \to 0$, corresponding to reversible transport

$$\frac{E_\star - \mu_L}{T_L} = \frac{E_\star - \mu_R}{T_R} \Rightarrow E_\star = \frac{\mu_R T_L - \mu_L T_R}{T_L - T_R}$$

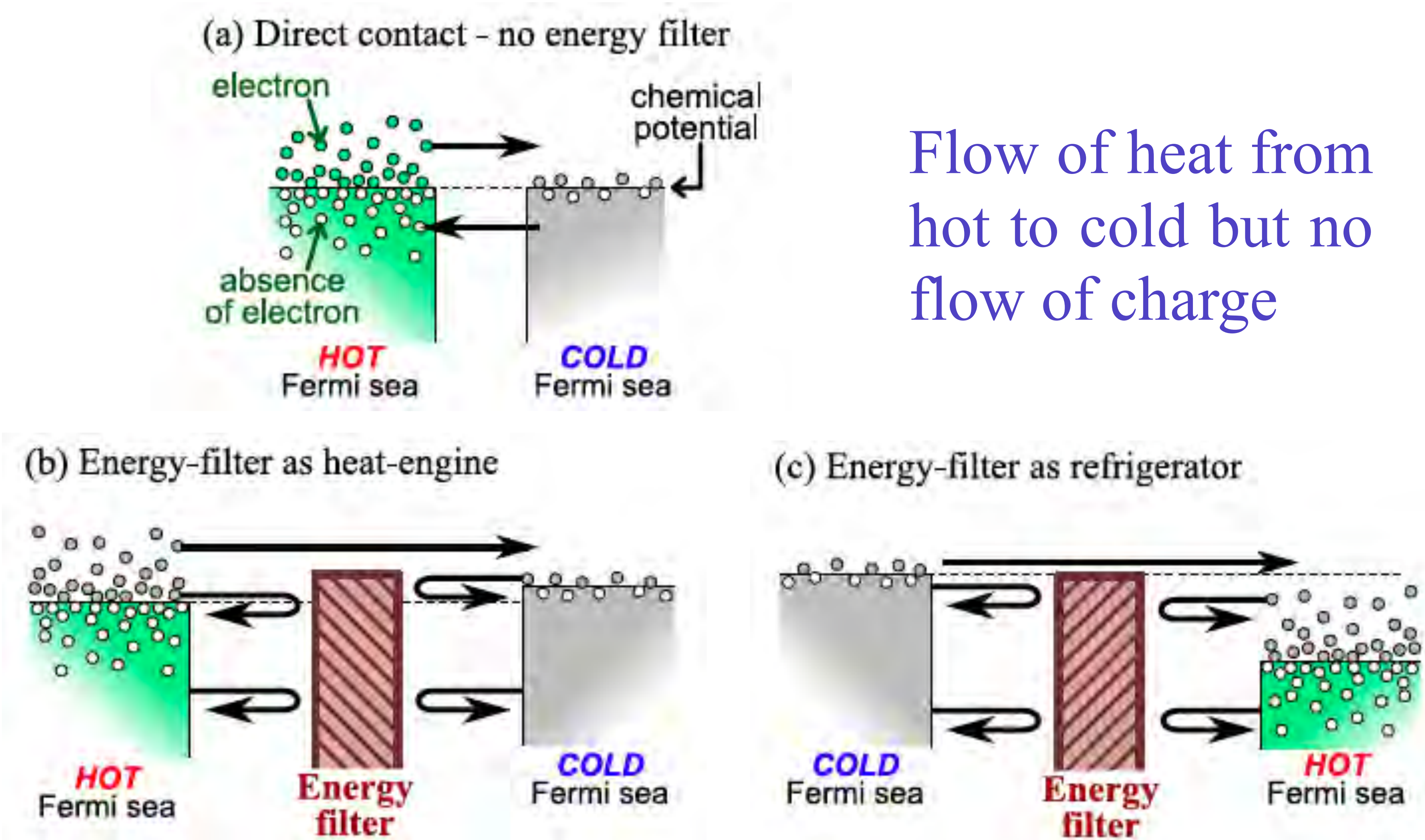
$$\eta = \eta_C = 1 - T_R/T_L$$

Carnot efficiency

Carnot efficiency obtained in the limit of reversible transport (zero entropy production) and zero output power

[Mahan and Sofo, PNAS 93, 7436 (1996); Humphrey et al., PRL 89, 116801 (2002)]

Heat-to-work conversion through energy filtering



Flow of heat from hot to cold but no flow of charge

[see G. B., G. Casati, K. Saito, R. S. Whitney, Phys. Rep. **694**, 1 (2017)]

Bekenstein-Pendry bound

There is an purely quantum upper bound on the heat current through a single transverse mode

[Bekenstein, PRL **46**, 923 (1981); Pendry, JPA **16**, 2161 (1983)]

For a reservoir coupled to another reservoir at T=0 through a $\mathcal{N}$-mode constriction which lets particle flow at all energies:

$$J_{h,i}^{\max} = \frac{\pi^2}{6h} \mathcal{N} \, k_{\mathrm{B}}^2 T_i^2$$

Maximum power of a heat engine

Since the heat flow must be less than the Bekenstein-Pendry bound and the efficiency smaller than Carnot efficiency also the output power must be bounded

Within scattering theory:

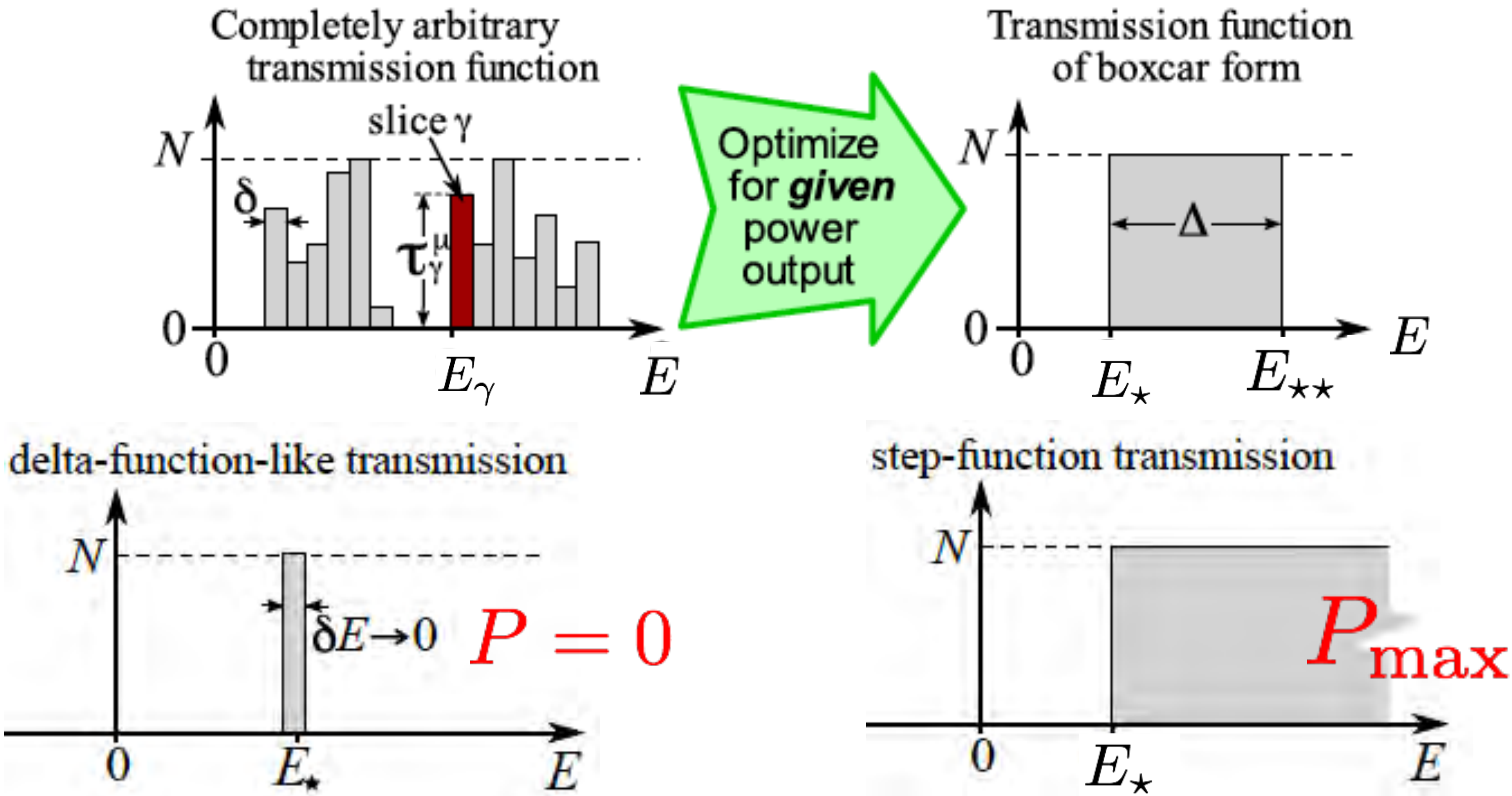
$$P \leq P_{\max} = A_q \frac{\pi^2}{h} \mathcal{N} k_B^2 (\Delta T)^2, \qquad A_q \approx 0.0321,$$

$$\Delta T = T_L - T_R$$

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

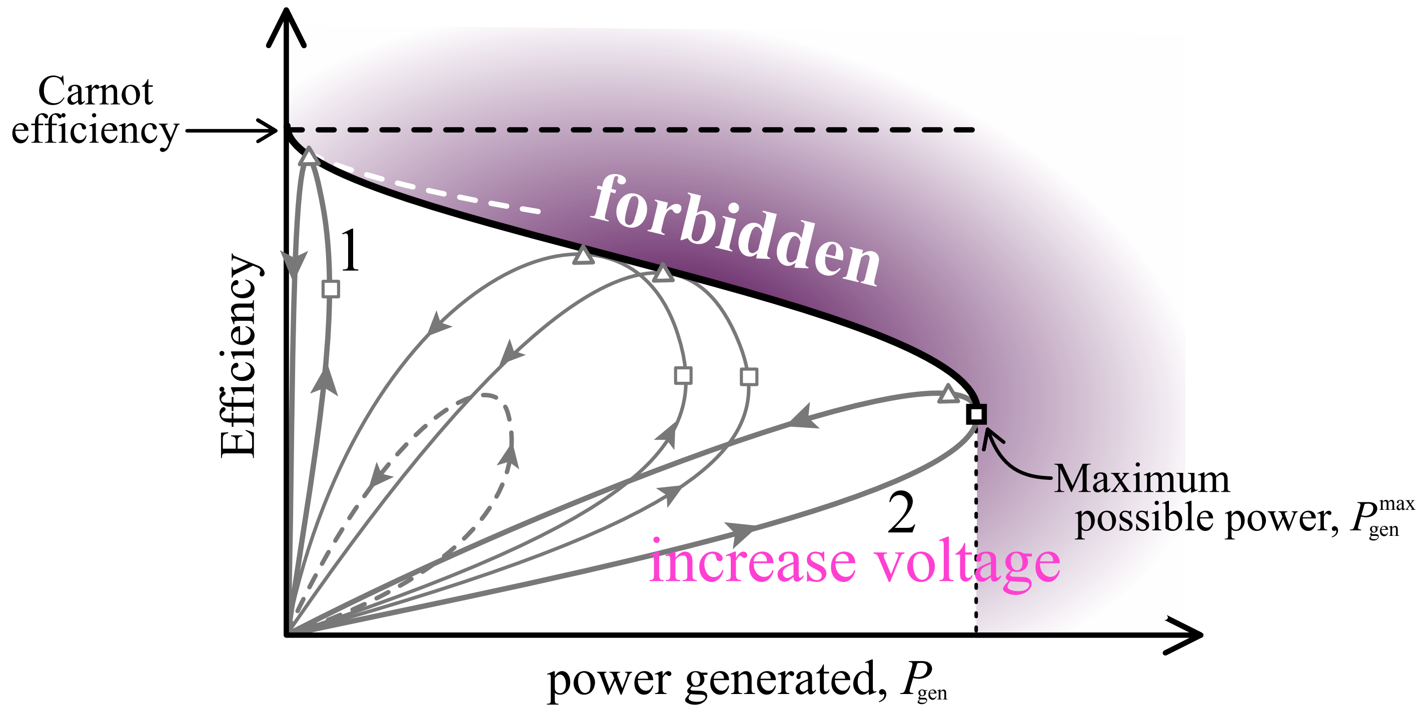
Efficiency optimization (at a given power)

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



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

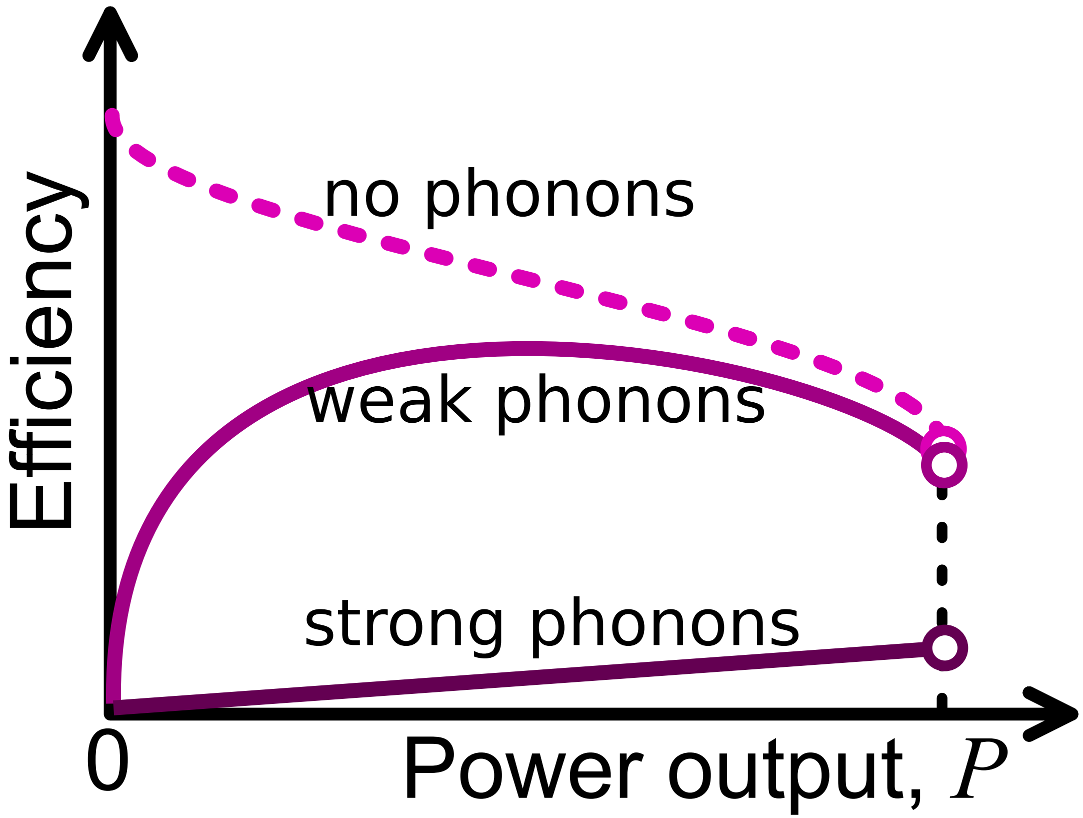
Trade-off between power and efficiency



Result from (nonlinear) scattering theory

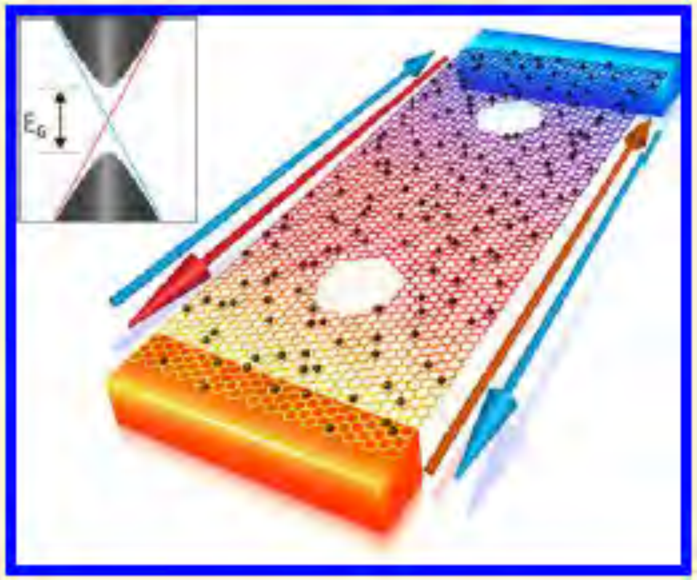
[Whitney, PRL **112**, 130601 (2014); PRB **91**, 115425 (2015)]

Power-efficiency trade-off including phonons



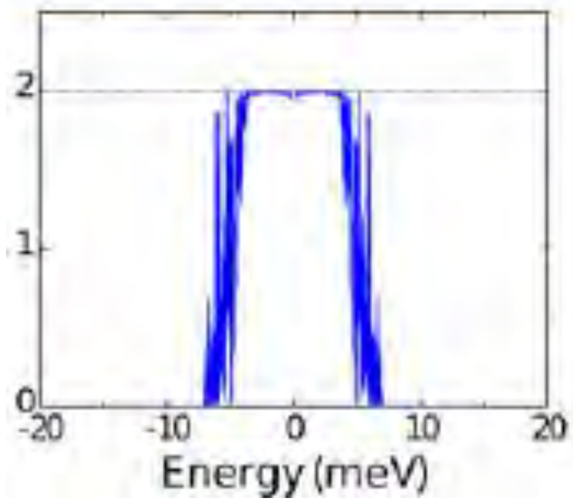
[see Whitney, PRB **91**, 115425 (2015)]

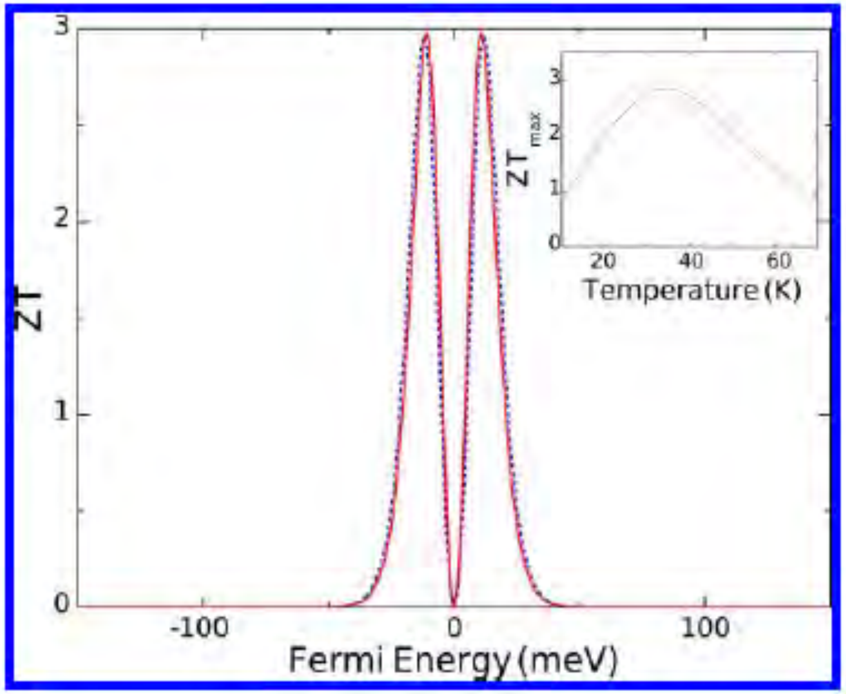
Boxcar transmission in topological insulators



Graphene nanoribbons with heavy adatoms and nanopores

[Chang et al., Nanolett., 14, 3779 (2014)]





Is it possible to overcome the non-interacting bound?

For $P/P_{max} \ll 1$,

$$\eta(P) \le \eta_{\max}(P) = \eta_C \left(1 - B_q \sqrt{\frac{T_R}{T_L} \frac{P}{P_{\max}}}\right),$$

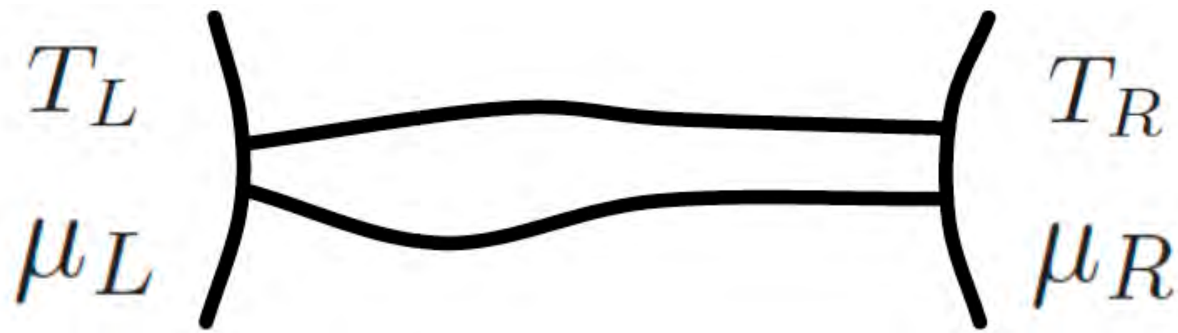
$$B_q \approx 0.478 \qquad (T_L > T_R)$$

Bound not favorable for power-efficiency trade-off; due to the fact that delta-energy filtering is the only mechanism to achieve Carnot for noninteracting systems

For interacting systems it is possible to achieve Carnot without delta-energy filtering

Linear response for coupled (particle and heat) flows

Stochastic baths: ideal gases at fixed temperature and electrochemical potential



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

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

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

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

$$\Delta T = T_L - T_R$$

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

Onsager relation (for time-reversal symmetric systems):

$$L_{eh} = L_{he}$$

Positivity of entropy production:

$$L_{ee} \geq 0, \quad L_{hh} \geq 0, \quad \det \boldsymbol{L} \geq 0$$

Onsager and transport coefficients

$$G = \left(\frac{J_e}{\Delta V}\right)_{\Delta T=0} = \frac{L_{ee}}{T}$$

$$K = \left(\frac{J_h}{\Delta T}\right)_{J_e=0} = \frac{1}{T^2}\frac{\det \boldsymbol{L}}{L_{ee}}$$

$$S = -\left(\frac{\Delta V}{\Delta T}\right)_{J_e=0} = \frac{1}{T}\frac{L_{eh}}{L_{ee}}$$

Note that the positivity of entropy production implies that the (isothermal) electric conductance G>0 and the thermal conductance K>0

Local equilibrium

Under the assumption of local equilibrium we can write phenomenological equations with ∇T and ∇μ rather than ΔT and Δμ

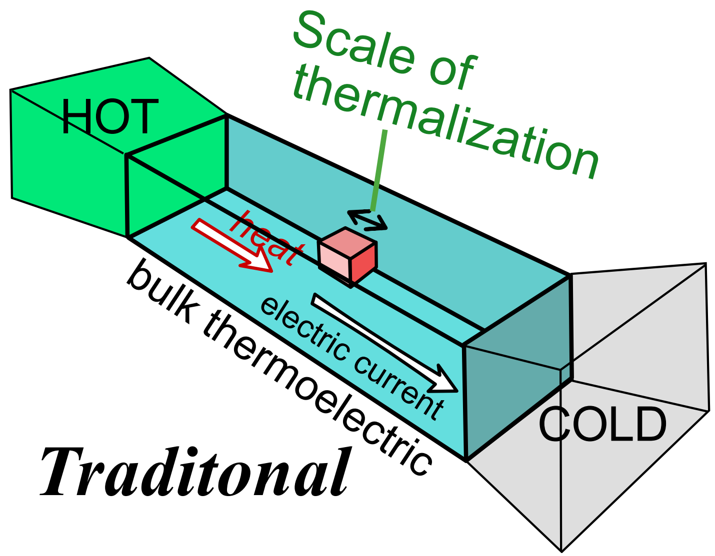
$$\begin{cases} j_e = \lambda_{ee}(-\nabla\mu/eT) + \lambda_{eh}\nabla(1/T) \\ \\ j_h = \lambda_{he}(-\nabla\mu/eT) + \lambda_{hh}\nabla(1/T) \end{cases}$$

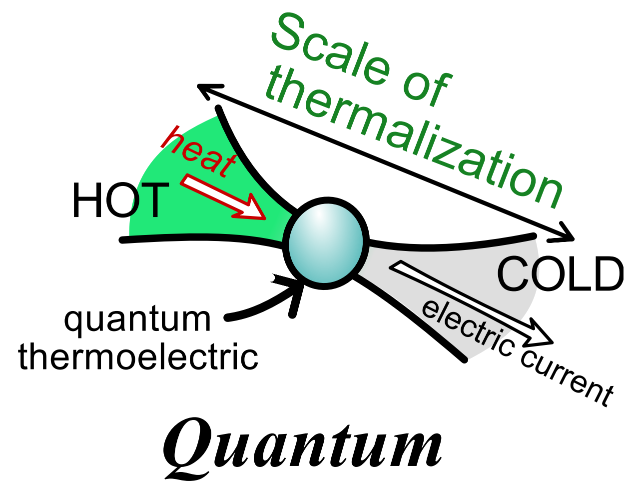
j_e, j_h charge and heat current densities

In this case we connect Onsager coefficients to electric and thermal conductivity rather than to conductances

$$\sigma = \left(\frac{j_e}{\nabla V}\right)_{\nabla T=0}, \quad \kappa = \left(\frac{j_h}{\nabla T}\right)_{j_e=0}$$

Traditional versus quantum thermoelectrics





Relaxation length (tens of nanometers at room temperature) of the order of the mean free path; inelastic scattering (phonons) thermalizes the electrons

Structures smaller than the relaxation length (many microns at low temperature); quantum interference effects; Boltzmann transport theory cannot be applied

[see G. B., G. Casati, K. Saito, R. S. Whitney, Phys. Rep. **694**, 1 (2017)]

Linear response?

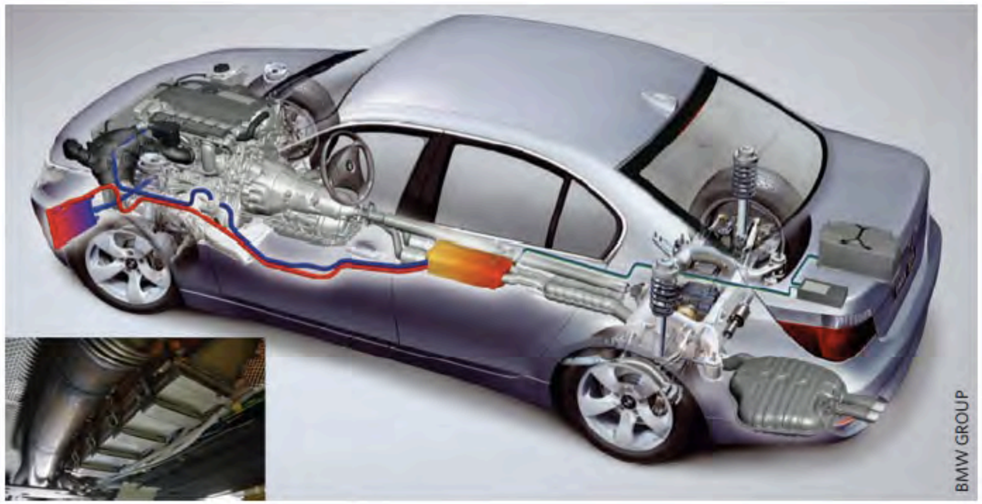


Figure 1 | Integrating thermoelectrics into vehicles for improved fuel efficiency. Shown is a BMW 530i concept car with a thermoelectric generator (yellow; and inset) and radiator (red/blue).

[Vining, Nat. Mater. **8**, 83 (2009)]

$$T_H \sim 600 - 700\,\mathrm{K}$$

(exhaust gases)

$$T_C \sim 270 - 300\,\mathrm{K}$$

(room temperature)

Linear response for small temperature and electrochemical potential differences (compared to the average temperature) on the scale of the relaxation length

Exhaust pipe: temperature drop over a mm scale: temperature drop of 0.003 K on the relaxation length scale (of 10 nm)

Maximum efficiency

Within linear response and for steady-state heat to work conversion:

$$\eta = \frac{P}{\dot{Q}_L} = \frac{-(\Delta V)J_e}{J_h} = \frac{-T\mathfrak{F}_e(L_{ee}\mathfrak{F}_e + L_{eh}\mathfrak{F}_h)}{L_{he}\mathfrak{F}_e + L_{hh}\mathfrak{F}_h}$$

Find the maximum of η over $\mathfrak{F}_e$ for fixed $\mathfrak{F}_h$ i.e., over the applied voltage ΔV for fixed temperature difference ΔT)

Maximum achieved for $\mathfrak{F}_e = \frac{L_{hh}}{L_{he}}\left(-1 + \sqrt{\frac{\det \boldsymbol{L}}{L_{ee}L_{hh}}}\right)\mathfrak{F}_h$

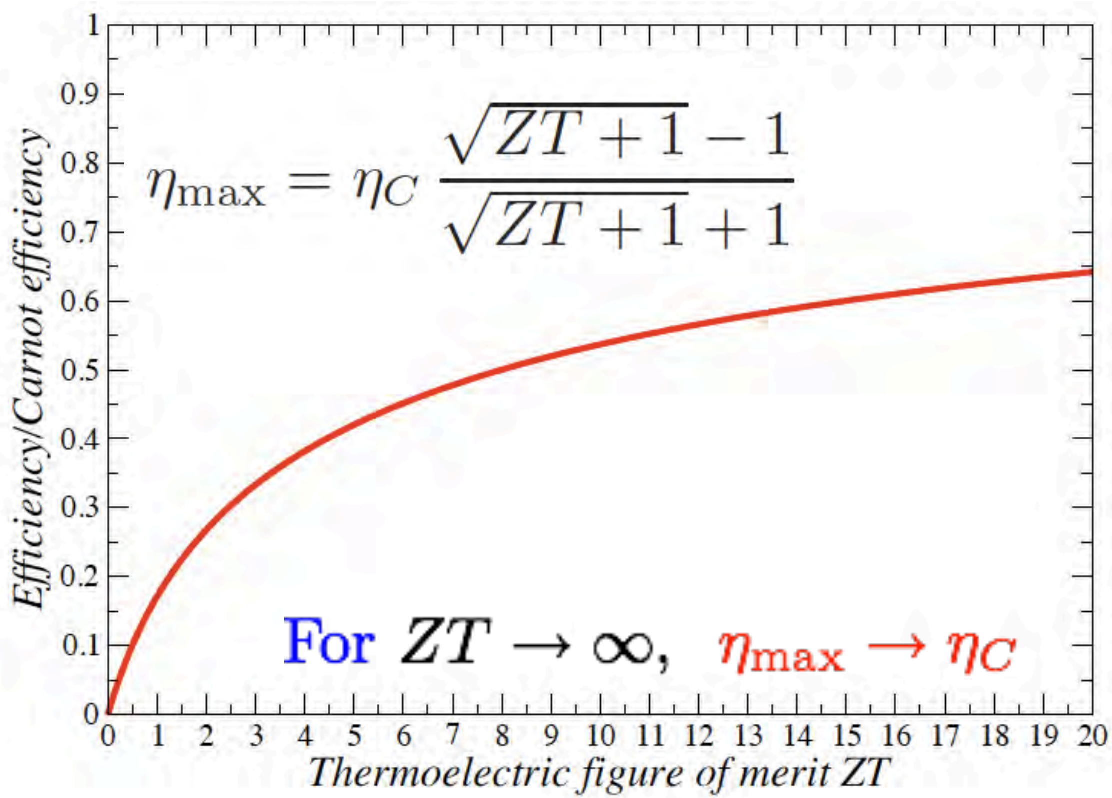
Maximum efficiency (for system with time-reversal symmetry)

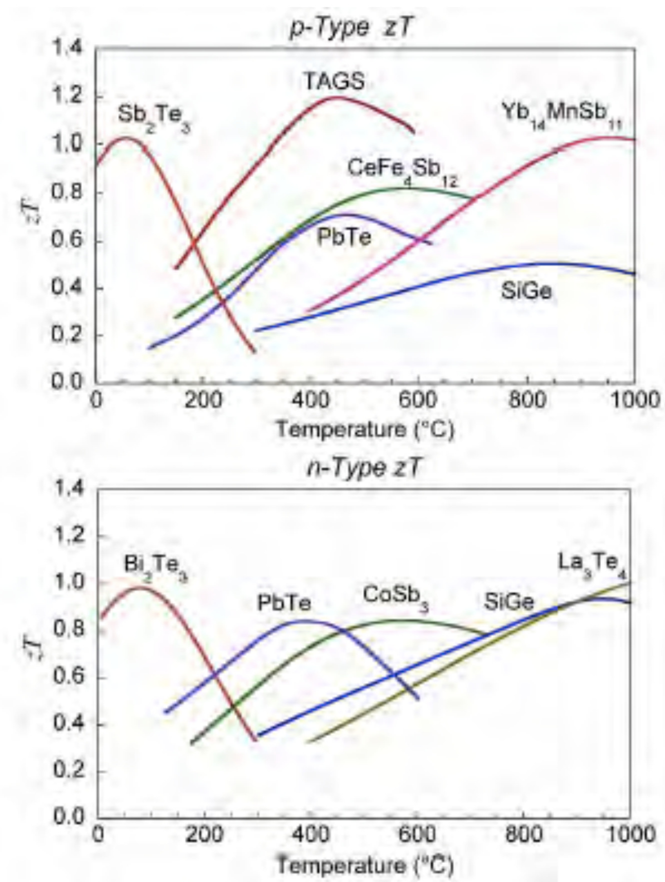
$$\eta_{\max} = \eta_C \frac{\sqrt{ZT+1}-1}{\sqrt{ZT+1}+1}$$

Thermoelectric figure of merit

$$ZT \equiv \frac{L_{eh}^2}{\det \mathbf{L}} = \frac{GS^2}{K} T$$

Positivity of entropy production implies $ZT > 0$





Efficiency at maximum power

Output power $P = -(\Delta V) J_e = -T\mathfrak{F}_e(L_{ee}\mathfrak{F}_e + L_{eh}\mathfrak{F}_h)$

Find the maximum of P over $\mathfrak{F}_e$ for fixed $\mathfrak{F}_h$ (over the applied voltage ΔV for fixed ΔT)

Maximum achieved for $\mathfrak{F}_e = -\dfrac{L_{eh}}{2L_{ee}}\mathfrak{F}_h$

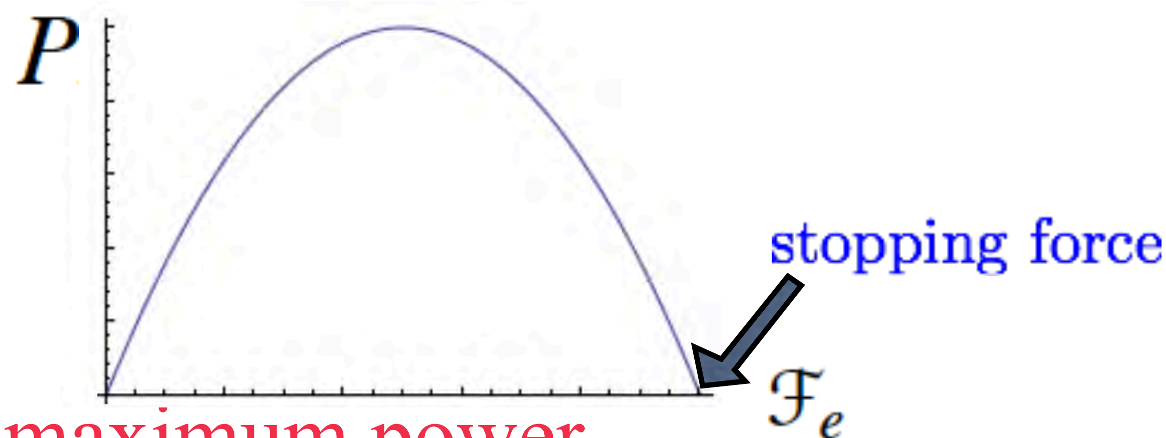
Maximum output power

$$P_{\max} = \frac{T}{4}\frac{L_{eh}^2}{L_{ee}}\mathcal{F}_h^2 = \frac{1}{4}S^2G(\Delta T)^2$$

Power factor S^2G

P quadratic function of $\mathcal{F}_e$, with maximum at half of the *stopping force*:

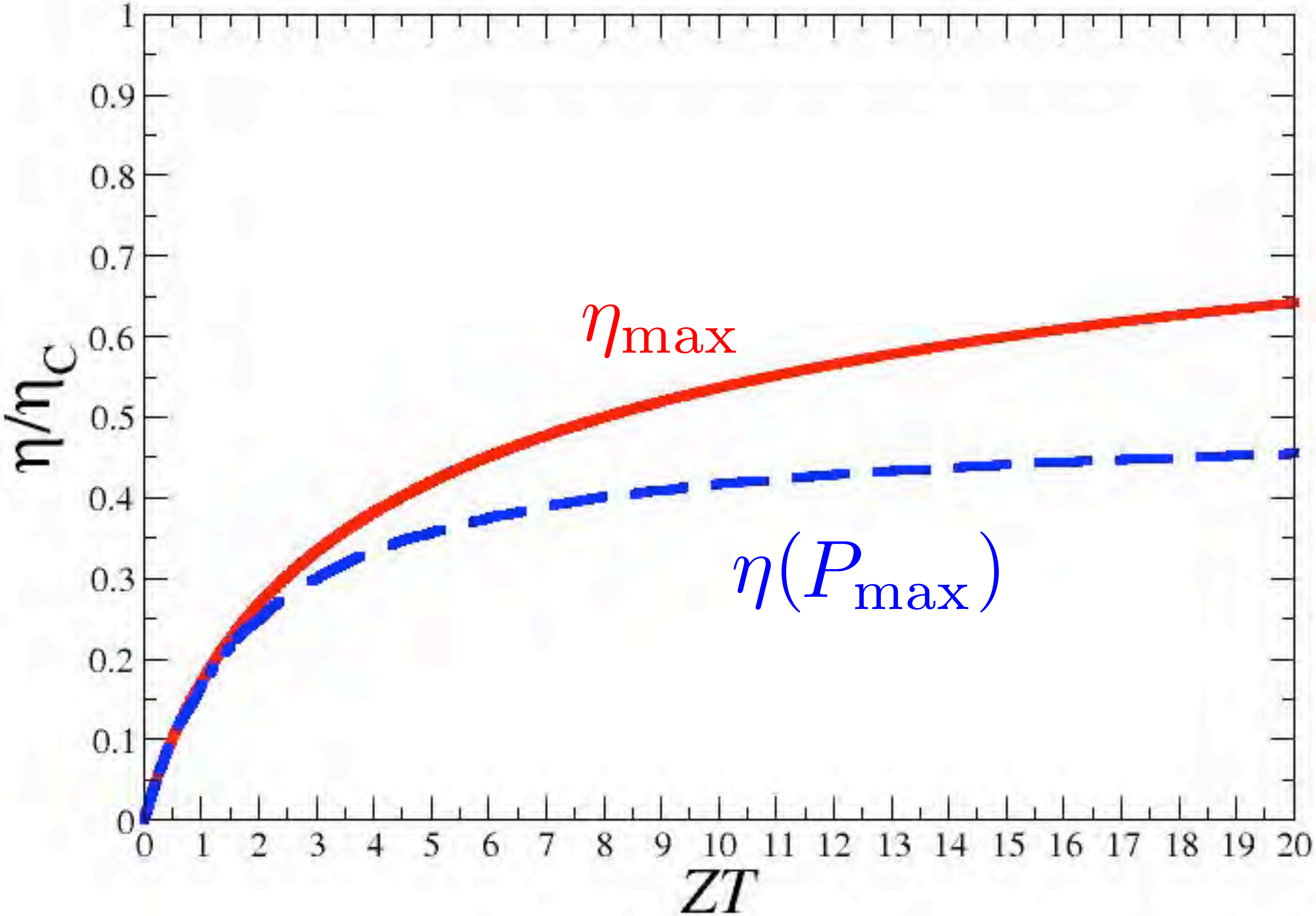
$$\mathcal{F}_e^{\text{stop}} = -\frac{L_{eh}}{L_{ee}} \mathcal{F}_h, \qquad J_e(\mathcal{F}_e^{\text{stop}}) = 0$$



Efficiency at maximum power

$$\eta(P_{\max}) = \frac{\eta_C}{2} \frac{ZT}{ZT+2} \leq \eta_{CA} \equiv \frac{\eta_C}{2}$$

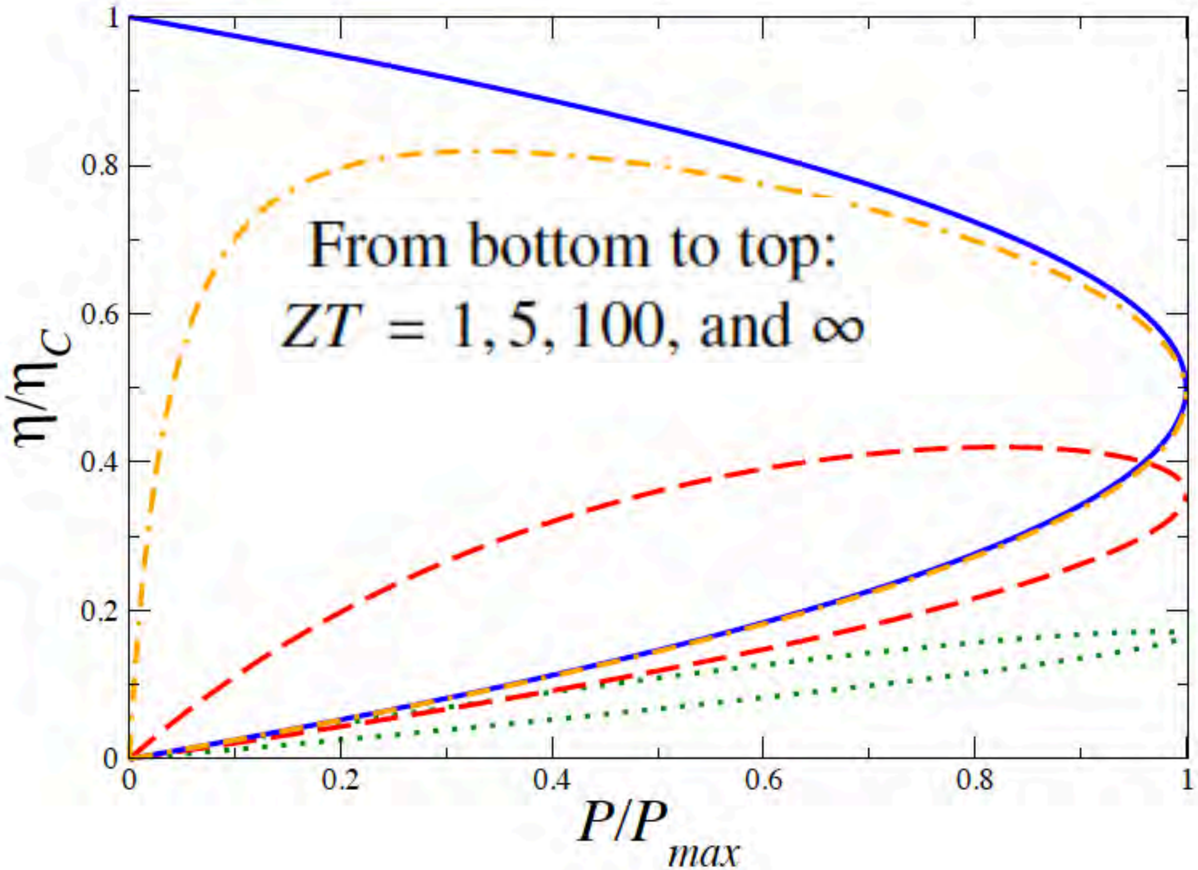
η_{CA} Curzon-Ahlborn upper bound


$\eta_{\max}$
$\eta(P_{\max})$
η/η_C
ZT
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Efficiency versus power

$$r = \mathcal{F}_e/\mathcal{F}_e^{\text{stop}} \qquad \frac{P}{P_{\max}} = 4r(1-r) \quad \Longrightarrow \quad r = \frac{1}{2}\left[1 \pm \sqrt{1 - \frac{P}{P_{\max}}}\right]$$

$$\frac{\eta}{\eta_C} = \frac{\frac{P}{P_{\max}}}{2\left(1 + \frac{2}{ZT} \mp \sqrt{1 - \frac{P}{P_{\max}}}\right)}$$



Interacting systems, Green-Kubo formula

The Green-Kubo formula expresses linear response transport coefficients in terms of dynamic correlation functions of the corresponding current operators, calculated at thermodynamic equilibrium

$$\lambda_{ab} = \lim_{\omega \to 0} \mathrm{Re}[\lambda_{ab}(\omega)]$$

$$\lambda_{ab}(\omega) = \lim_{\epsilon \to 0} \int_0^{\infty} dt e^{-i(\omega - i\epsilon)t} \lim_{\Omega \to \infty} \frac{1}{\Omega} \int_0^{\beta} d\tau \langle \hat{J}_a \hat{J}_b(t + i\tau) \rangle,$$

$$J_a = \langle \hat{J}_a \rangle$$

$$\hat{J}_a = \int_\Omega d\vec{r}\, \hat{j}_a(\vec{r})$$

$$\langle \cdot \rangle = \{\mathrm{tr}[(\cdot) \exp(-\beta H)]\} / \mathrm{tr}[\exp(-\beta H)]$$

$$\mathrm{Re}\lambda_{ab}(\omega) = 2\pi D_{ab} \delta(\omega) + \lambda_{ab}^{\mathrm{reg}}(\omega)$$

Non-zero generalized Drude weights signature of ballistic transport

Conservation laws and thermoelectric efficiency

Suzuki's formula (which generalizes Mazur's inequality) for finite-size Drude weights

$$d_{ab}(\Lambda) \equiv \frac{1}{2\Omega(\Lambda)} \lim_{\bar{t}\to\infty} \frac{1}{\bar{t}} \int_0^{\bar{t}} dt \langle \hat{J}_a(0)\hat{J}_b(t)\rangle = \frac{1}{2\Omega(\Lambda)} \sum_{m=1}^{M} \frac{\langle \hat{J}_a Q_m\rangle\langle \hat{J}_b Q_m\rangle}{\langle Q_m^2\rangle}$$

Q_m relevant (i.e., non-orthogonal to charge and thermal currents), mutually orthogonal conserved quantities

$$D_{ab} = \lim_{\bar{t}\to\infty} \lim_{\Lambda\to\infty} \frac{1}{2\Omega(\Lambda)\bar{t}} \int_0^{\bar{t}} dt \langle \hat{J}_a(0)\hat{J}_b(t)\rangle$$

Assuming commutativity of the two limits,

$$D_{ab} = \lim_{\Lambda\to\infty} d_{ab}(\Lambda)$$

Momentum-conserving systems

Consider systems with a single relevant constant of motion, notably momentum conservation

Ballistic contribution to $\det \lambda$ vanishes since

$$D_{ee} D_{hh} - D_{eh}^2 = 0$$

$$\sigma \sim \lambda_{ee} \sim \Lambda$$

$$S \sim \lambda_{eh} / \lambda_{ee} \sim \Lambda^0 \qquad ZT = \frac{\sigma S^2}{\kappa} T \propto \Lambda^{1-\alpha} \to \infty \text{ when } \Lambda \to \infty$$

$$\kappa \sim \det \lambda / L_{ee} \sim \Lambda^{\alpha}$$

$$(\alpha < 1)$$

(G.B., G. Casati, J. Wang, PRL 110, 070604 (2013))

For systems with more than a single relevant constant of motion, for instance for integrable systems, due to the Schwarz inequality

$$D_{ee}D_{hh} - D_{eh}^2 = ||\mathbf{x}_e||^2||\mathbf{x}_h||^2 - \langle \mathbf{x}_e, \mathbf{x}_h \rangle \geq 0$$

$$\mathbf{x}_i = (x_{i1}, \dots, x_{iM}) = \frac{1}{2\Lambda}\left(\frac{\langle J_i Q_1 \rangle}{\sqrt{\langle Q_1^2 \rangle}}, \dots, \frac{\langle J_i Q_M \rangle}{\sqrt{\langle Q_M^2 \rangle}}\right)$$

$$\langle \mathbf{x}_e, \mathbf{x}_h \rangle = \sum_{k=1}^{M} x_{ek} x_{hk}$$

Equality arises only in the exceptional case when the two vectors are parallel; in general

$$\det \lambda \propto \Lambda^2, \ \kappa \propto \Lambda, \ ZT \propto \Lambda^0$$

Example: 1D interacting classical gas

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

For $M = m$ (integrable model)

$$J_u = T_L\gamma_L - T_R\gamma_R \qquad (J_u = J_q + \mu J_\rho)$$

$$J_\rho = \gamma_L - \gamma_R.$$

$ZT = 1$ (at $\mu = 0$)

For $M \neq m$ ZT depends on the system size

Quantum mechanics needed:
Relation between density and electrochemical potential

Reservoirs modeled as ideal (1D) gases

$$f_\alpha(v) = \sqrt{\frac{m}{2\pi k_B T_\alpha}} \exp\left(-\frac{mv^2}{2k_B T_\alpha}\right)$$

Maxwell-Bolzmann distribution of velocities

$$\gamma_\alpha = \rho_\alpha \int_0^\infty dv\, v f_\alpha(v) = \rho_\alpha \sqrt{\frac{k_B T_\alpha}{2\pi m}}$$

injection rates

$$\Xi_\alpha = \sum_{N=0}^{\infty} \frac{1}{N!} \left\{ \frac{\Lambda}{h} e^{\beta_\alpha \mu_\alpha} \int dv\, m \exp\left[-\beta_\alpha \left(\frac{1}{2} m v^2\right)\right] \right\}^N$$

grand partition function

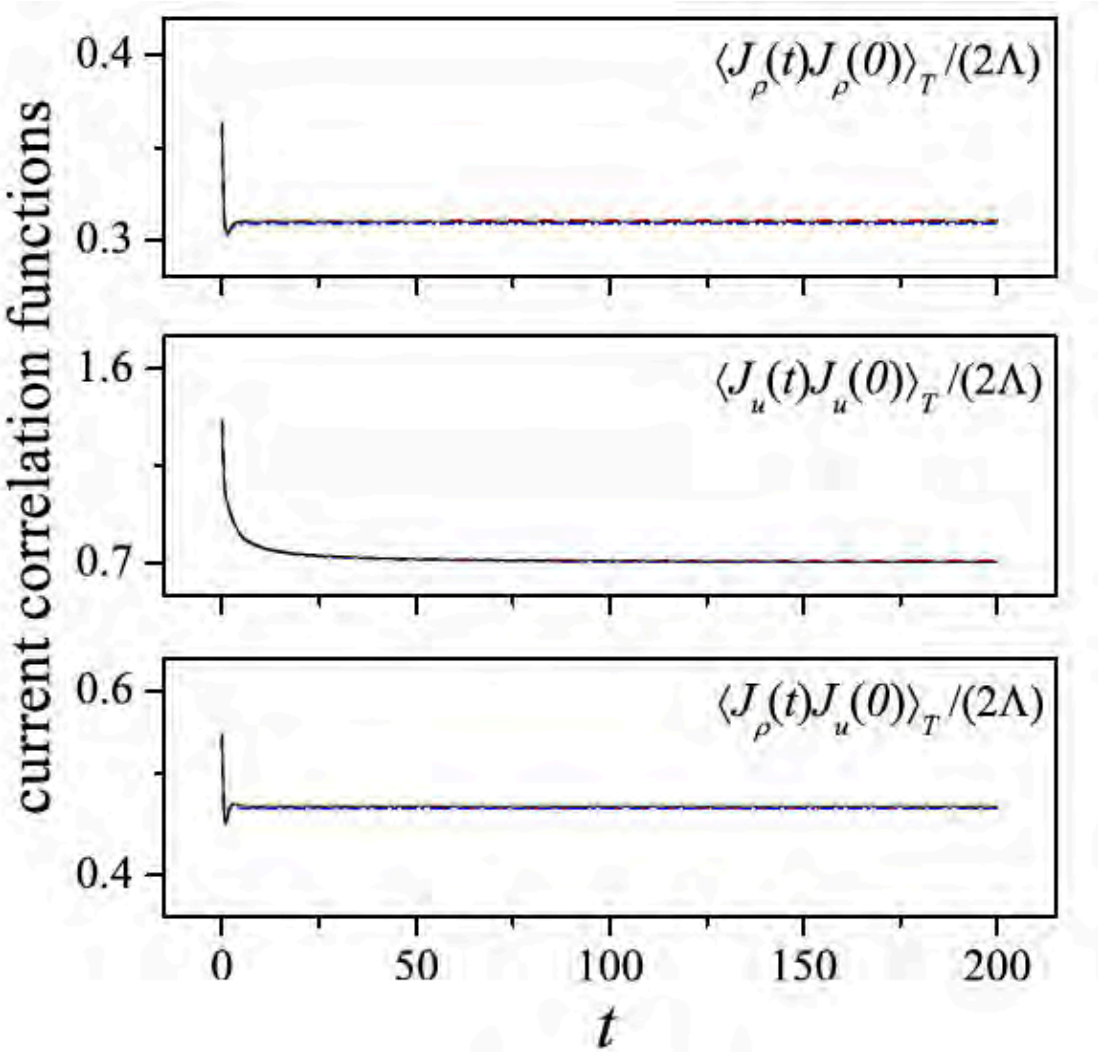
$$\langle N \rangle_\alpha = \frac{1}{\beta_\alpha} \frac{\partial}{\partial \mu_\alpha} \ln \Xi_\alpha, \quad \rho_\alpha = \frac{\langle N \rangle_\alpha}{\Lambda} = \frac{e^{\beta_\alpha \mu_\alpha} \sqrt{2\pi m k_B T_\alpha}}{h}$$

density

$$\mu_\alpha = k_B T_\alpha \ln(\lambda_\alpha \rho_\alpha), \quad \lambda_\alpha = \frac{h}{\sqrt{2\pi m k_B T_\alpha}}$$

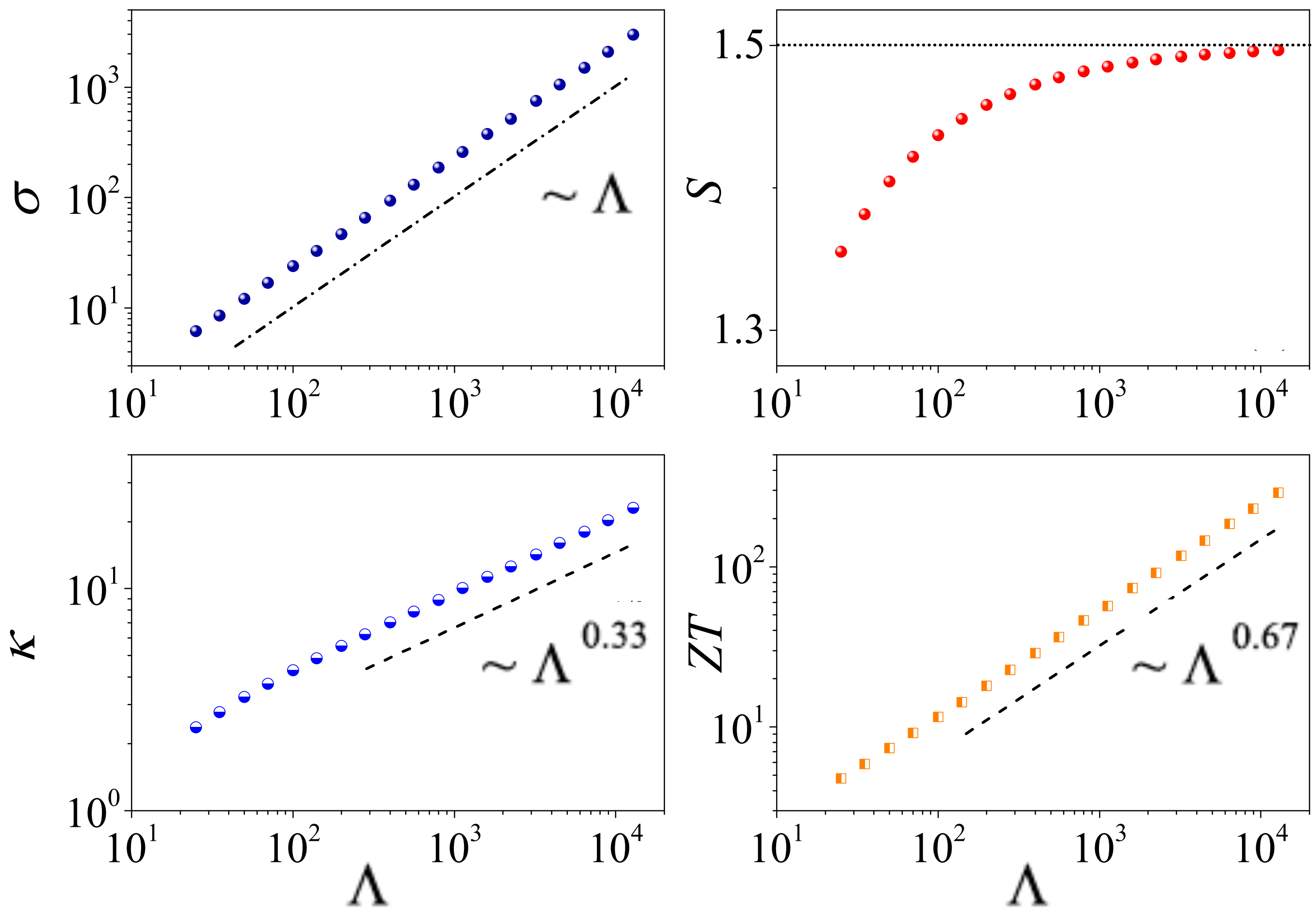
de Broglie thermal wave length

Non-decaying correlation functions



$\Lambda = 256$ (red dashed curve), 512 (blue dash-dotted curve), and 1024 (black solid curve)

Carnot efficiency at the thermodynamic limit



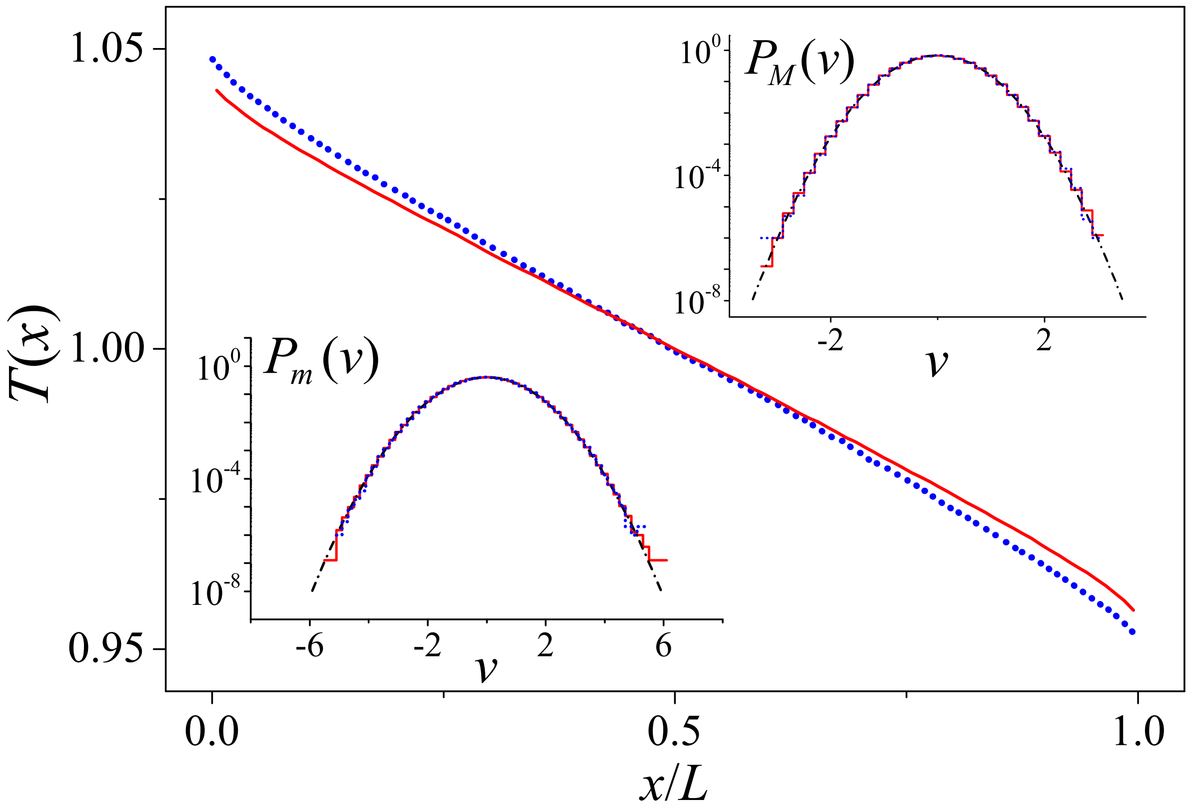
Anomalous thermal transport

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

ZT diverges increasing the systems size

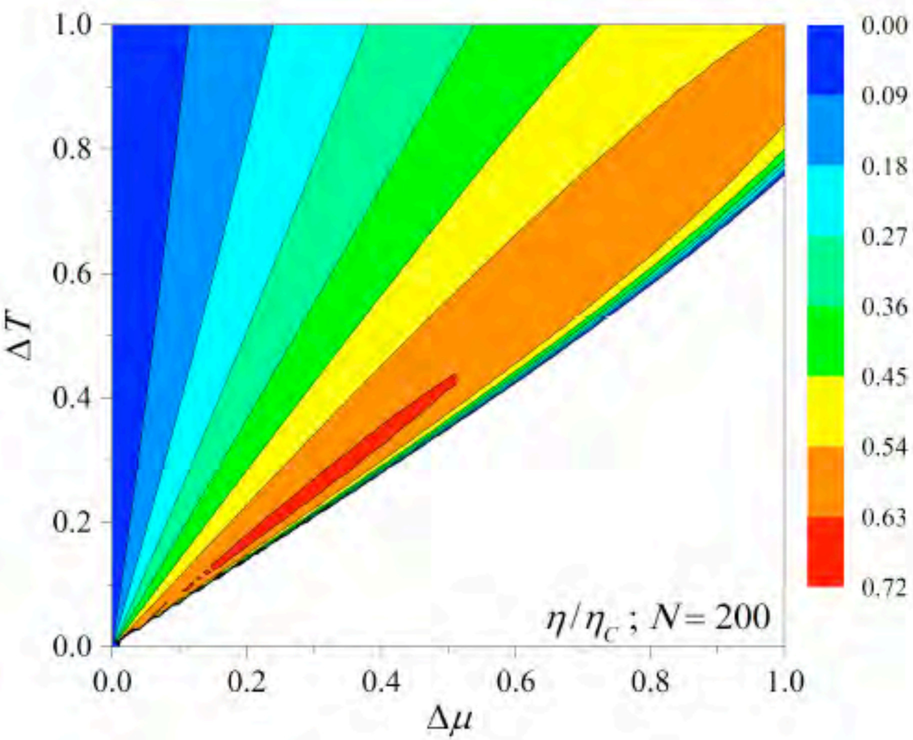
(R. Luo, G. B., G. Casati, J. Wang, arXiv:1710.08823)

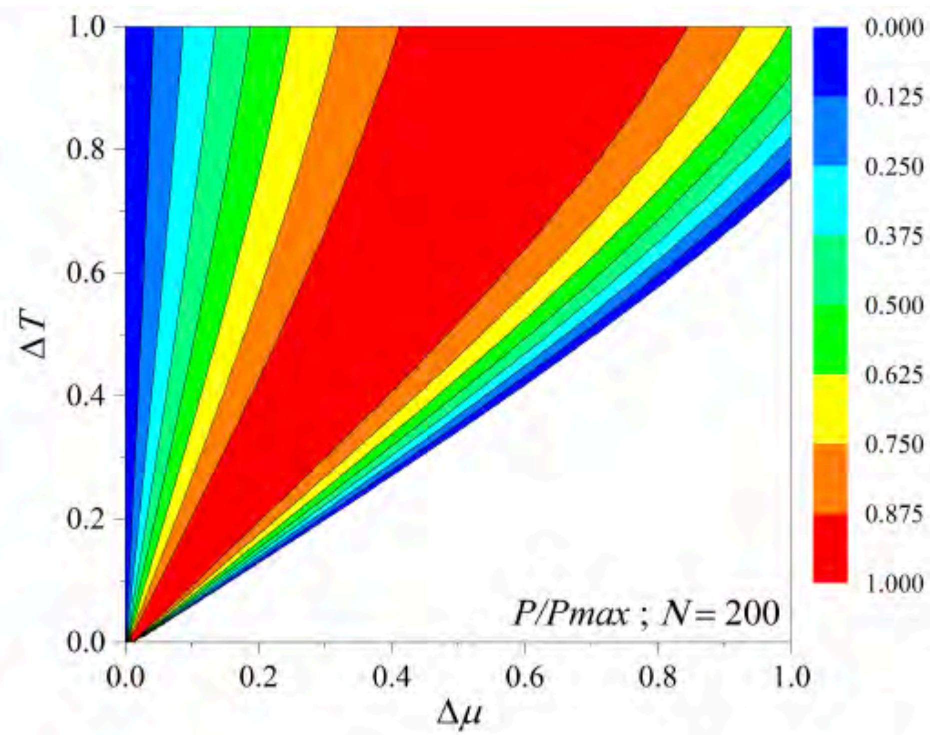
Delta-energy filtering mechanism?



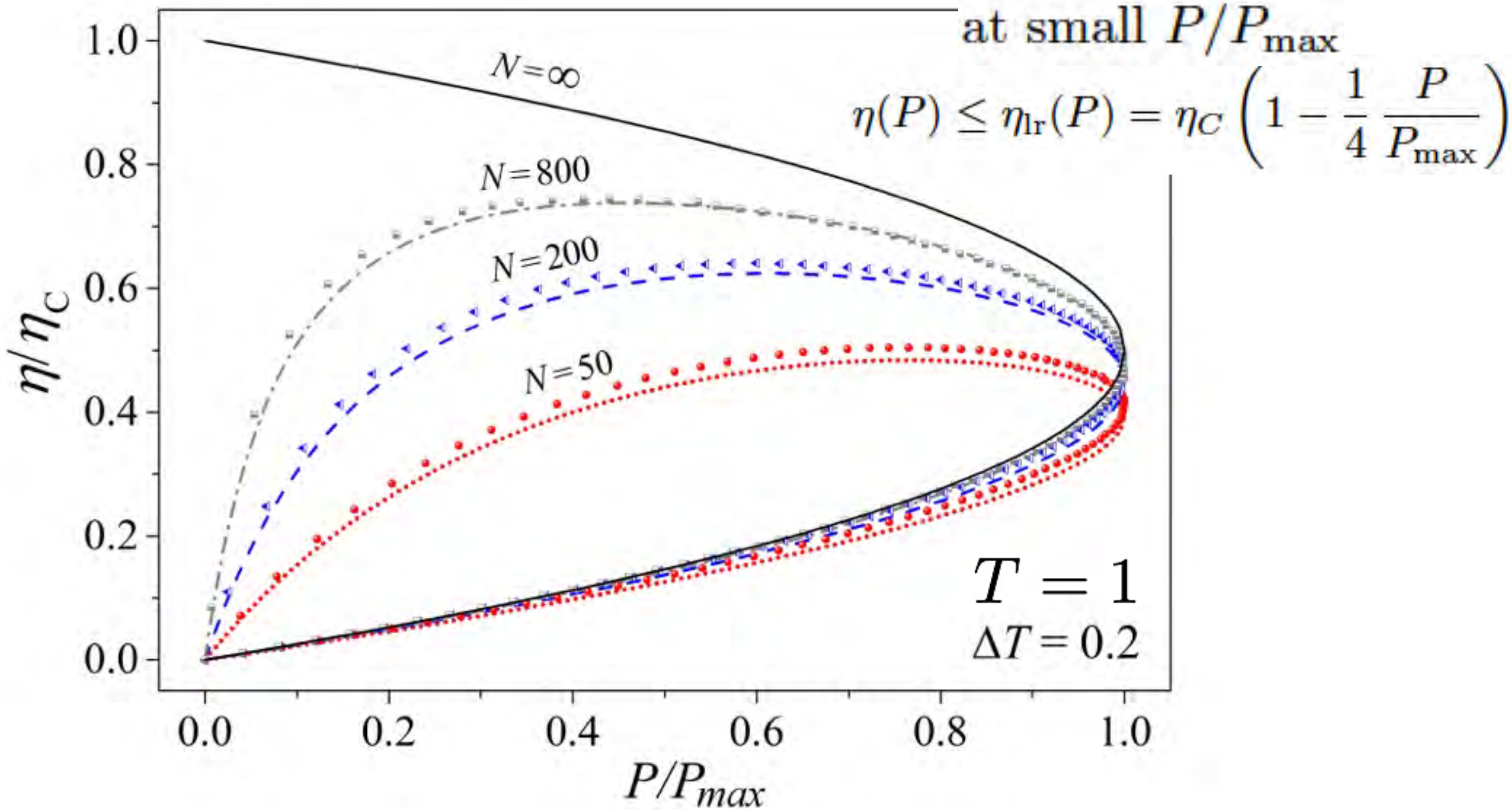
A mechanism for achieving Carnot different from delta-energy filtering is needed

Power vs. efficiency





Validity of linear response



The agreement with linear response improves with N

(∇T decreases as the system size increases)

Non-interacting classical bound (but quantum mechanics needed)

$$J_\rho = \gamma_L \int_0^\infty d\epsilon u_L(\epsilon)\mathcal{T}(\epsilon) - \gamma_R \int_0^\infty d\epsilon u_R(\epsilon)\mathcal{T}(\epsilon), \quad u_\alpha(\epsilon) = \beta_\alpha e^{-\beta_\alpha \epsilon}$$

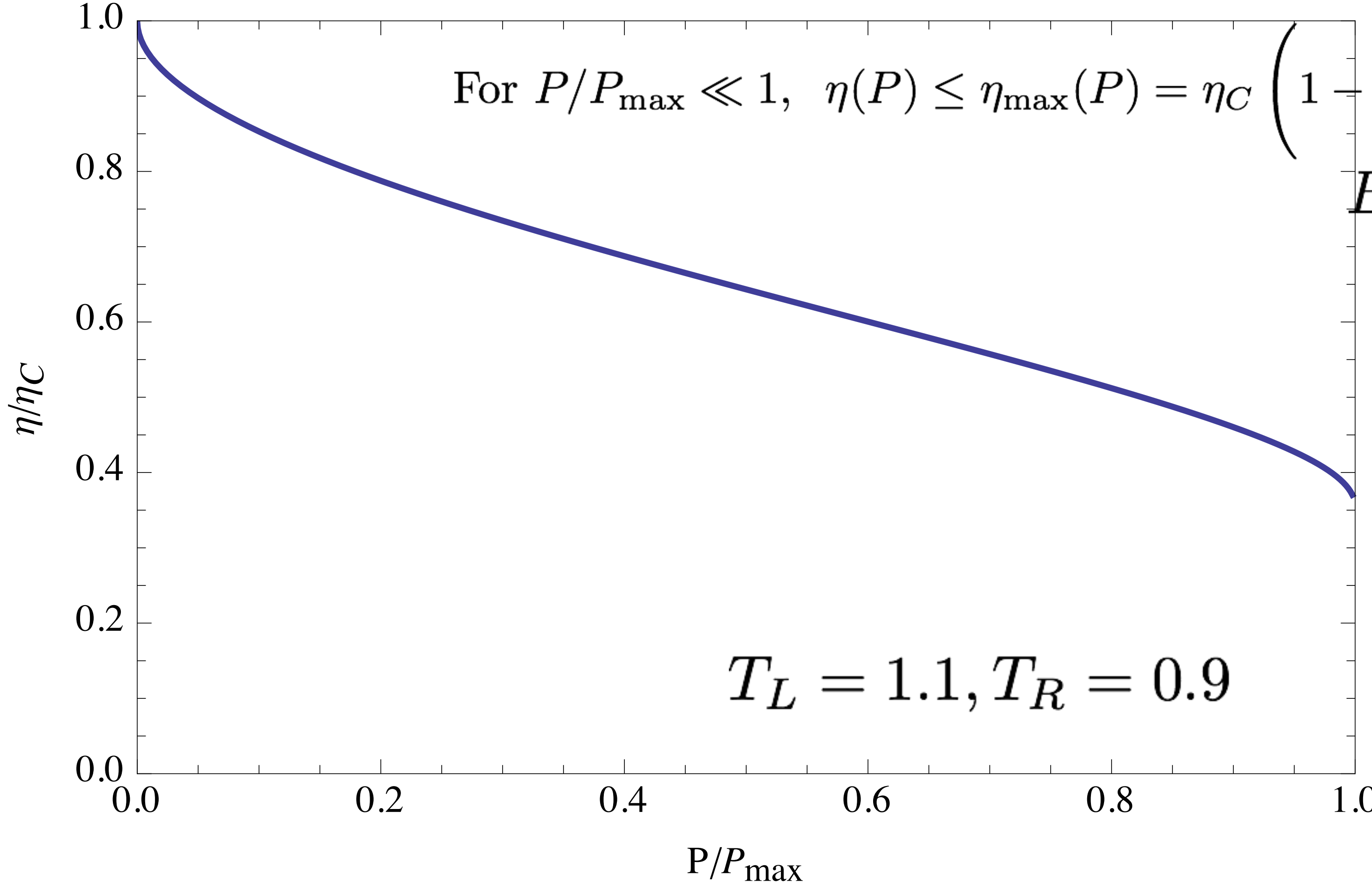
$$J_e = \frac{e}{h}\int_0^\infty dE\,[f_L(E) - f_R(E)]\tau(E)$$ charge current

$$J_{h,\alpha} = \frac{1}{h}\int_0^\infty dE\,(E-\mu_\alpha)[f_L(E) - f_R(E)]\tau(E)$$ heat current

$$f_\alpha(E) = e^{-\beta_\alpha(E-\mu_\alpha)}$$ Maxwell-Boltzmann distribution

$$0 \le \tau(E) \le 1$$ (in 1D)

$$\mu_\alpha = k_B T_\alpha \ln(\lambda_\alpha \rho_\alpha), \quad \lambda_\alpha = \frac{h}{\sqrt{2\pi m k_B T_\alpha}}$$ de Broglie thermal wave length

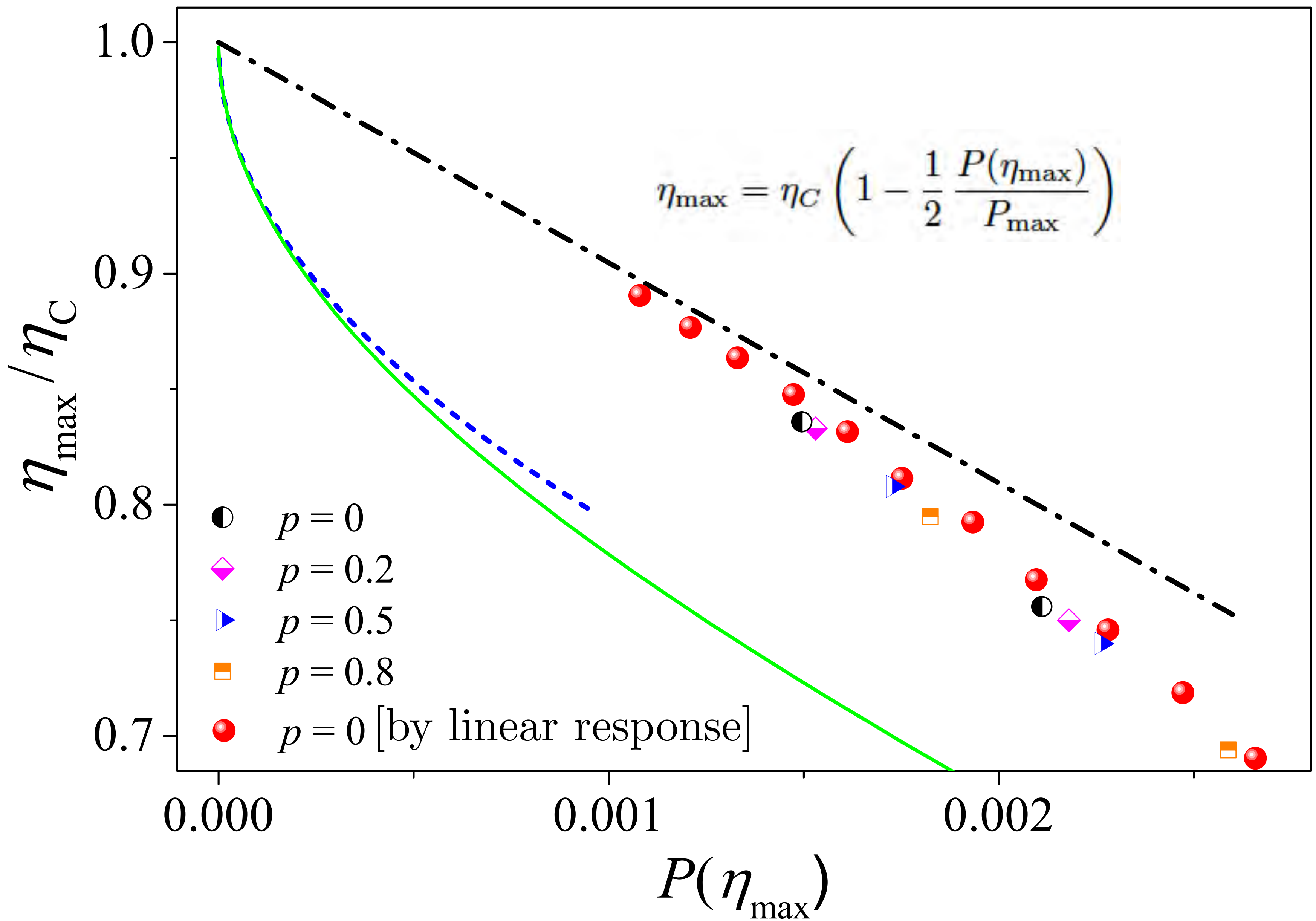


$$\text{For } P/P_{\max} \ll 1, \;\; \eta(P) \le \eta_{\max}(P) = \eta_C \left(1 - B_c \sqrt{\frac{T_R}{T_L}\frac{P}{P_{\max}}}\right),$$

$$B_c \approx 0.493$$

$$P \le P_{\max} = A_c \frac{\pi^2}{h} k_B^2 (\Delta T)^2, \quad A_c \approx 0.0373$$

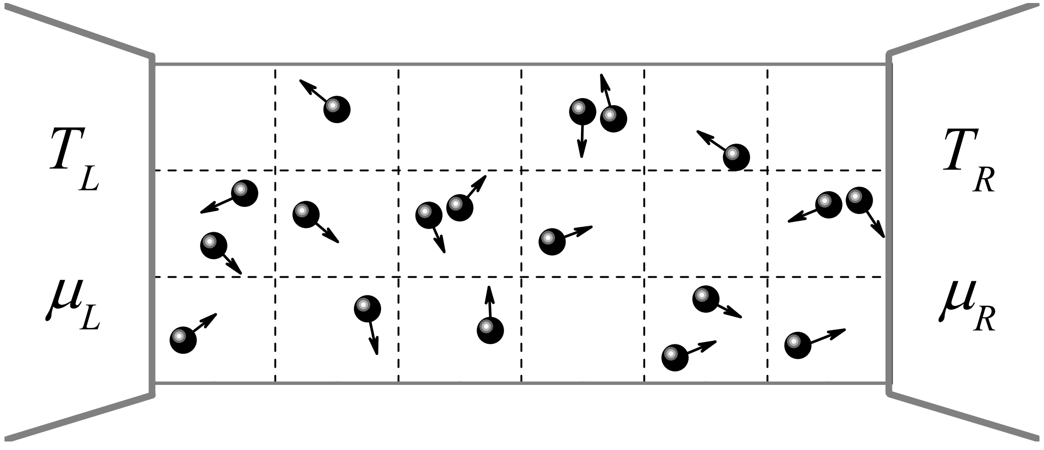
Overcoming the non-interacting bound



Multiparticle collision dynamics (Kapral model) in 2D

Streaming step: free propagation during a time τ

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

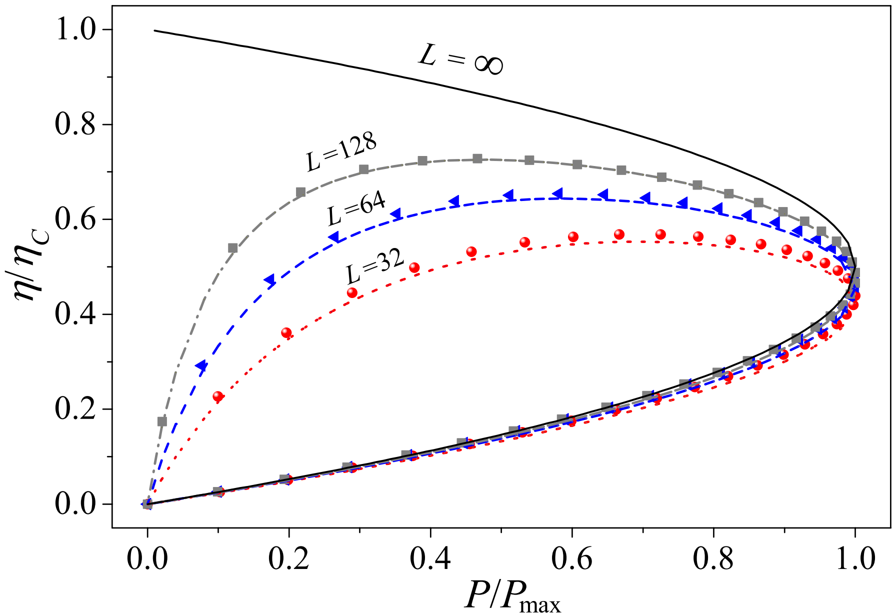


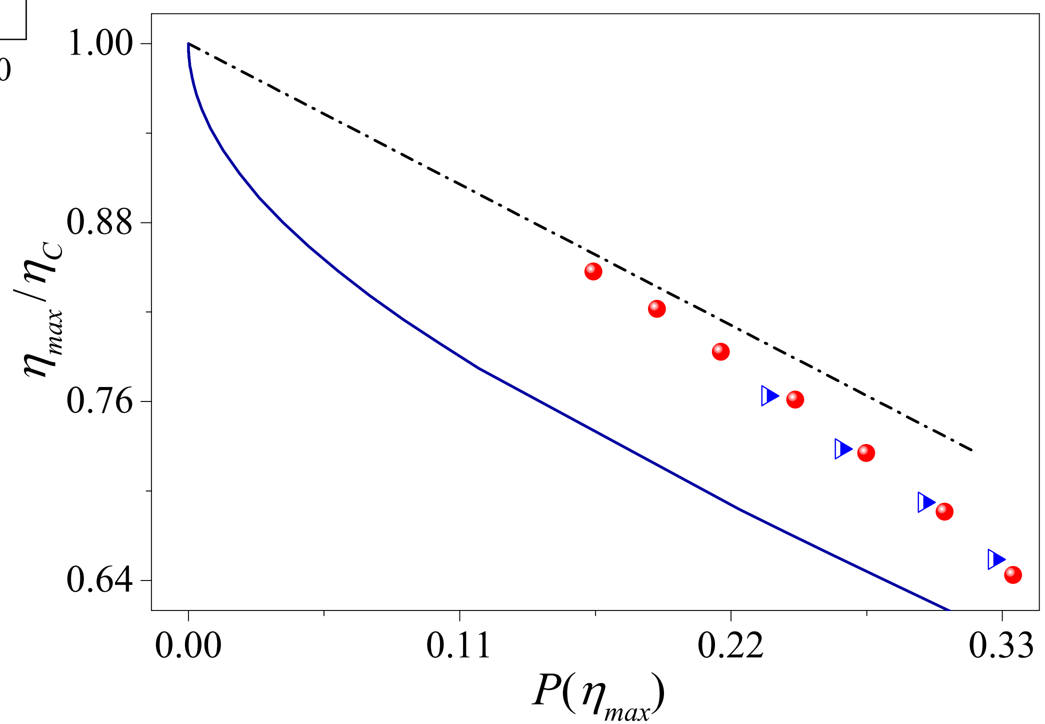
Collision step: random rotations of the velocities of the particles in cells of linear size *a* with respect to the center of mass velocity:

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

Momentum is conserved

Overcoming the (2D) non-interacting bound





Conclusions

Thanks to interactions, for a given power it is possible to overcome the bound of efficiency which applies for classical non-interacting systems

Non-integrable momentum-conserving systems exhibit a power-efficiency trade-off which is optimal within linear response

Results can be extended to cooling

Our results are based on the fact that such systems can achieve the Carnot efficiency at the thermodynamic limit without delta-energy filtering

Extension of our results to purely quantum systems?