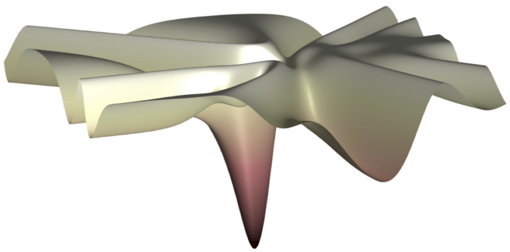
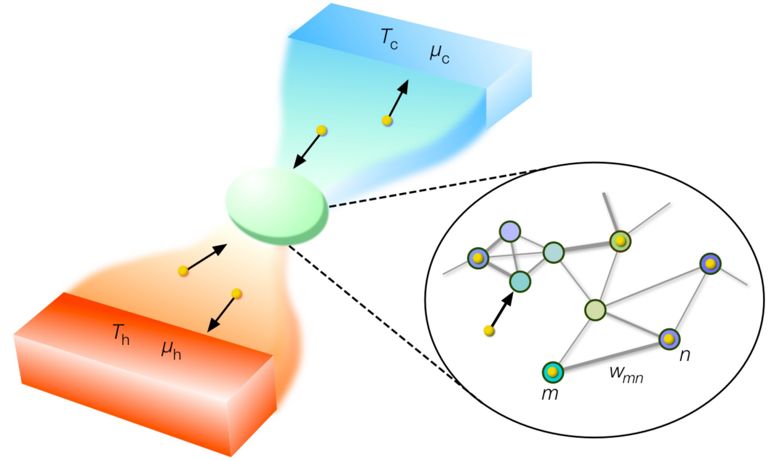




差分進化を用いた最適なナノ熱機関の探索

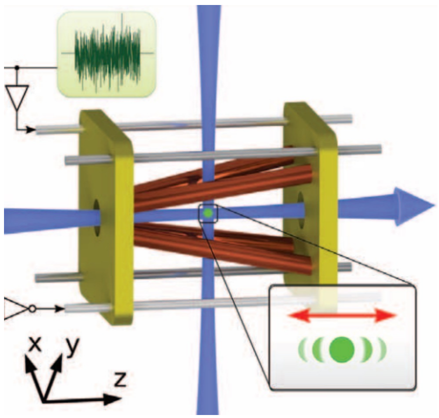
東大理
蘆田祐人

Ref: YA and T. Sagawa, Comm. Phys. 4, 45 (2021).

Motivation: What is the "best" nanoscale heat engines?

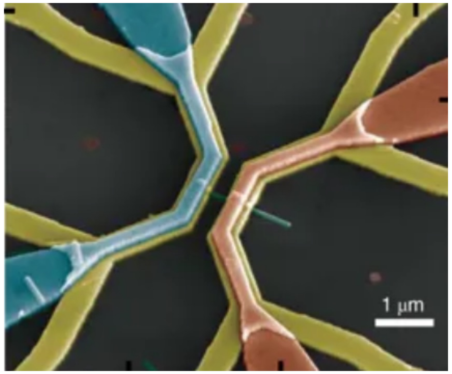
Remarkable developments in the ability to control ***nanoscale heat engines***:

Single trapped ion



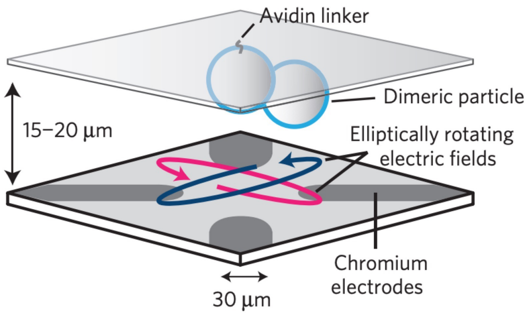
J. Rossnagel et al.,
Science 352, 6283 (2016).

Quantum dot



M. Josefsson et al.,
Nat. Nanotech. 13, 920 (2018).

Colloidal particle



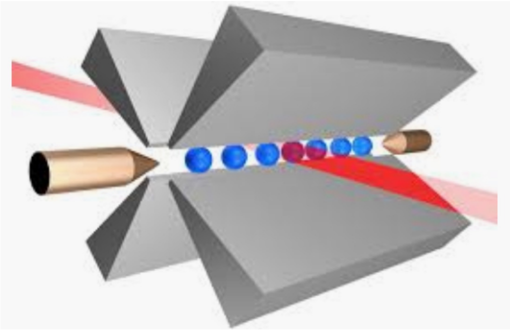
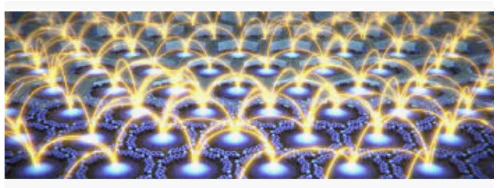
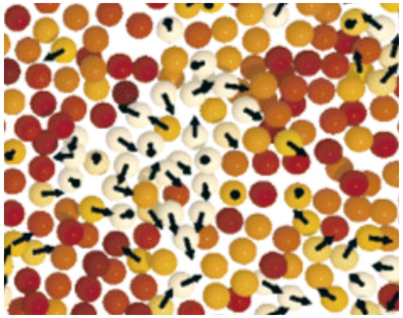
S. Toyabe et al.,
Nat. Phys. 6, 988 (2010).

So far, single-particle or noninteracting regimes are well explored.

Toward realizing high power, one has to assemble a large number of microscopic engines, in which interaction effects become essential.

Motivation: What is the “best” nanoscale heat engines?

Remarkable developments in the ability to control ***nanoscale heat engines***:

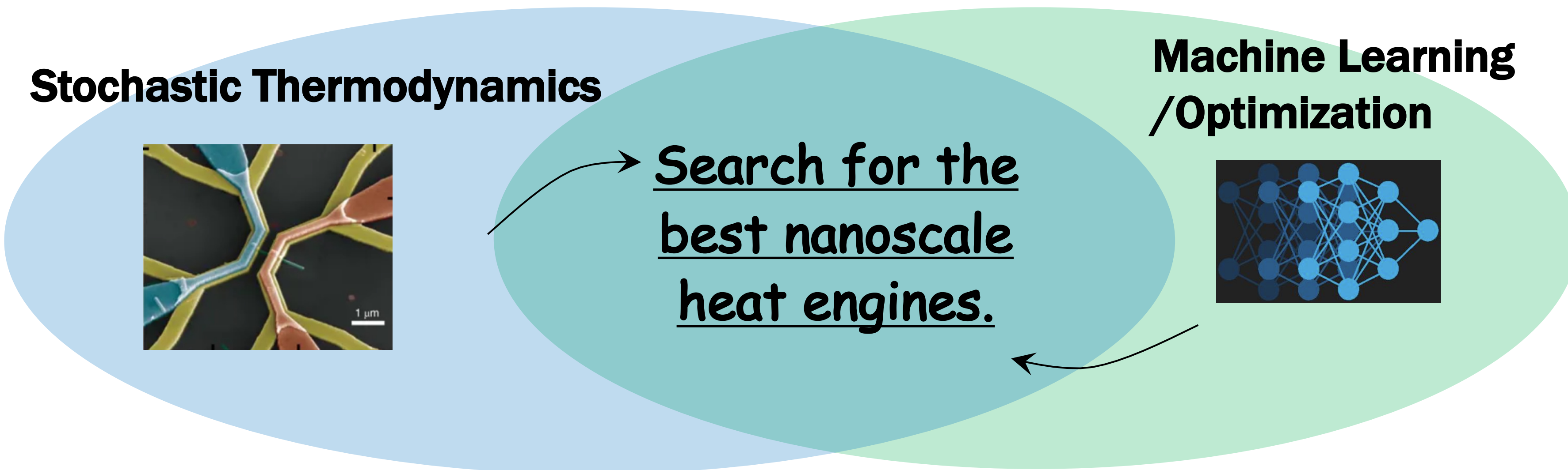
Trapped ions	Quantum-dot array	Colloidal particles
		
Univ. Innsbruck	I. Piquero-Zulaica et al., Nat. Commun. 8, 787 (2017).	P. J. Lu et al., Annu. Rev. Cond. Matt. 4, 217 (2013).

So far, single-particle or noninteracting regimes are well explored.

Toward realizing high power, one has to assemble a large number of microscopic engines, in which interaction effects become essential.

What is the “best” nanoscale heat engines with interactions?

Motivation: What is the “best” nanoscale heat engines?



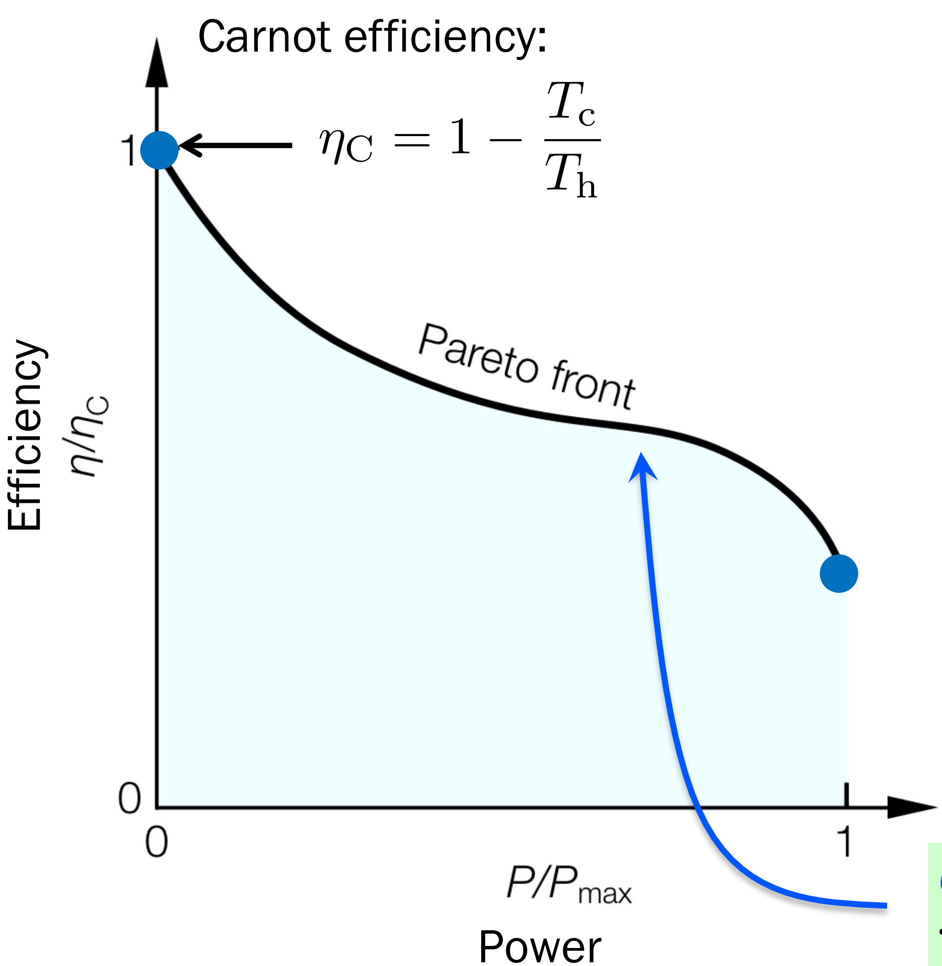
So far, single-particle or noninteracting regimes are well explored.

Toward realizing high power, one has to assemble a large number of microscopic engines, in which interaction effects become essential.

What is the “best” nanoscale heat engines with interactions?

The "best" heat engines as Pareto-optimal solutions

Two conflicting objectives: thermodynamic efficiency and power



Both of objectives cannot be optimized simultaneously in general.

The best heat engines =
<u>A set of engines whose efficiency and power cannot be further improved without comprising the other.</u>

= *"Pareto front"*

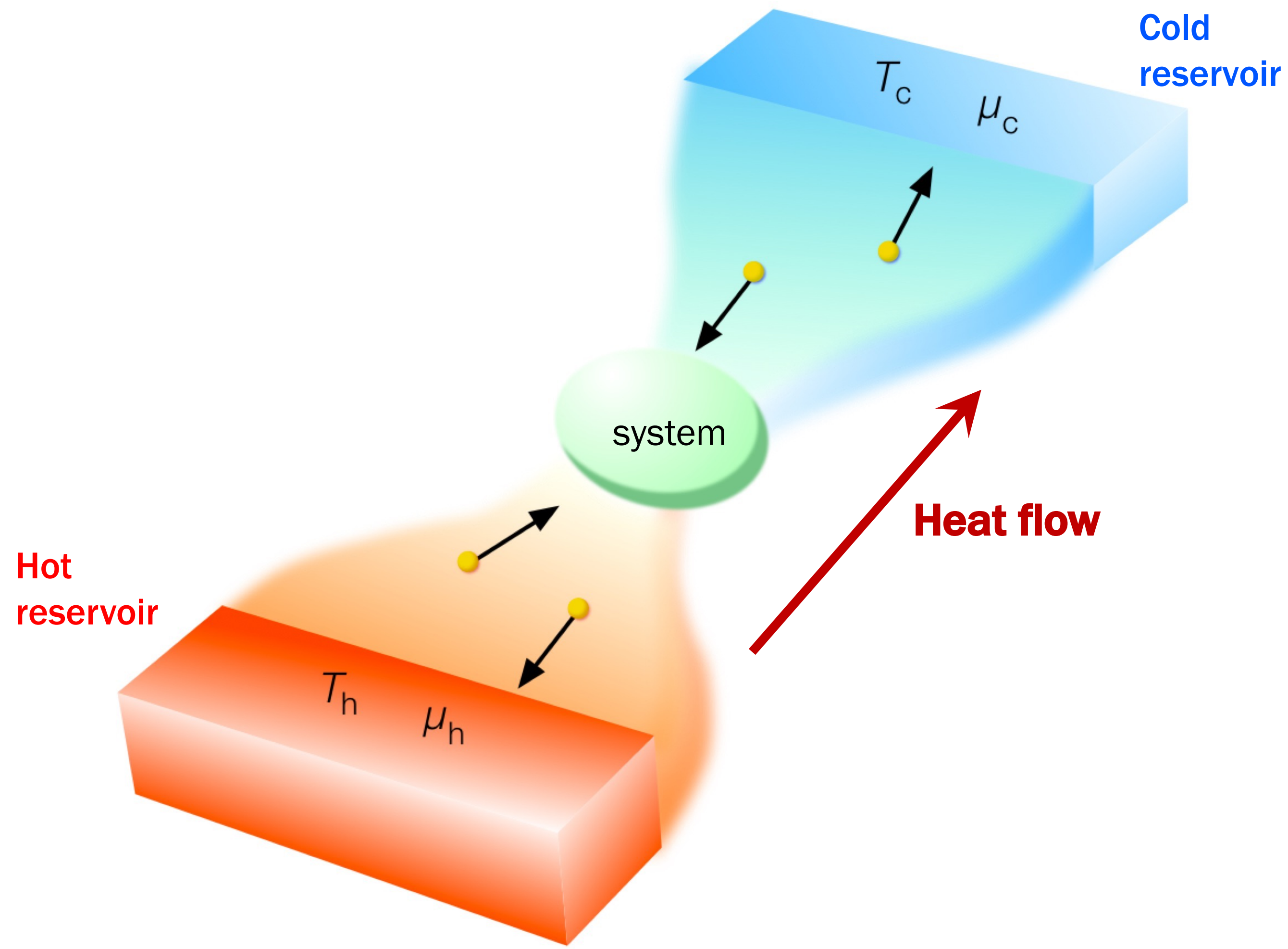
cf. Sawaragi et al.,
Theory of multiobjective optimization. (1985).

Specific examples: Carnot machine, heat engine operating at the maximum power.

Optimize the model parameters to find the best thermodynamic tradeoff

The "best" thermoelectric heat engines in linear-response regime

Thermoelectric system as a steady-state heat engine:
Convert heat flows into work in the form of electrical power.



The "best" thermoelectric heat engines in linear-response regime

Thermoelectric system as a steady-state heat engine:
Convert heat flows into work in the form of electrical power.

Linear-response formula
(cf. Benenti, Casati, Saito and Whitney, Phys. Rep. 694 (2017)):

$$\frac{\eta(P)}{\eta_{\mathrm{C}}} = \frac{P/(Q\delta T^2/4)}{2\left[1 + 2/ZT \mp \sqrt{1 - P/(Q\delta T^2/4)}\right]}$$

ZT : figure of merit

Q : power factor

$$\frac{\eta}{\eta_{\mathrm{C}}} \leq \frac{\sqrt{ZT+1}-1}{\sqrt{ZT+1}+1}$$

$$P \leq Q\delta T^2/4$$

Relation to transport coefficients:

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

σ : electrical conductance

κ : thermal conductivity

S : Seebeck coefficient

The “best” thermoelectric heat engines in linear-response regime

Thermoelectric system as a steady-state heat engine:
Convert heat flows into work in the form of electrical power.

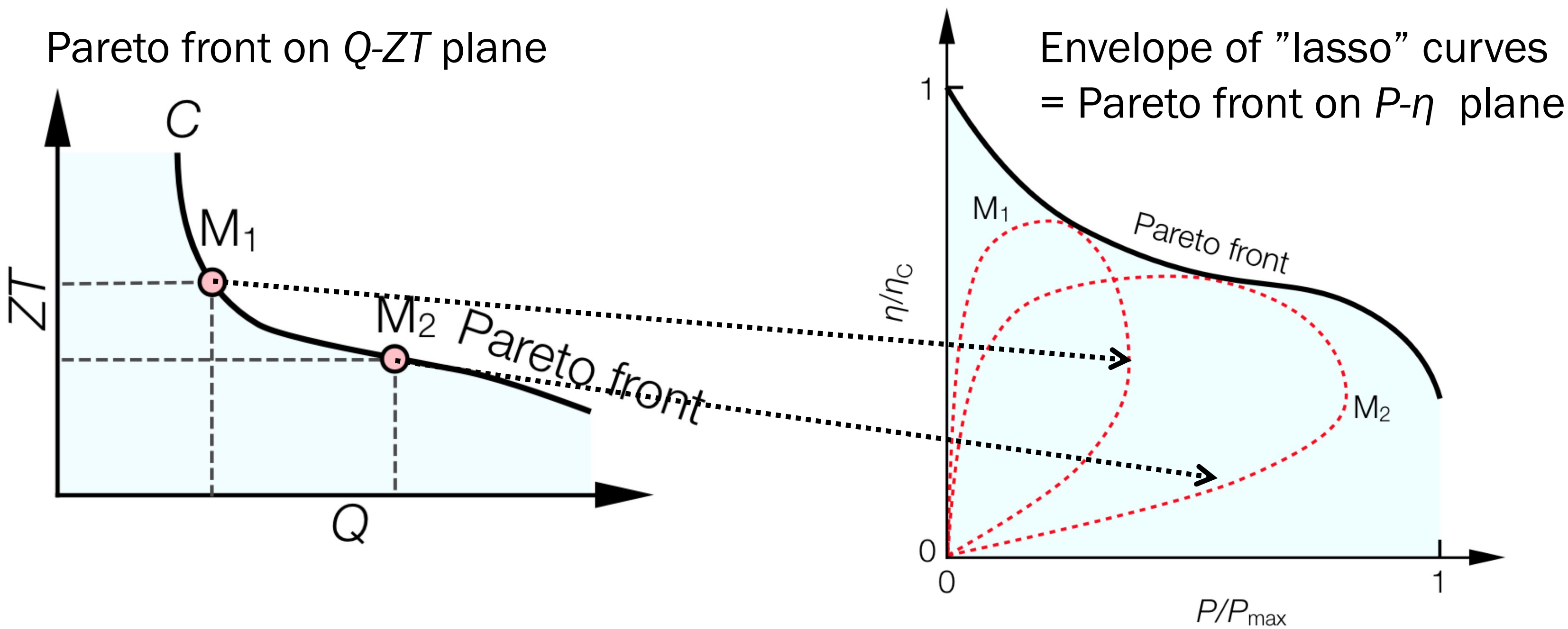
Linear-response formula
(cf. Benenti, Casati, Saito and Whitney, Phys. Rep. 694 (2017)):

$$\frac{\eta(P)}{\quad} = \frac{P/(Q\delta T^2/4)}{\quad}$$

In the linear-response regime, the search for the best heat engines reduces to finding the Pareto front on the Q-ZT plane.

Pareto front on *Q*-*ZT* plane

Envelope of ”lasso” curves
= Pareto front on *P*-*η* plane.



Model: interacting fermions in the sequential regime

Prototypical and generic model for interacting fermions:

$$H = \sum_l (\epsilon_l - v_g) n_l + \frac{1}{2} \sum_{l \neq m} w_{lm} n_l n_m$$

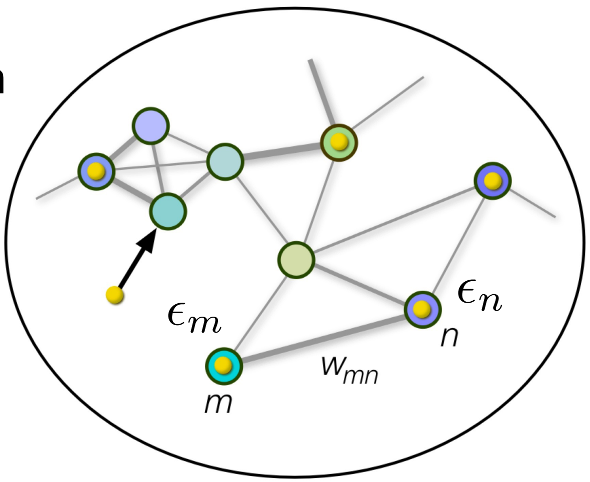
ϵ_l : single-electron modes

v_g : ground voltage

n_l : electron occupancy

w_{lm} : repulsive interaction

Graphical representation



"interaction network"

Node: single-electron level
Edge: interaction between nodes

Our aim: finding a set of the best heat engines in the presence of interaction = optimization of "network topology" in the graphical representation.

Calculations of ZT and Q

We neglect quantum coherence; the dynamics is described by the ***classical master equation*** **(=Stochastic Thermodynamics)**

cf. Seifert, Rep Prog. Phys. 75 126001 (2012)

$$\frac{dp_a}{dt} = \sum_b W_{ab} p_b, \quad W_{ab} = \Gamma_{ab} - \delta_{ab} \sum_d \Gamma_{db}, \quad \Gamma = \Gamma^{\mathrm{h}} + \Gamma^{\mathrm{c}},$$

$2^{N_f} \times 2^{N_f}$ transfer matrix

For the matrix elements between many-body states *a* and *b* whose particle-number difference is one, we set the ***detailed balance conditions***:

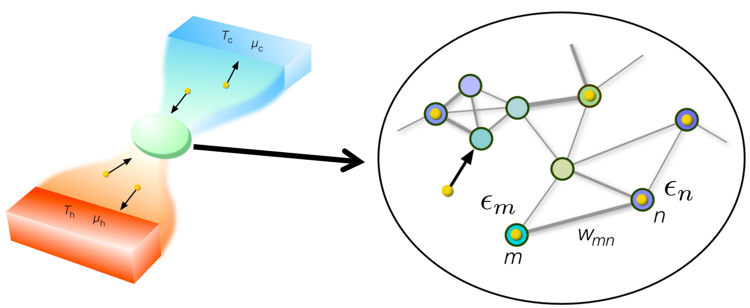
Fermi distribution

Entropy production

$$\Gamma^i_{ab} = \gamma_i f(\delta s^i_{ab}), \quad f(x) = \frac{1}{1+e^x}, \quad \delta s^i_{ab} = \frac{E_a - E_b}{k_{\mathrm{B}} T_i} + (N_a - N_b)\left(-\frac{\mu_i}{k_{\mathrm{B}} T_i}\right),$$

Reservoir: $i = \mathrm{h}, \mathrm{c}$

Steady-state solution: $W p^{\mathrm{ss}} = 0$



Calculations of ZT and Q

We work in the ***linear-response regime***:

$$\delta T = T_{\mathrm{h}} - T_{\mathrm{c}} \ll T_{\mathrm{h}} \qquad |\delta\mu| = |\mu_{\mathrm{h}} - \mu_{\mathrm{c}}| \ll k_{\mathrm{B}} T_{\mathrm{h}}$$

Using the steady-state values of the currents $(J^{\mathrm{ss}}, J_q^{\mathrm{ss}})^{\mathrm{T}}$ for $\begin{cases} \delta T = 0, \delta\mu \neq 0 \\ \delta T \neq 0, \delta\mu = 0 \end{cases}$,

we calculate the Onsager matrix and figure of merit ZT and power factor Q accordingly

$$ZT = \frac{\sigma S^2 T}{\kappa} = \frac{L_{12}L_{21}}{\det(\mathbf{L})}, \quad Q = \sigma S^2 = \frac{L_{12}^2}{T^3 L_{11}}, \quad \begin{pmatrix} J^{\mathrm{h}} \\ J_q^{\mathrm{h}} \end{pmatrix} = \mathbf{L} \begin{pmatrix} \delta\mu/T \\ \delta T/T^2 \end{pmatrix},$$

J_q^{h} : heat current out of the hot reservoir

J^{h} : particle current out of the hot reservoir

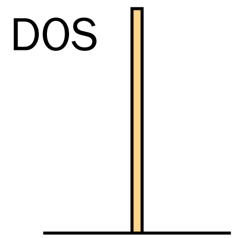
(*System works as a heat engine when we set) $\begin{cases} \delta\mu < 0 \;\; \text{if} \;\; S > 0 \\ \delta\mu > 0 \;\; \text{if} \;\; S < 0 \end{cases}$

Previous studies in noninteracting regimes

Noninteracting case: $w_{lm} = 0$

The best engine in the ideal situation:
perfectly degenerate single-electron levels

$$\epsilon_1 = \epsilon_2 = \cdots = \epsilon_{N_f}$$

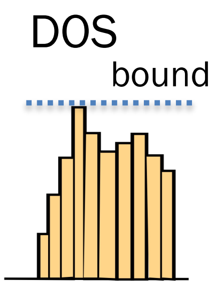


cf. Mahan & Sofo, PNAS 93, 7436 (1996).

$$ZT \to \infty \qquad Q \propto N_f$$

∵) tight-coupling condition satisfied: $J \propto J_q$

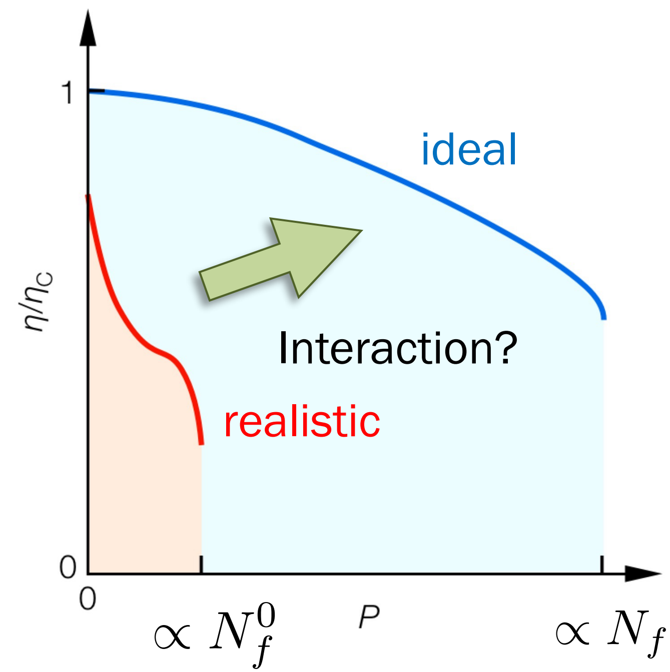
The best engine in a realistic situation:
(imposing upperbound on DOS)
nondegenerate single-electron levels



$$\epsilon_1 < \epsilon_2 < \cdots < \epsilon_{N_f}$$

cf. Whitney, PRB 91, 115425 (2015).

$$ZT \text{ finite} \qquad Q \propto N_f^0$$



Can interaction push up the bound close to the ideal case?

Problem setting and optimization algorithm

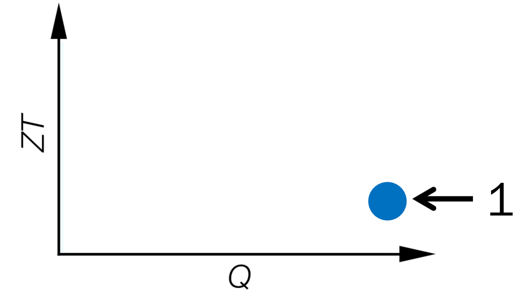
Problem: Given generic (nondegenerate) single-electron levels $\epsilon_1 < \epsilon_2 < \cdots < \epsilon_{N_f}$,

find a set of the optimal parameters $\mathcal{W} = \{v_g, \{w_{lm}\}_{l>m}\}$,

which provide the Pareto front on the *Q-ZT* plane.

Strategy:

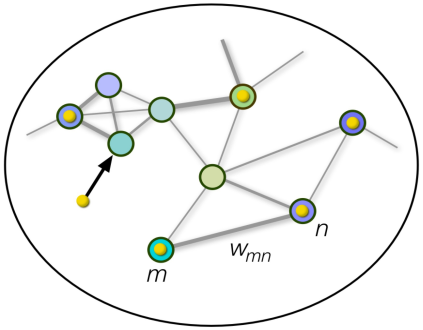
1. Maximize *Q* with respect to $\mathcal{W}$ via solving the single-objective optimization problem.
   → Identifying an unambiguous element for the Pareto front.



2. Search the Pareto front starting from the above solution.

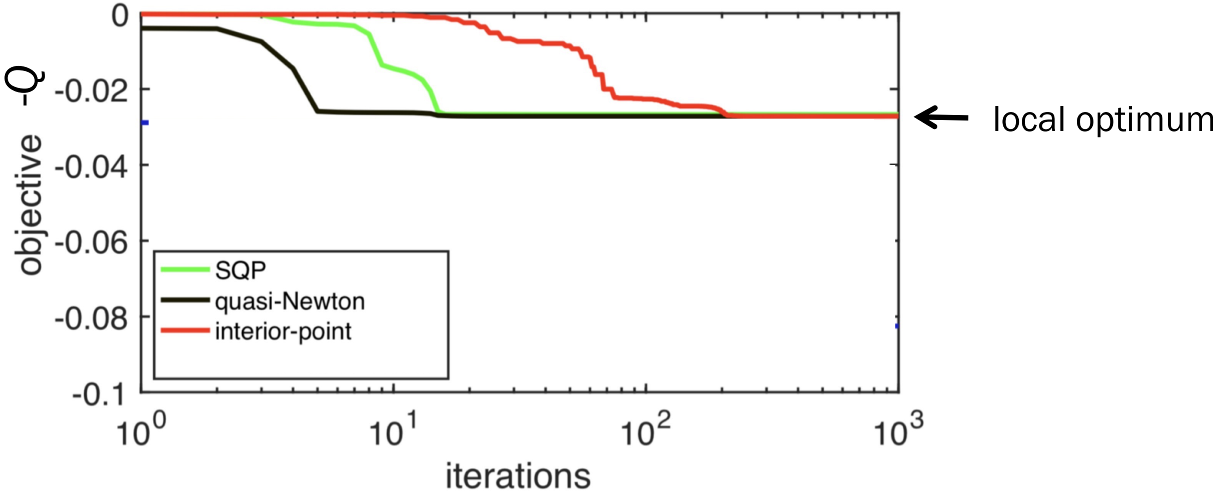
   The iterative alternate method:
   Custodio et al., SIAM J. Optim. 21, 1109 (2011).

Optimizing (training) $\mathcal{W}$ to maximize efficiency and power
= "Reinforcement learning" of the underlying topology and weights of the interaction network.

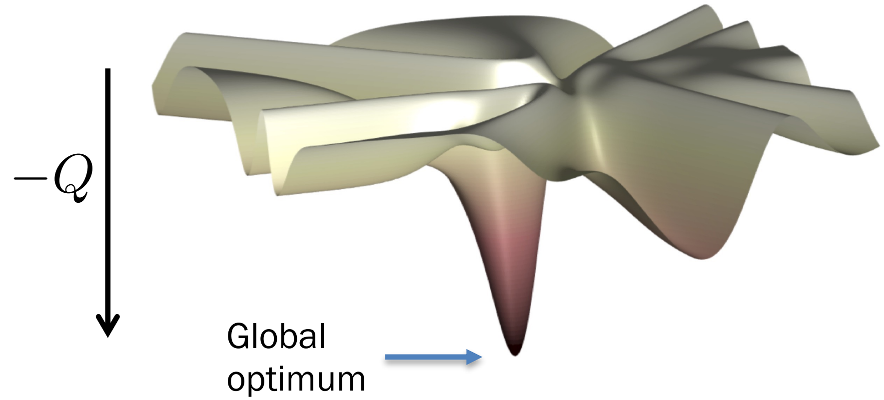


Learning the best heat engines via global search

The optimization problem is **challenging**: local (gradient-based) algorithms failed.



Visualizing the optimization landscape



cf. Goodfellow et al., ICLR 2015.

$$L(\alpha, \beta) = -Q(\mathcal{W}_Q^* + \alpha\phi + \beta\psi)$$

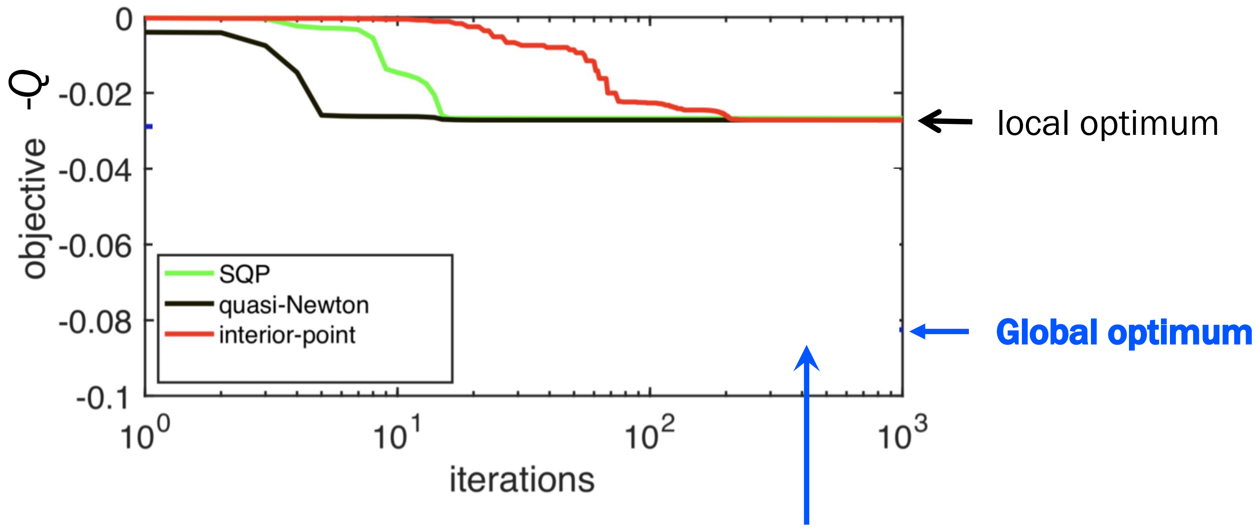
Randomly generate vectors: $\phi, \psi \in \mathbb{R}^d$ $\quad d = 1 + N_f(N_f - 1)/2$

Optimal solution: $\mathcal{W}_Q^*$

We then plot L as a function of α and β, which gives the 2D projection of the d-dimensional optimization landscape.

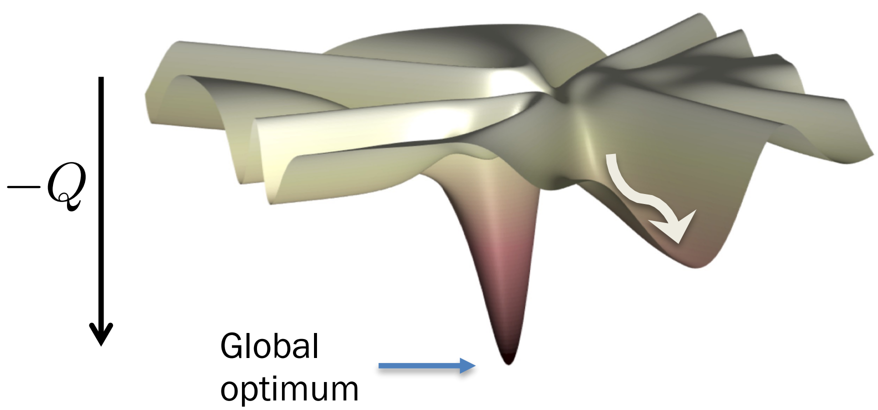
Learning the best heat engines via global search

The optimization problem is **challenging**: local (gradient-based) algorithms failed.



Visualizing the optimization landscape:

highly nonconvex

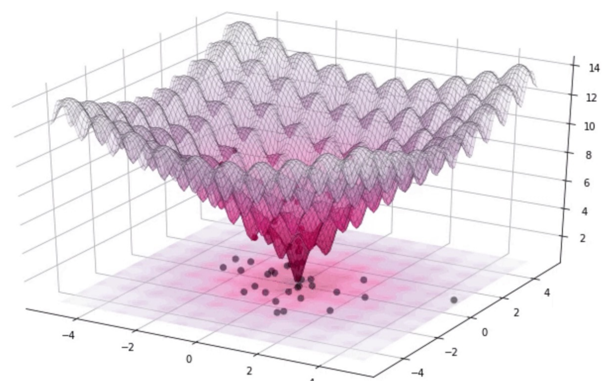


Differential evolution:

one of the most competitive ***global search algorithm***

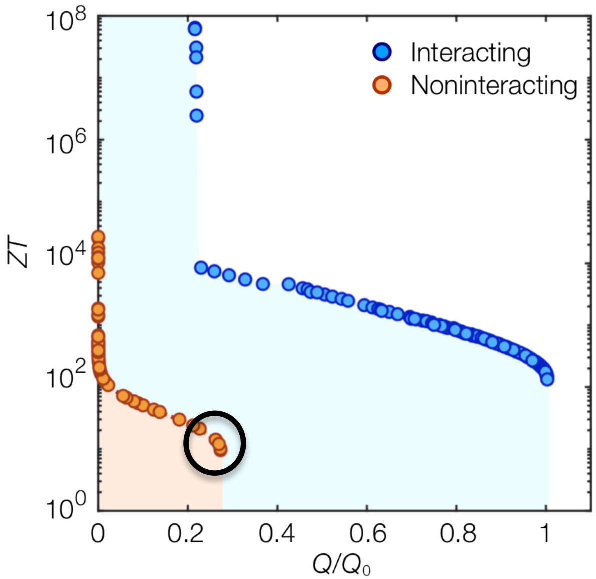
Stron & Price Tech. Rep. 95-012 (1995).

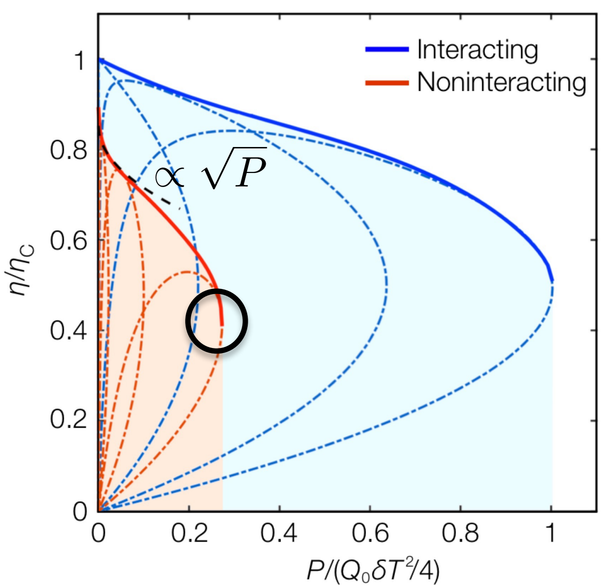
Wang et al., IEEE Trans. Evol. 15, (2011).



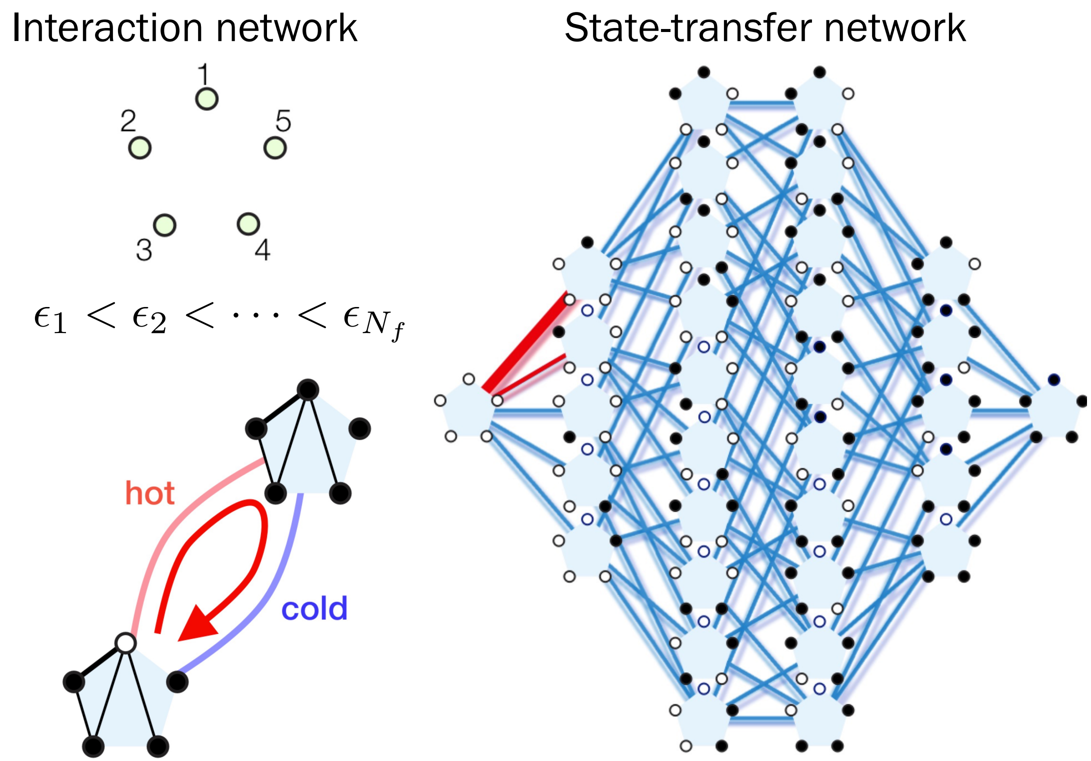
https://pablormier.github.io

Results: representative examples for $N_f = 5$ levels





Noninteracting case



Only a few edges activated ⟶ low power output

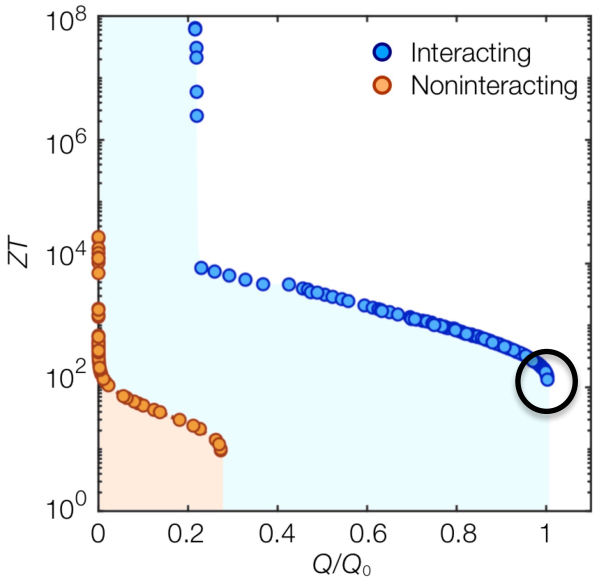
Modest ZT~10 at the highest power

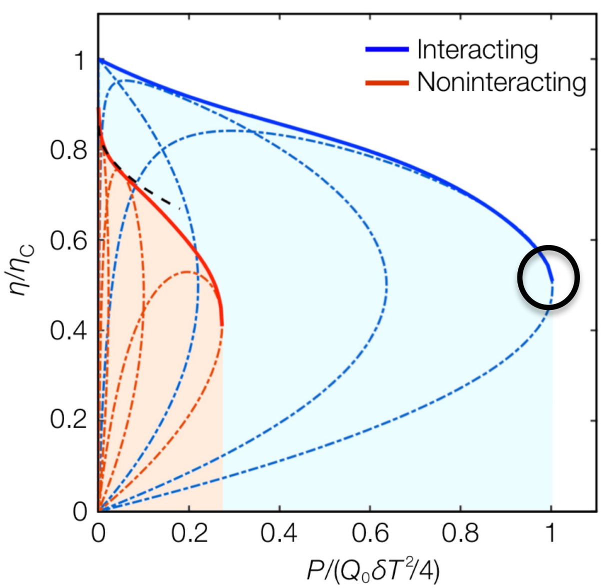
∵) nonzero heat flow at zero particle current
(= bipolar effect)

*Qualitatively consistent with previous studies.

cf. Whitney, PRB 91, 115425 (2015).

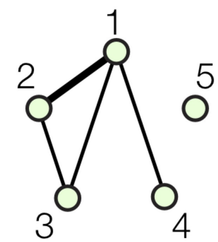
Results: representative examples for $N_f = 5$ levels



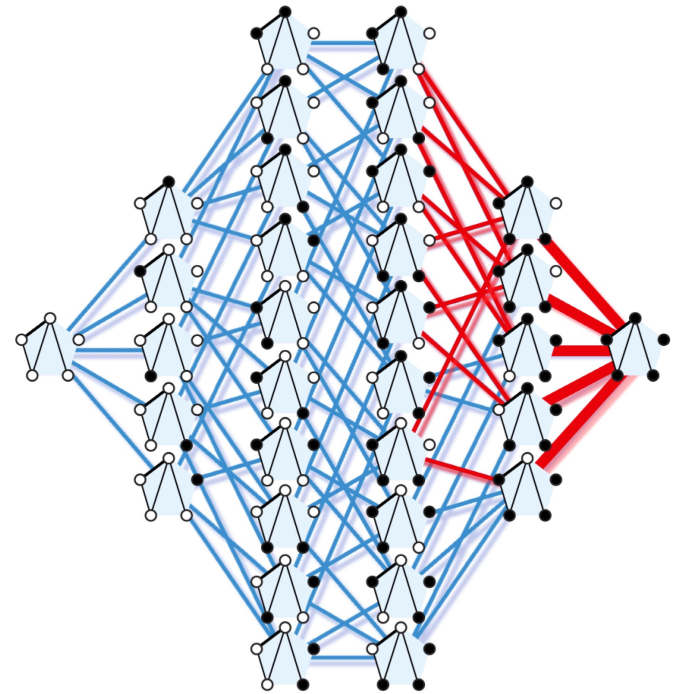


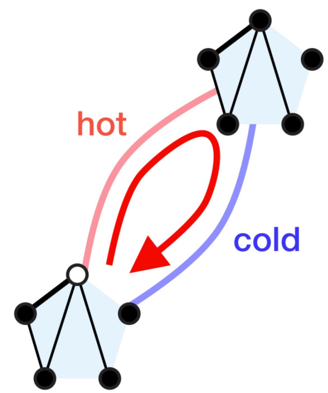
Interacting case, highest power factor Q

Interaction network



State-transfer network



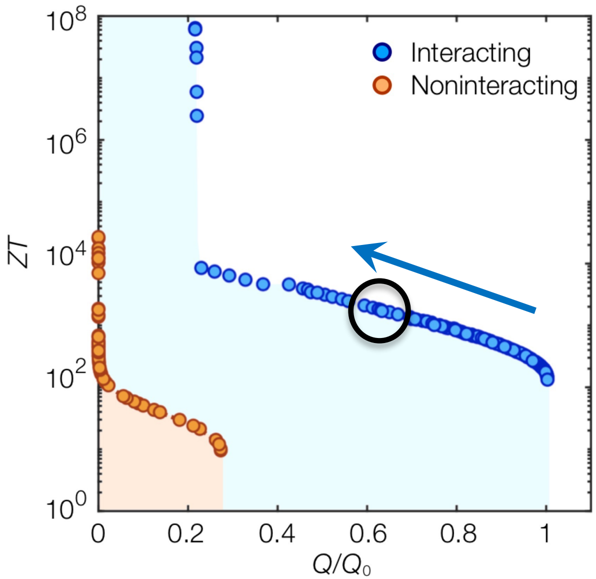


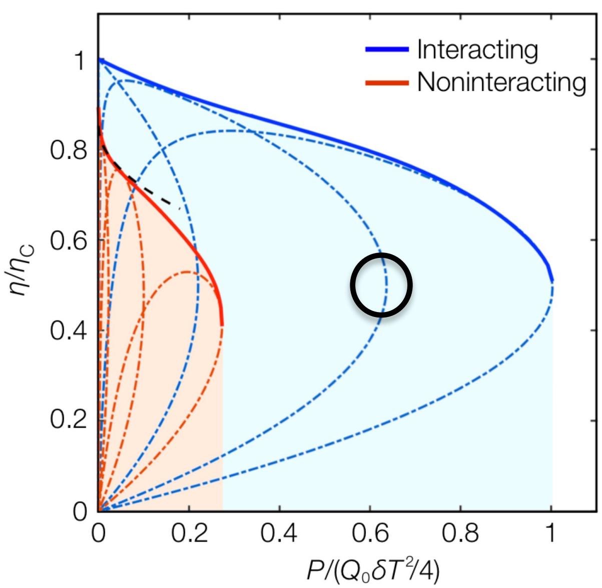
Maximum power achieved by a sparse interaction:

1. Degeneracy of single-hole excitation energies
   (activating many transfer edges→high power)

2. Suppressing hole-hole interactions
   (nondiverging, but still large ZT)

Results: representative examples for $N_f = 5$ levels

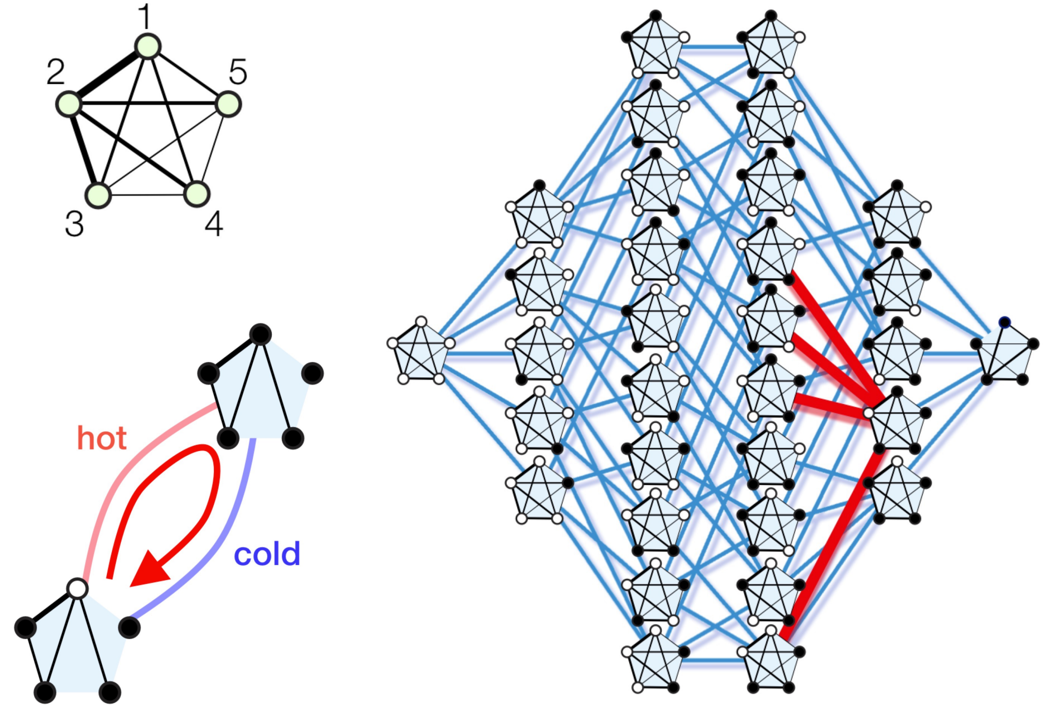




Interacting case, intermediate Q and ZT

Interaction network

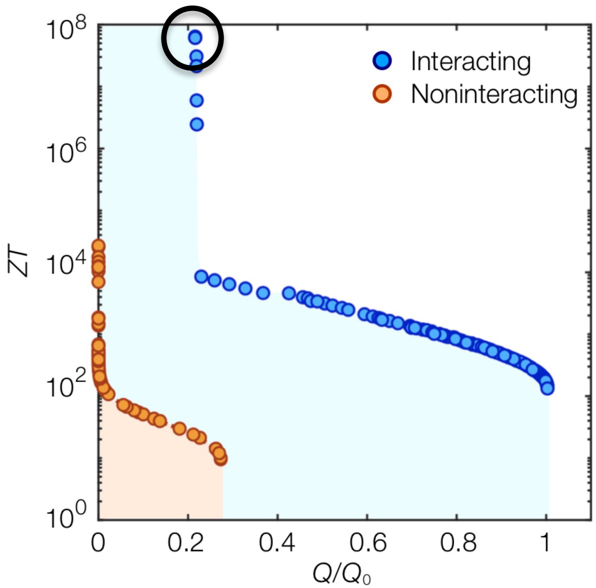
State-transfer network

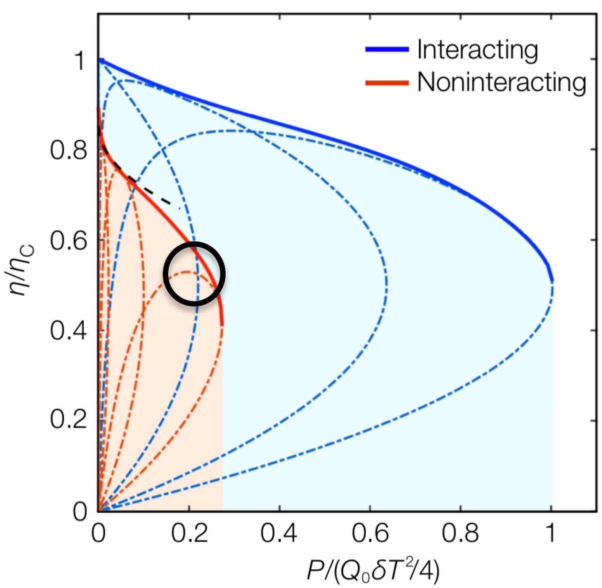


Making interaction stronger and denser, ZT is improved at the expense of compromising Q.

∵) Strong and dense interaction isolates a particular energy manifold, realizing the approximate tight-coupling condition: $J \propto J_q$

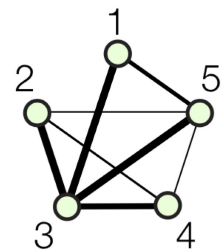
Results: representative examples for $N_f = 5$ levels



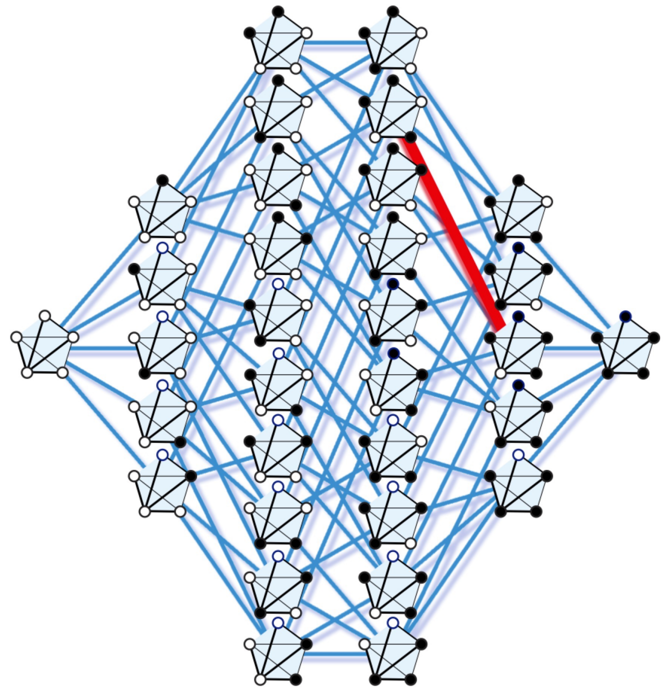


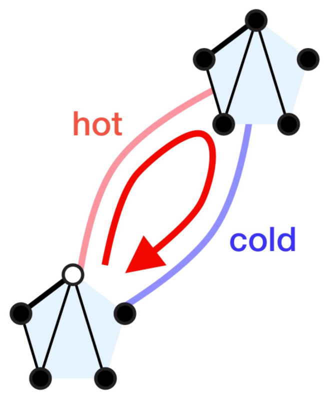
Interacting case, highest ZT

Interaction network



State-transfer network

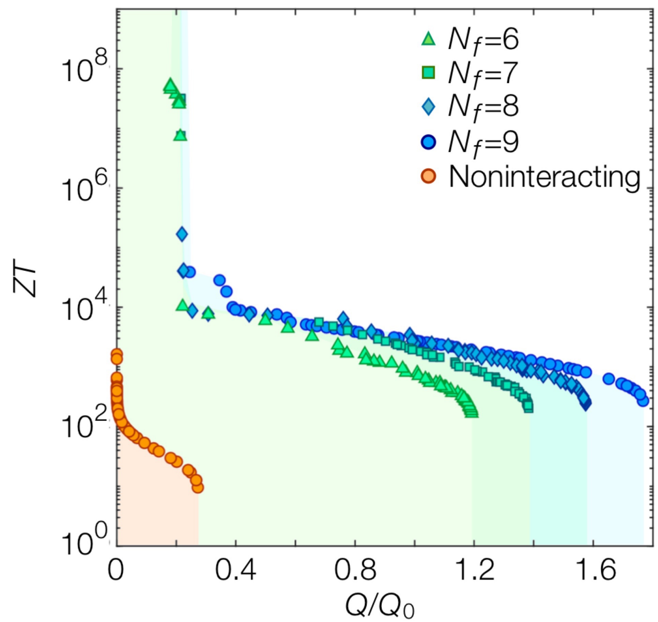


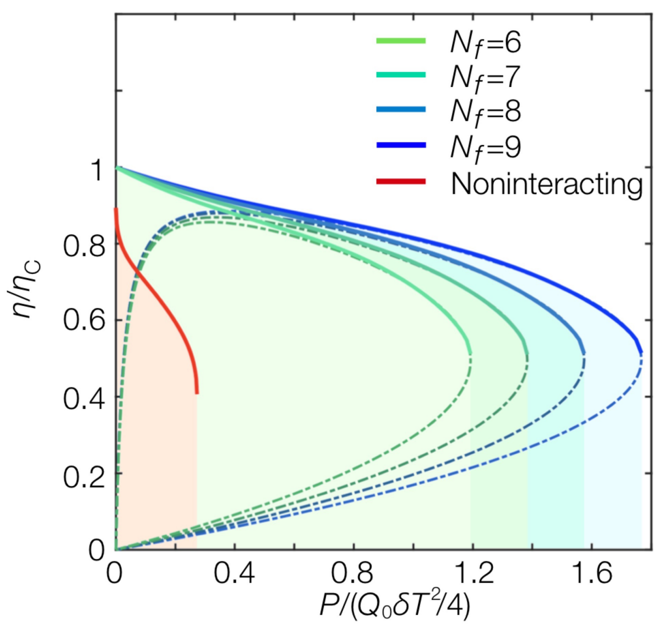


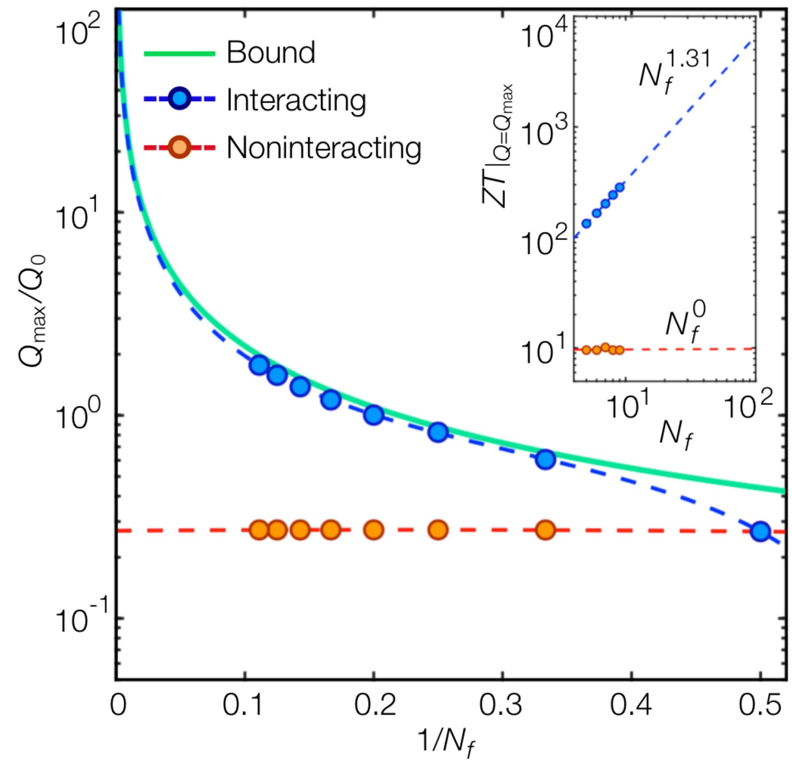
Further increasing interaction, one can isolate two particular levels far from other many-body levels.

The divergence of ZT originates from almost perfect unicyclic structure in the probability flow, ensuring the tight-coupling condition $J \propto J_q$

Results at larger highest-power machines and finite-size scaling analysis







(interacting) $$\frac{Q_{\max}}{N_f} \to \xi \frac{k_{\mathrm{B}}}{T} \frac{\gamma_{\mathrm{h}}\gamma_{\mathrm{c}}}{\gamma_{\mathrm{h}}+\gamma_{\mathrm{c}}} \qquad \xi \simeq 0.439$$

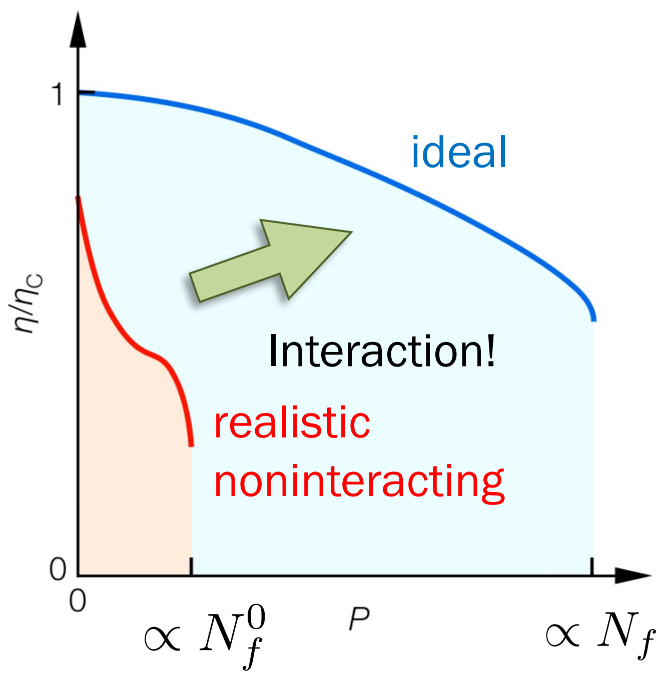
Fundamental bound on Q per level

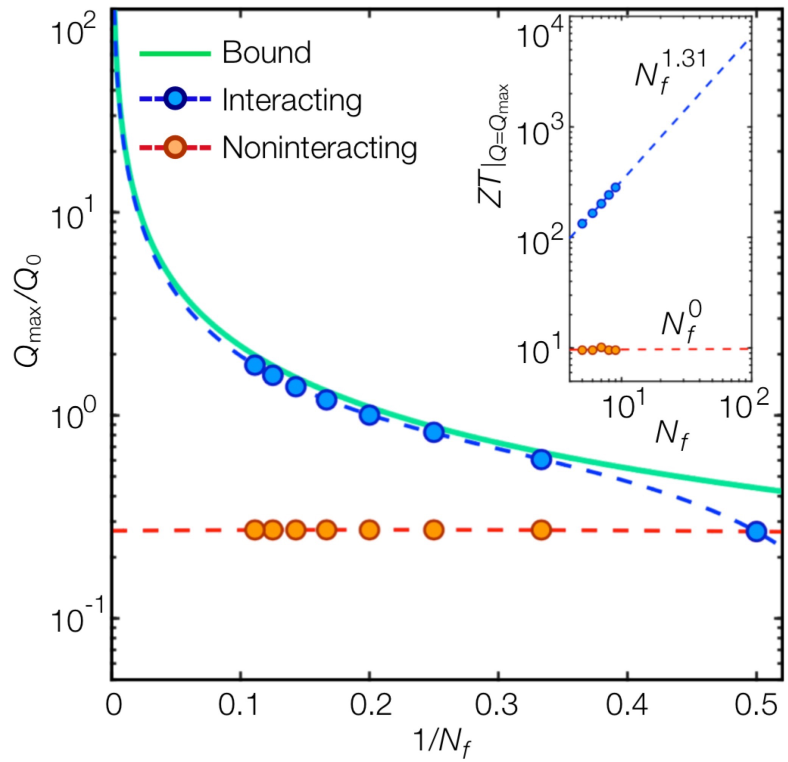
cf. Esposito et al., EPL 85, 60010 (2009).

(noninteracting) $Q_{\max} \propto N_f^0$

$\gamma_{\mathrm{h,c}}$: tunneling rates

Results at larger highest-power machines and finite-size scaling analysis





(interacting) $$\frac{Q_{\max}}{N_f} \to \xi \frac{k_{\mathrm{B}}}{T} \frac{\gamma_{\mathrm{h}}\gamma_{\mathrm{c}}}{\gamma_{\mathrm{h}}+\gamma_{\mathrm{c}}} \qquad \xi \simeq 0.439$$

Fundamental bound on Q per level

cf. Esposito et al., EPL 85, 60010 (2009).

(noninteracting) $Q_{\max} \propto N_f^0$ $\gamma_{\mathrm{h,c}}$: tunneling rates

Conditions for the highest-power heat engines

Given generic single-electron levels $\{\epsilon_l\}$, we conjecture that the ***highest-power machine*** is achieved by satisfying the following conditions:

(i) Single-hole excitation energies are degenerate ($N_f - 1$ constraints):

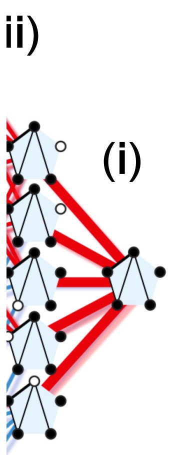
$$|e_l - e_{l+1}| \ll k_{\mathrm{B}}T, \qquad e_l = \epsilon_l + \sum_{m \neq l} w_{lm}$$

(ii) At most $N_f - 1$ variables of $\{w_{lm}\}_{l>m}$ can be nonzero (sparse interaction).

(iii) The ground voltage is set to be $v_g = e_{\mathrm{h}} + \alpha k_{\mathrm{B}}T$

cf. Murphy et al., PRB 78, 161406 (2008).
Esposito et al., EPL 85, 60010 (2009).

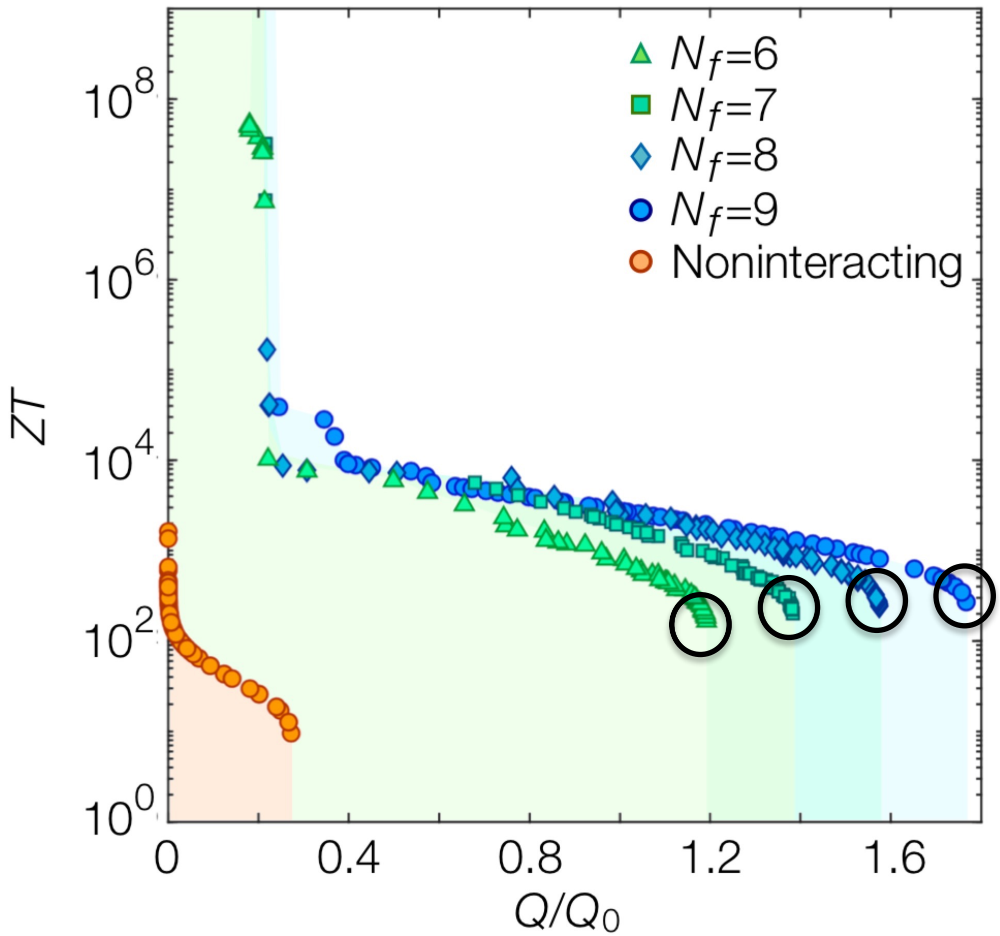
$$\alpha \simeq 2.40$$



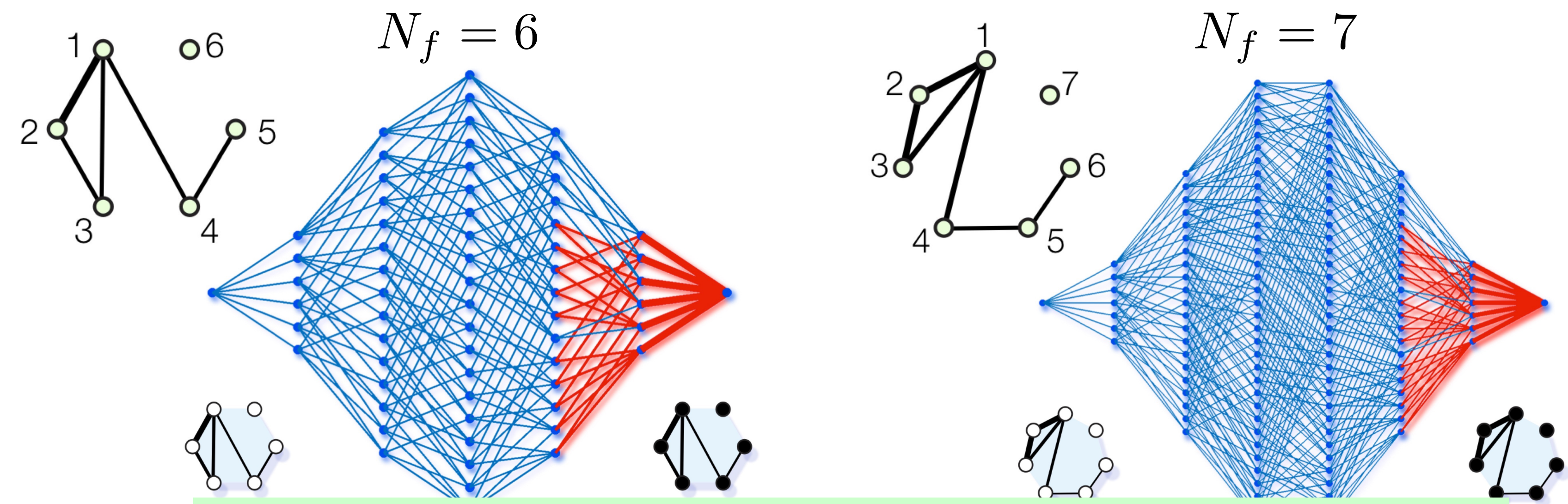
For any $\{\epsilon_l\}$ there in general exist an excessive number of solutions for $\{w_{lm}\}_{l>m}$ which allow for the highest power
→ flexible design of optimal nanoscale engines.

*In noninteracting case, the highest power is possible only if $\epsilon_1 = \epsilon_2 = \cdots = \epsilon_{N_f}$

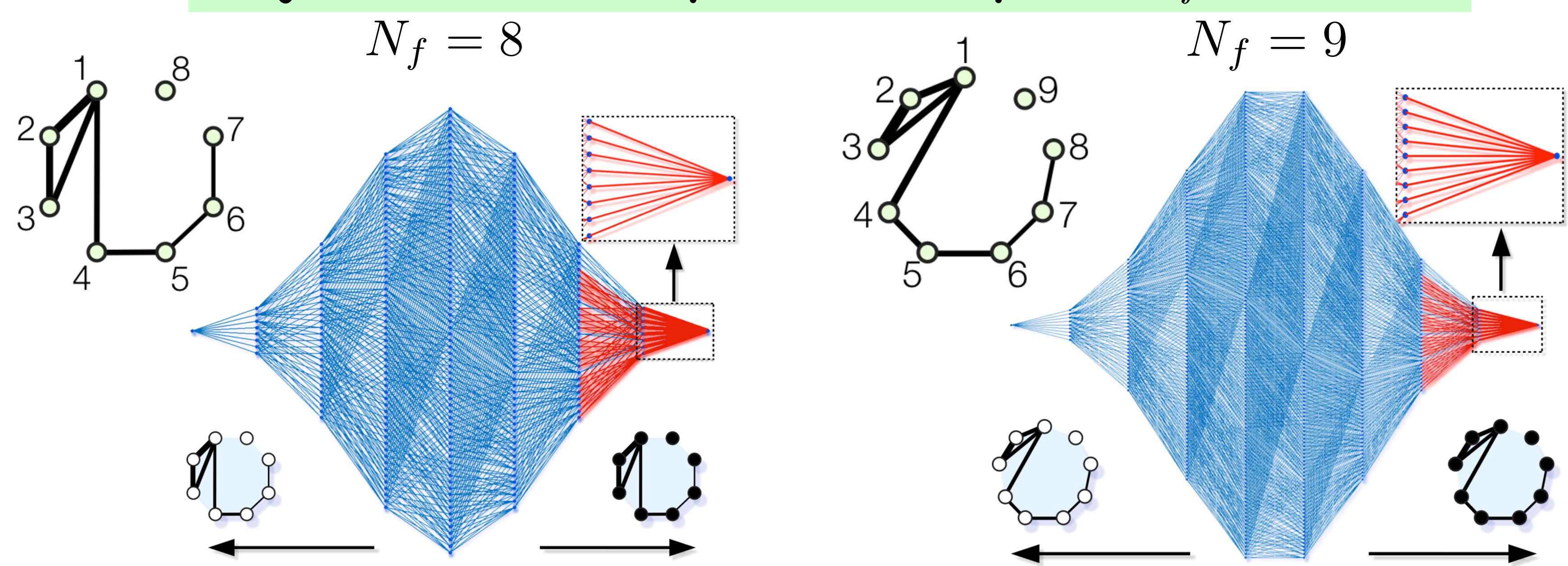
Conditions for the highest-power heat engines



Conditions for the highest-power heat engines



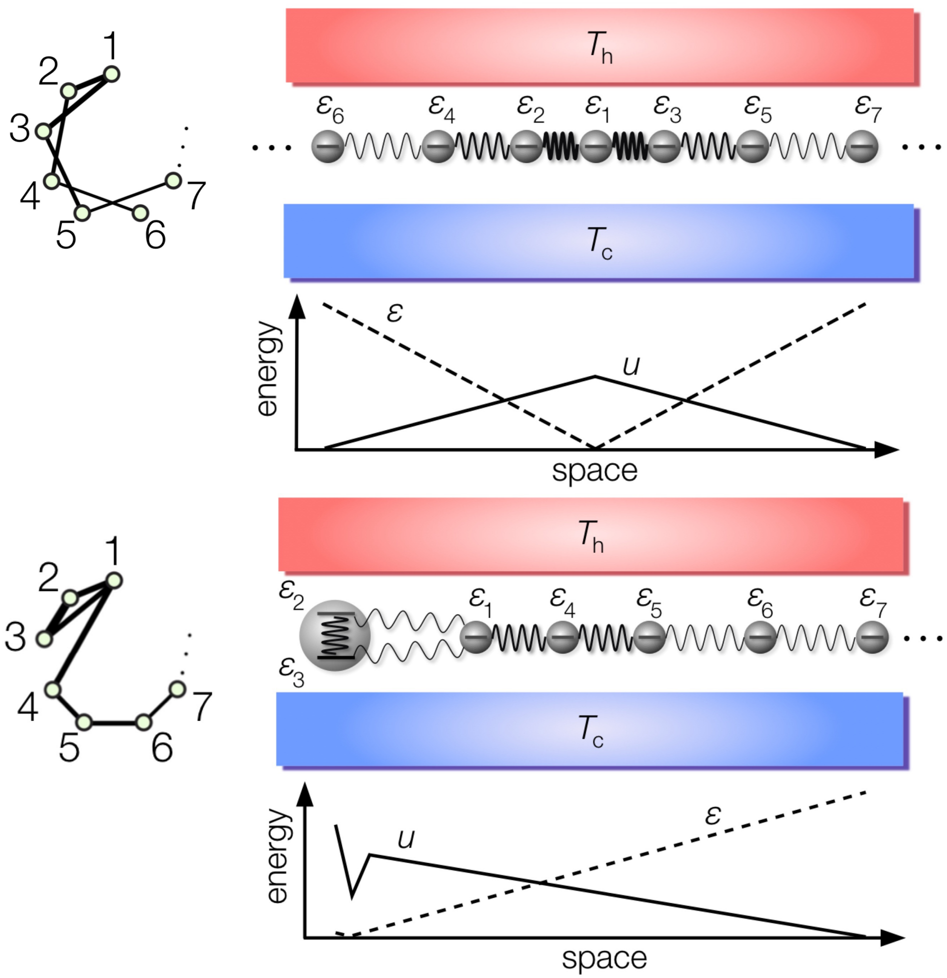
Conjecture numerically confirmed up to N_f levels



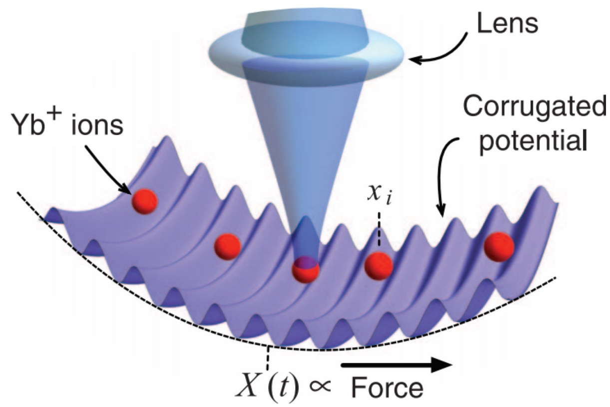
Possible experimental relevance

Quantum-dot array

- Coulomb interactions in dense regimes.
- Two prototypical configurations for the highest power with $\epsilon_1 < \epsilon_2 < \cdots < \epsilon_{N_f}$



Trapped ions



Bylinskii et al.,
Science 348, 6239 (2015).

- Noise of electric fields act as equilibrium baths.
- Inevitable Coulomb interactions.
- Single-particle manipulation realized.

Summary

- We develop a global-optimization framework to identify the best tradeoff relation in the multiple objectives for interacting nanoscale machines.
- We apply it to optimizing power and efficiency in nanothermoelectrics to find a set of the best heat engines.
- For generic single-electron levels, thermoelectric figure of merit and power factor can in principle be enhanced by orders of magnitudes in the presence of interaction.
- Our findings could be of relevance to quantum-dot array and trapped ions.

Outlook:

✓ Application to other nanosystems described by the master equation (such as solar photovoltaics, molecular motors and biophysics networks).

✓ Multiobjective optimization with other objectives; finding a way to maximize solar power, molecular mobility and biophysical-reaction yield while keeping high efficiency.

✓ Role of nonlinear effects, quantum many-body effects (e.g., Kondo physics), and time-reversal symmetry breaking in interacting nano-heat engines.

Ref: YA and T. Sagawa, Commun. Phys. 4, 45 (2021).