

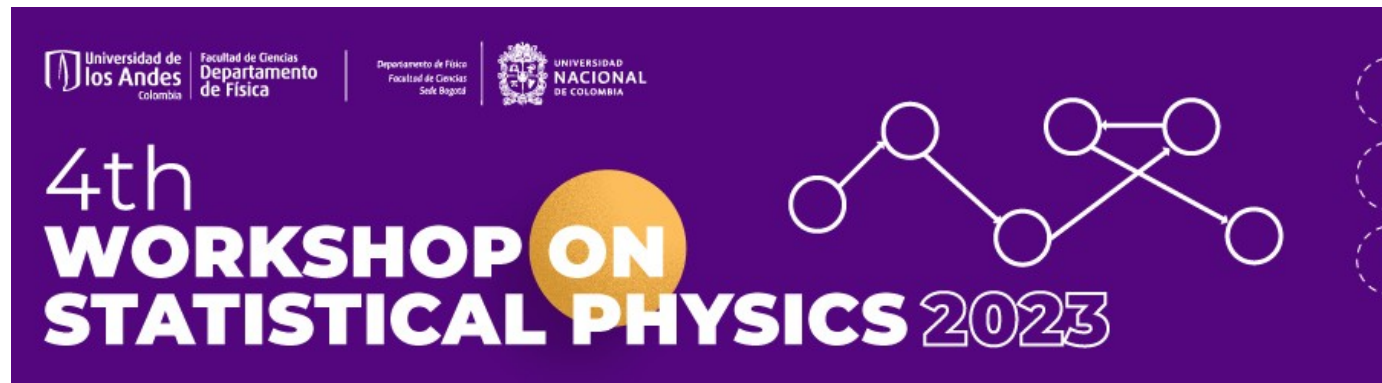
Quantum Thermal Machines

Gonzalo Manzano,

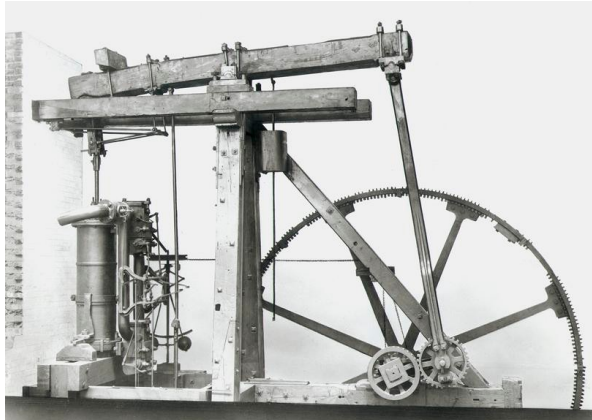
IFISC (UIB-CSIC), Palma de Mallorca (Spain)

MINI-COURSE:

Quantum thermodynamics: fluctuations and thermal machines



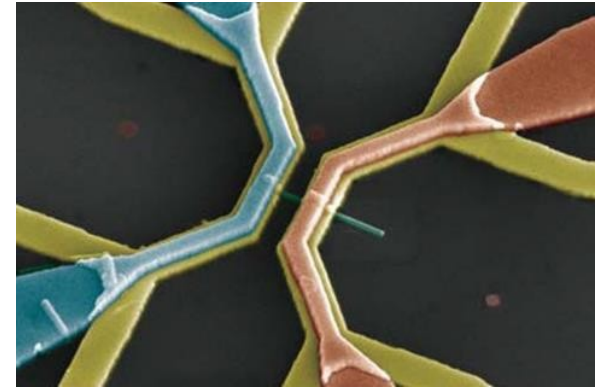
Macroscopic (classical) heat engines



(Watt's steam engine, 1769)

- + Large number of degrees of freedom
- + Fluctuations become negligible
- + Classical thermodynamics

Microscopic (quantum) heat engines



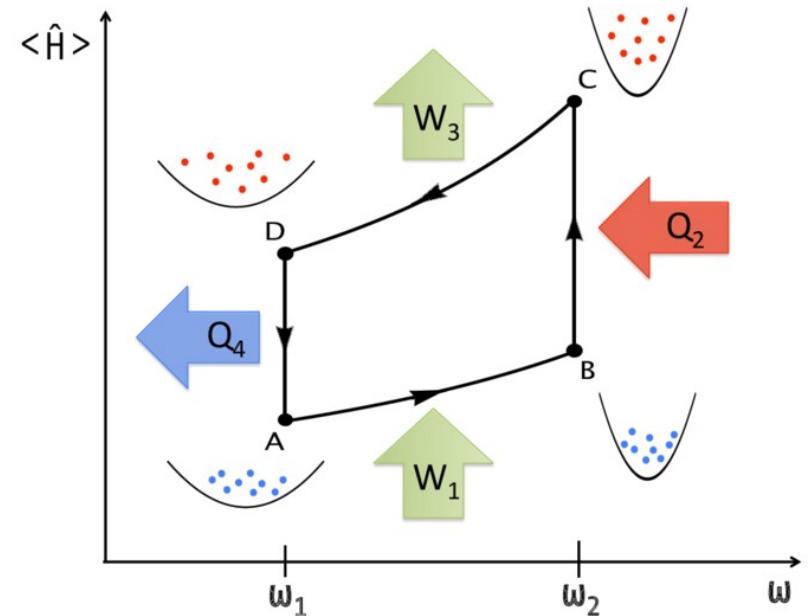
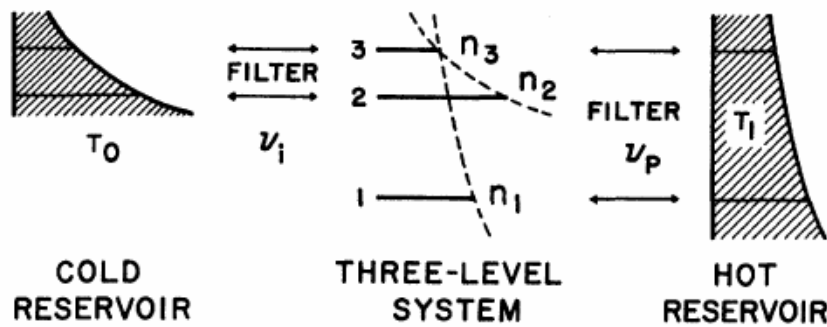
(Quantum-dot engine, 2018
H. Linke group, Sweden)

- + Small systems (nanoscale)
- + Fluctuations are important
- + Stochastic and quantum thermodynamics
- + **Quantum-mechanical enhancements**

+ Pioneering works in 60s:

Three-Level Masers as Heat Engines

Scovil and Schulz-Dubois, *Phys. Rev. Lett.* **2** (1959).



+ Cyclic vs. continuous operation engines

Quantum Carnot, Otto and Stirling cycles

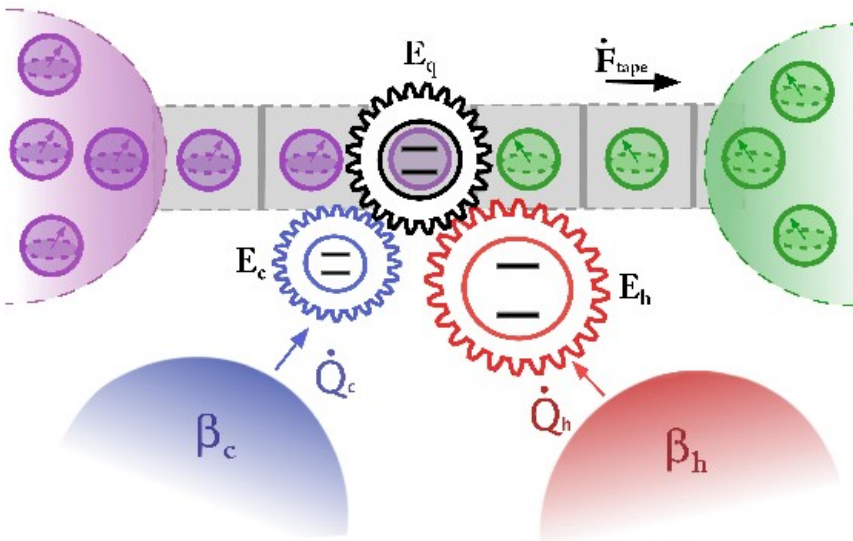
Quan, Liu, Sun, Nori, *Phys. Rev. E* **76** (2007).

Steady-state heat engines: lasers, masers, solar cells, thermoelectric devices ...

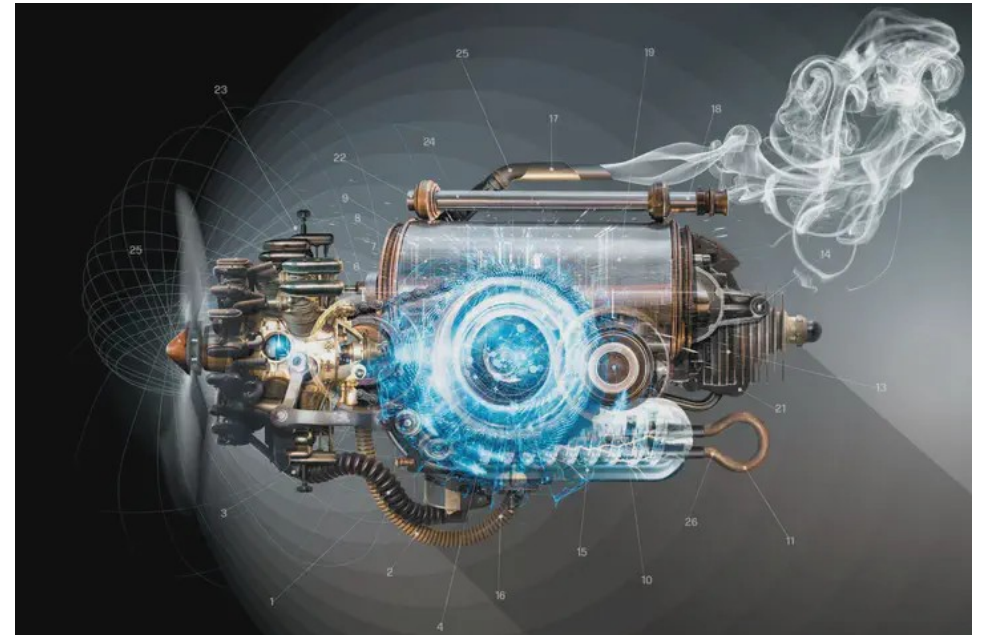
Kosloff & Levy, *Annu. Rev. Phys. Chem.* **65** (2014).

Why developing and studying models of quantum heat engines?

- + Simple setups to explore and test fundamental issues in quantum thermodynamics
- + Is there any miniaturization limit for heat engines and refrigerators ?
- + Is there any systematic quantum-thermodynamic advantage in the performance with respect to classical engines?

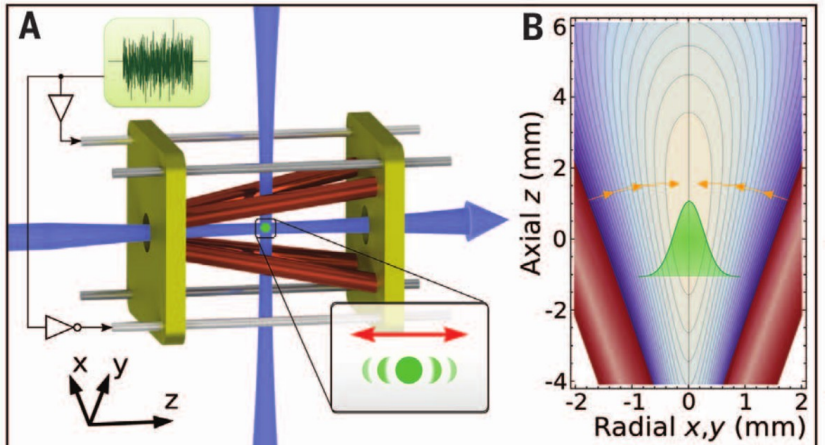


K. Hammam *et al.* NJP **23** 043024 (2021)



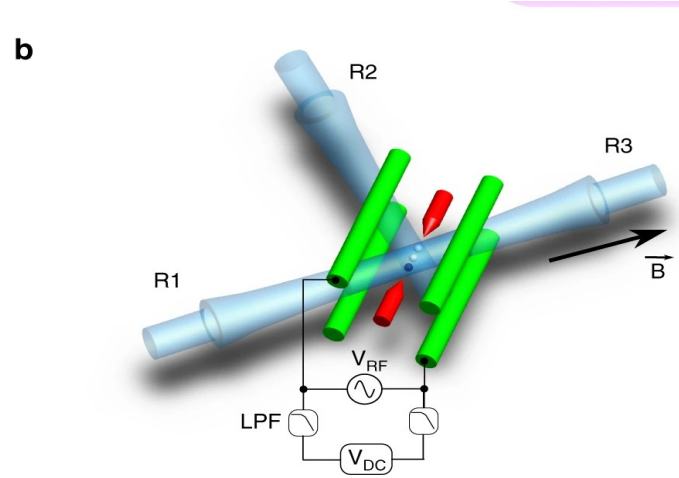
QTD Maryland 2024 conference webpage picture

Single-atom quantum engine



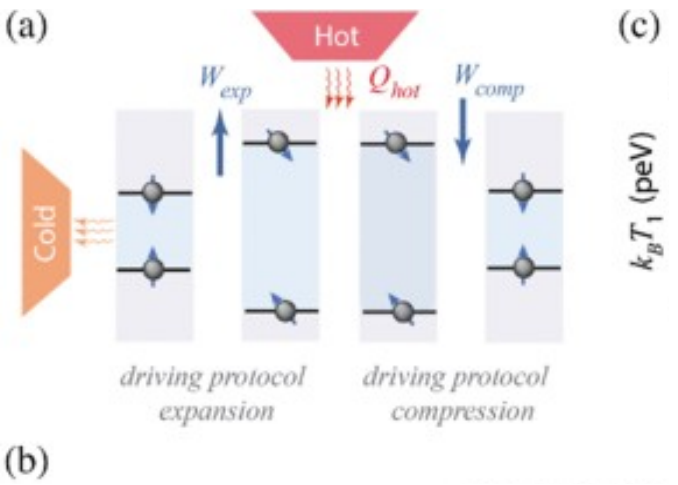
Roßnagel, *et al.* Science (2016)

Quantum absorption refrigerator



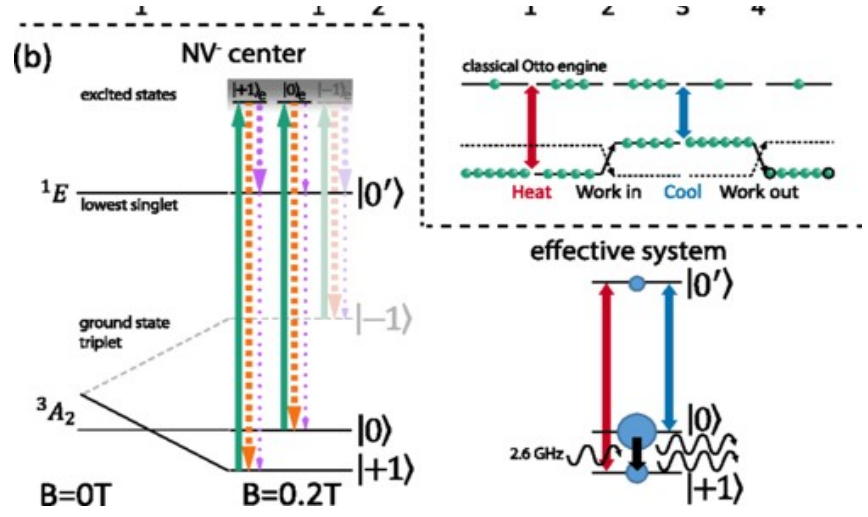
Maslennikov, *et al.* Nat Commun. (2019)

Spin Otto cycle with NMR techniques



Peterson, *et al.* Phys. Rev. Lett **123** (2019)

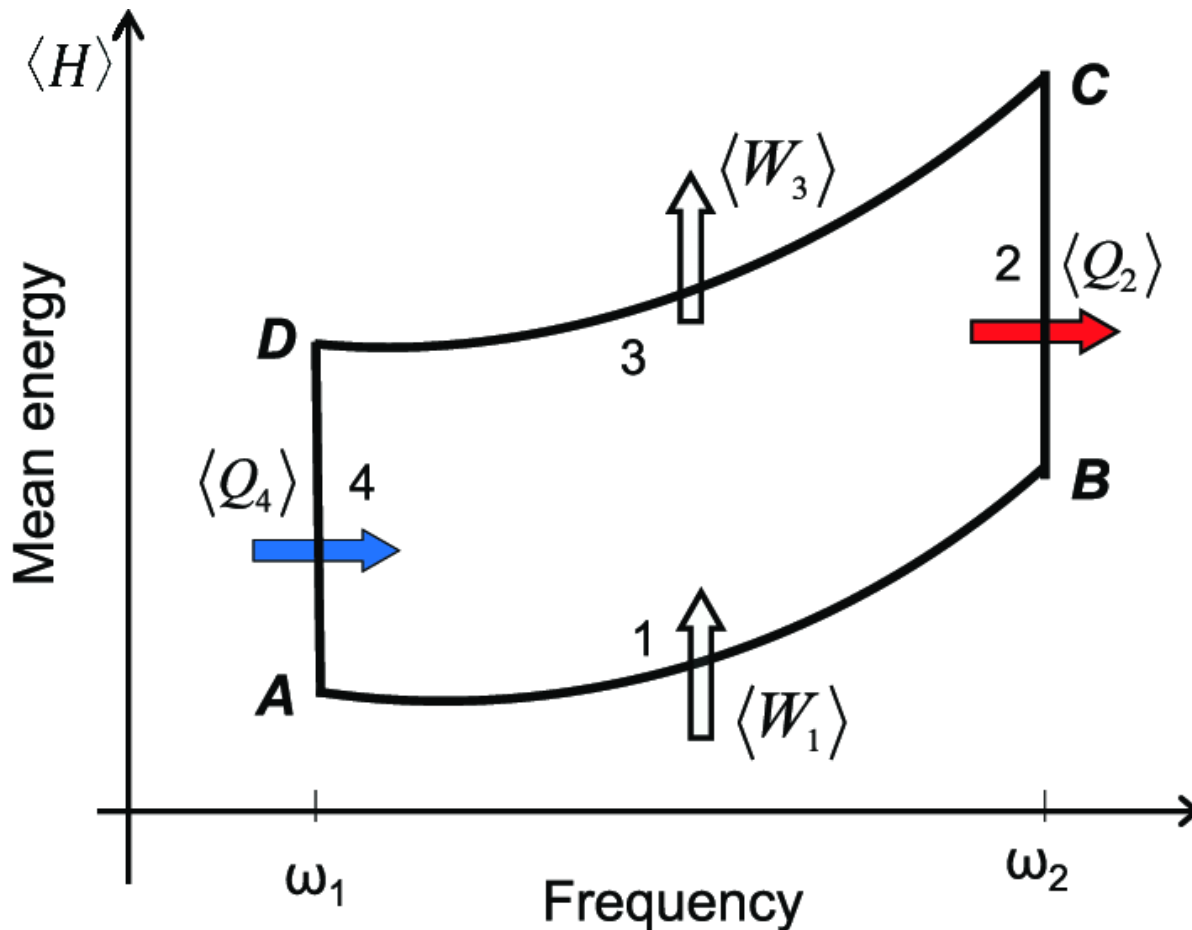
Continuous three-level engine with NV centers



Klatzow, *et al.* Phys. Rev. Lett **122** (2019)

Quantum Otto cycle

+ Quantum system (working substance) is driven by an external agent and selectively put in contact with two thermal reservoirs at different temperatures in a cyclic way



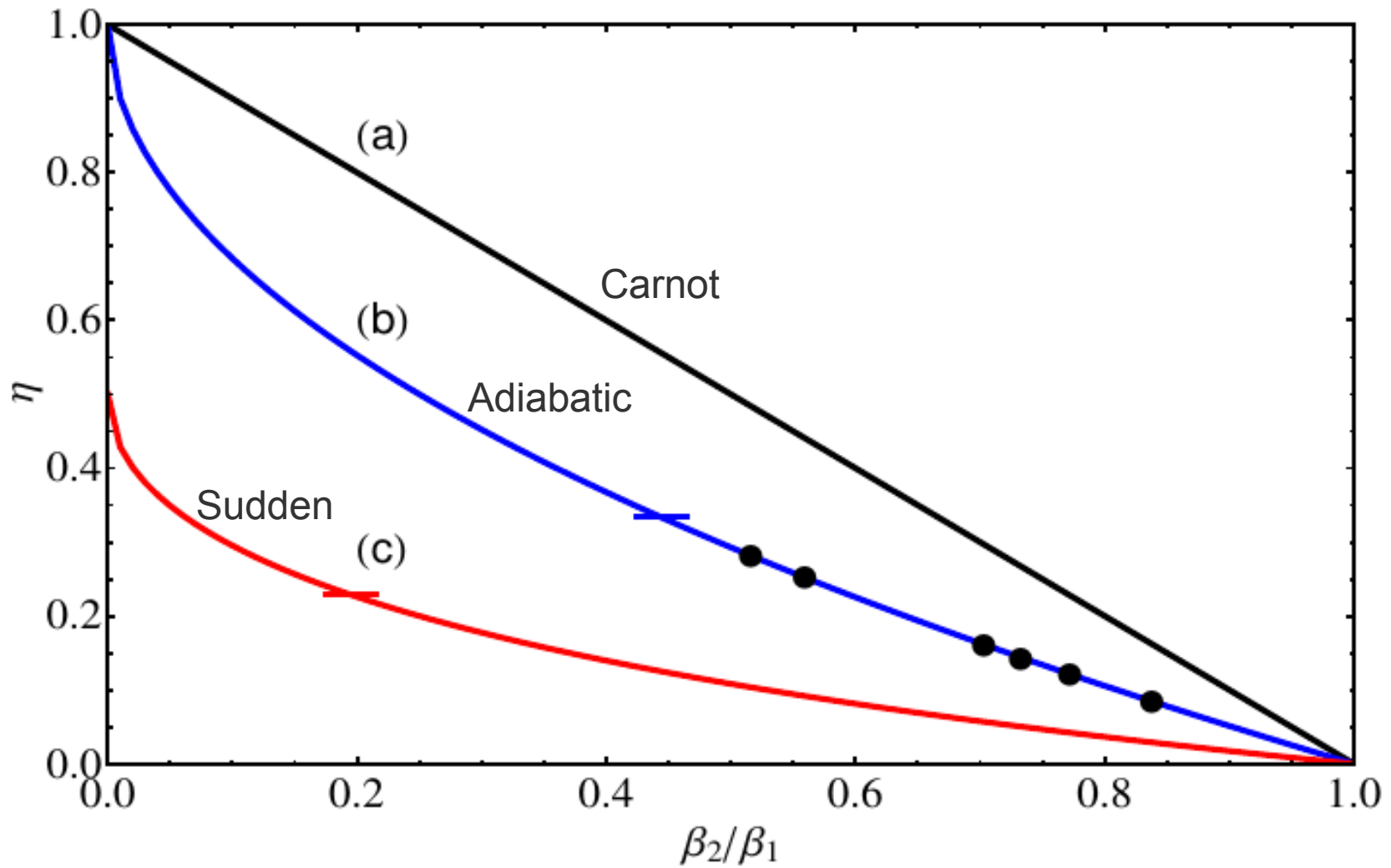
Example: Harmonic oscillator

$$H = \hbar\omega a^\dagger a \quad \omega_1 \leftrightarrow \omega_2$$

Four strokes:

- 1: A \rightarrow B Adiabatic compression
- 2: B \rightarrow C Hot isochore
- 3: C \rightarrow D Adiabatic expansion
- 4: D \rightarrow A Cold isochore

Efficiency at maximum power:

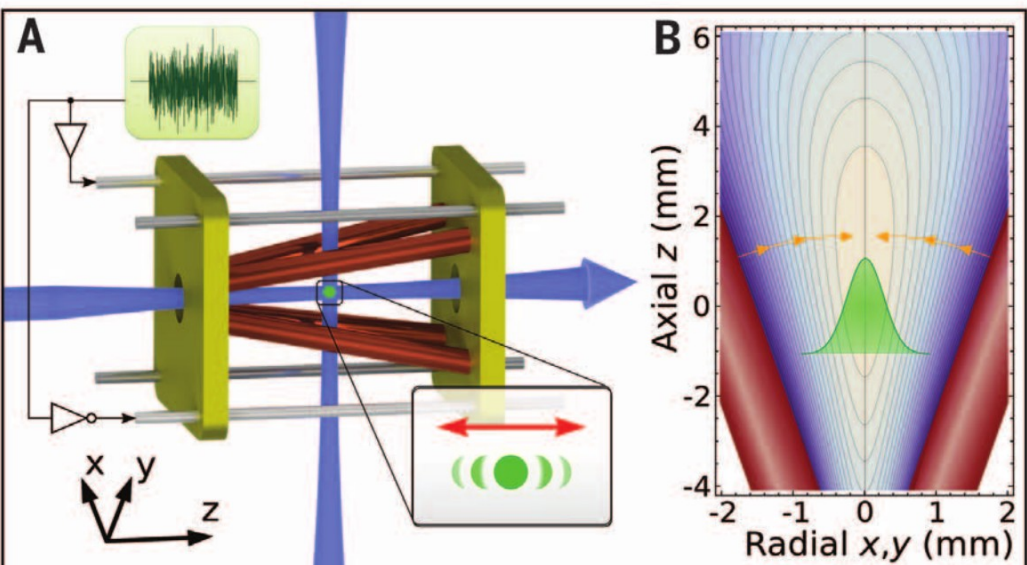


Typical car gasoline-fueled Otto engine ~ 0.2

Single-atom quantum engine experiment:

J. Roßnagel, *et al.* *Science* **352** 325-329(2016)

Single Calcium ion in a linear Paul trap (with tapered geometry) → harmonic potential



Axial z position determines frequency of radial potential

$$\omega_{x,y} = \frac{\omega_{0x,0y}}{(1 + z \tan \theta / r_0)^2}$$

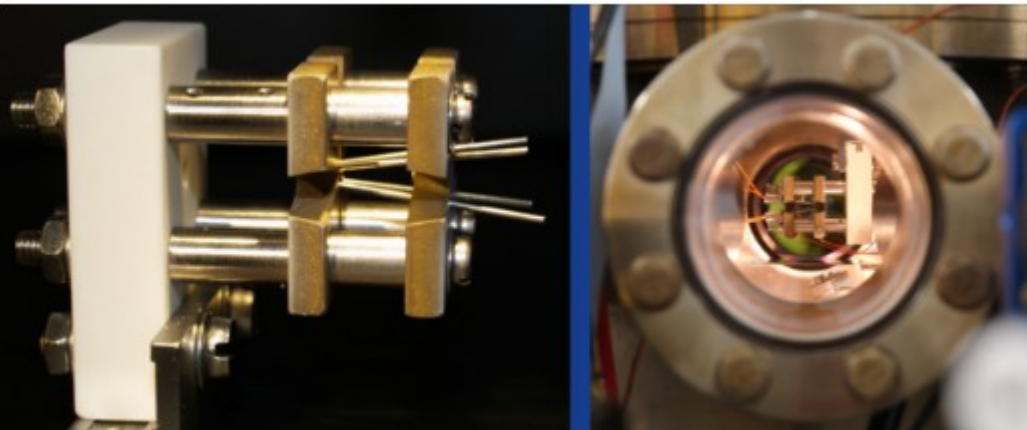
Hot bath → electric field noise

Cold bath → laser cooling

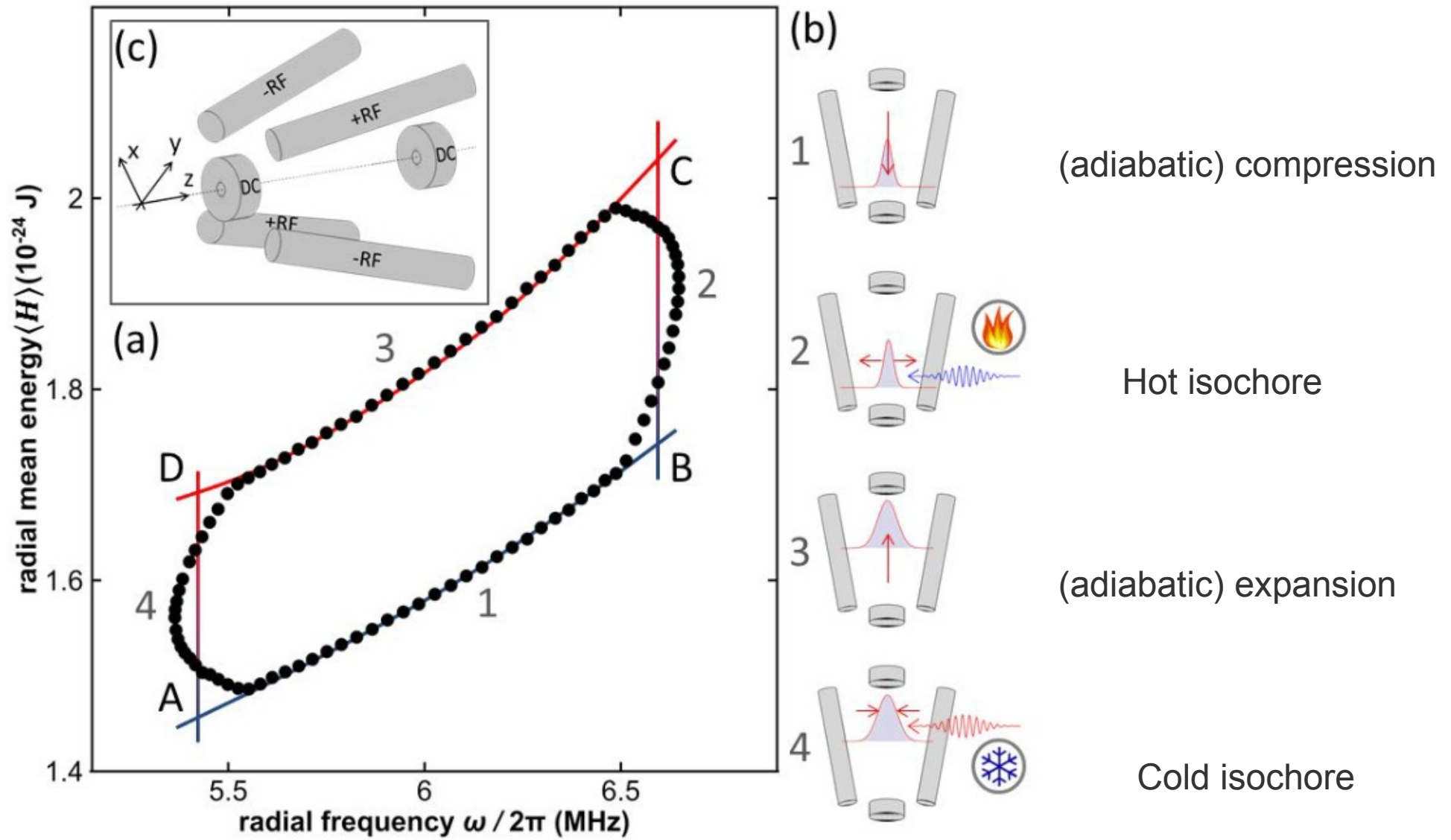
Force in the z direction:

$$F_z(T)$$

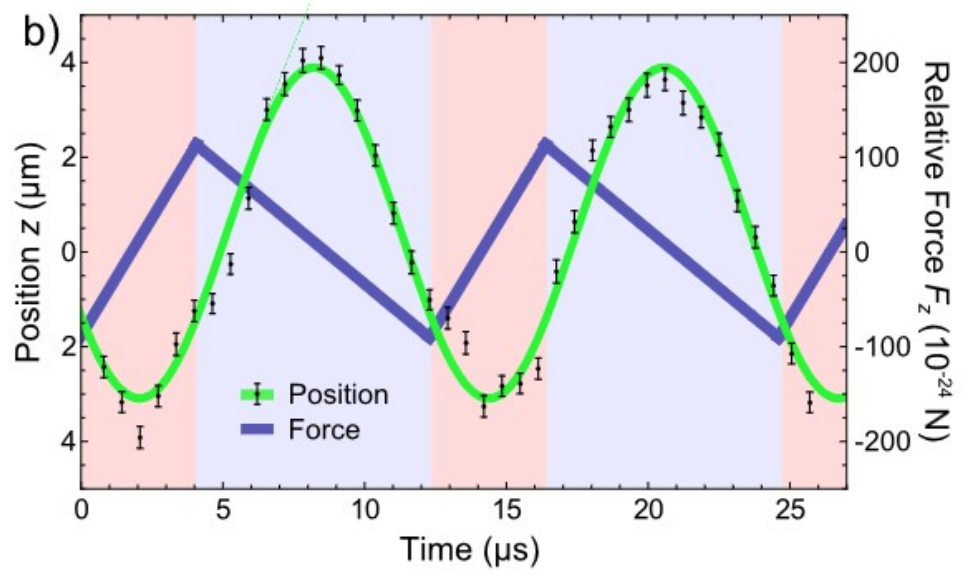
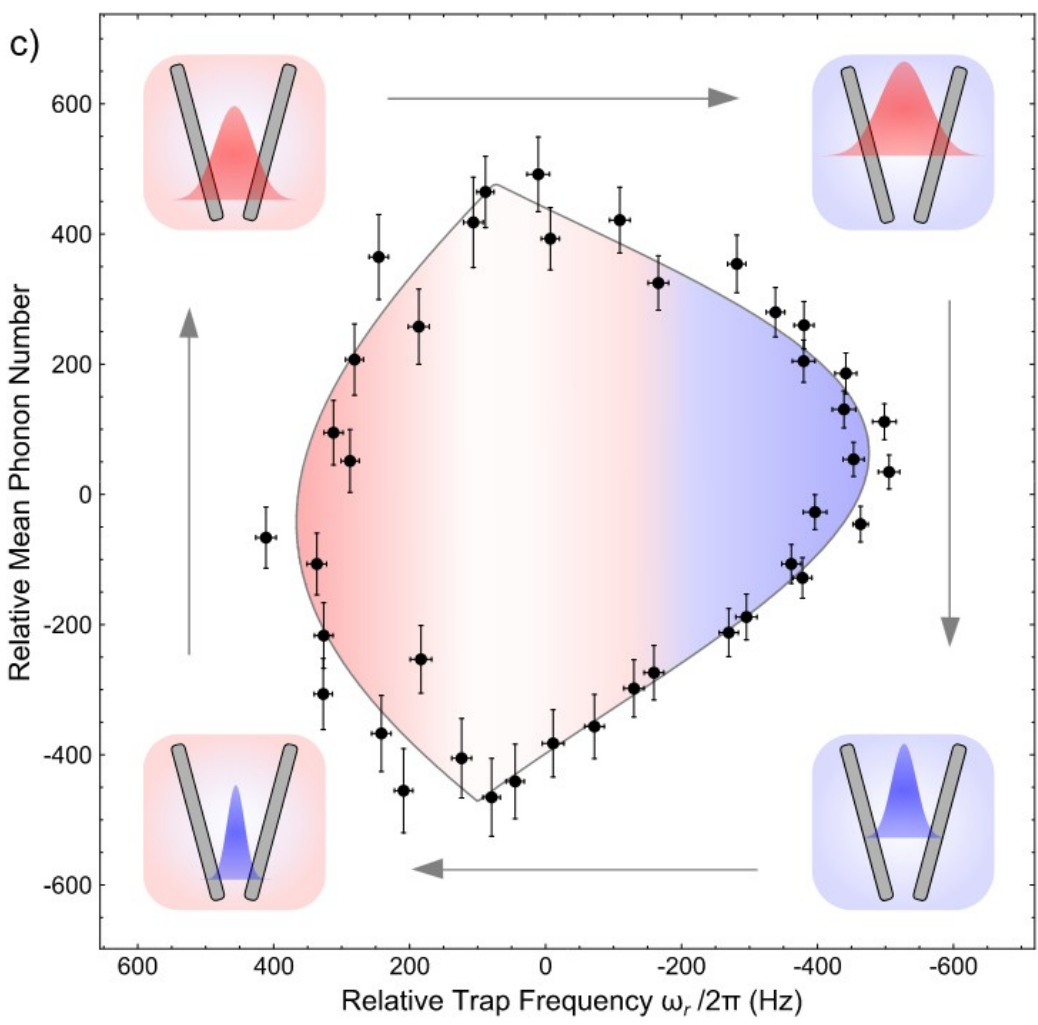
depends on the temperature



Modulate the radial frequency to perform an Otto cycle:



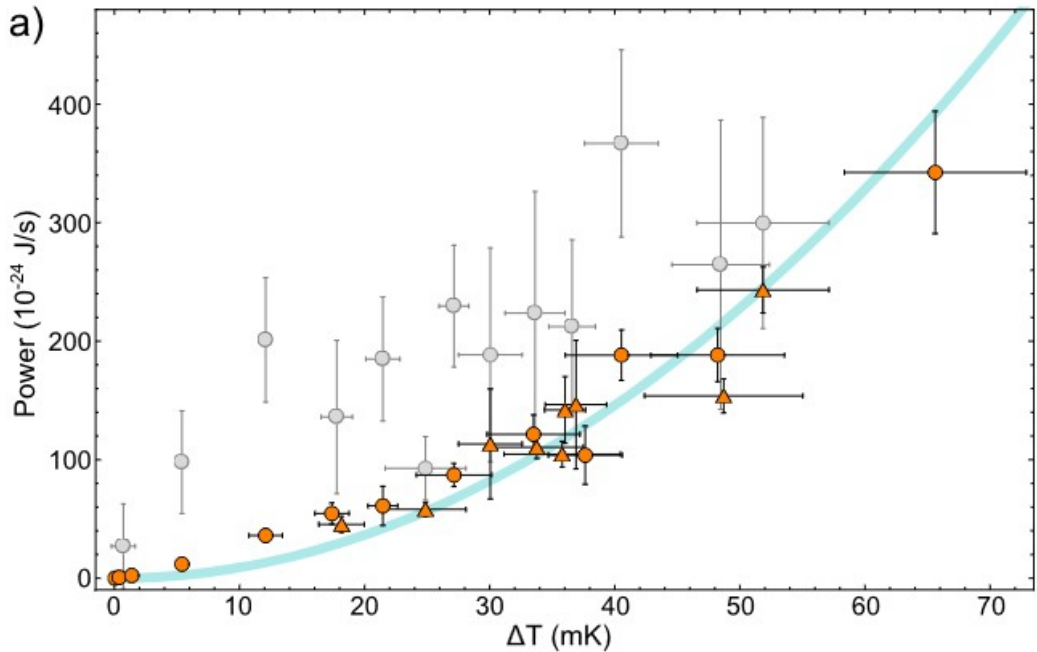
Actual implementation of the cycle:



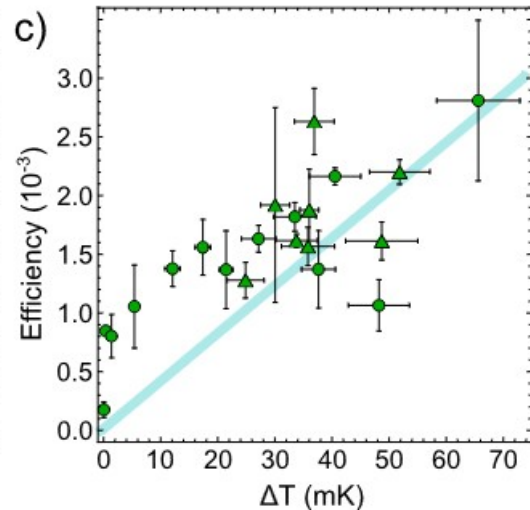
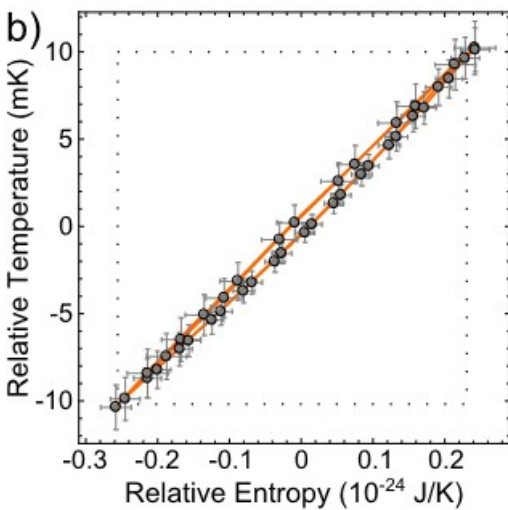
- Keep laser cooling (cold bath)
- Switch on/off extra electric noise (hot bath)
- Work accumulated in axial movement

Working temperature $\sim 568\text{mK}$
 $\Delta T \sim 20\text{mK}$

Performance of the engine:



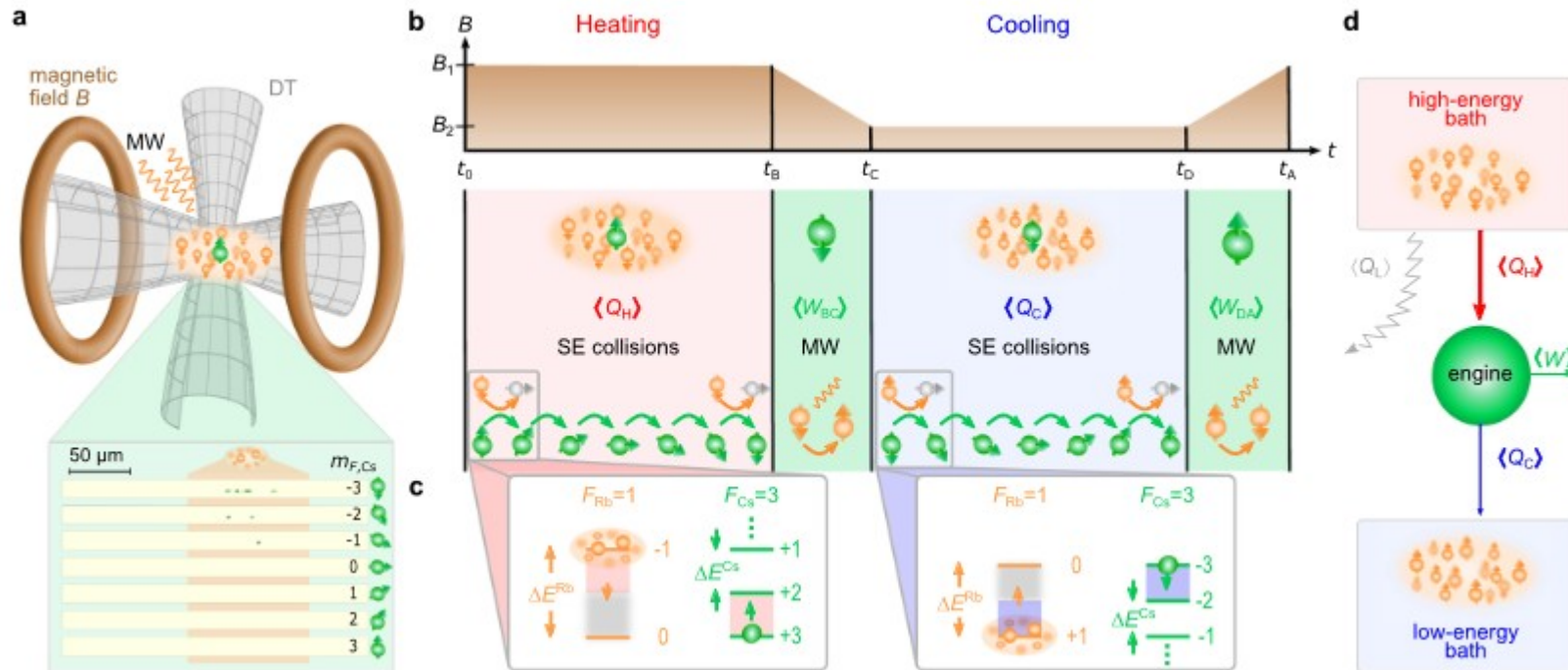
Power $\sim 10^{-21} J/s$
 approx $k_B T$ per second
 (at room temperature)



Efficiency $\sim 0.28\%$
 $\eta_{\text{Carnot}} \sim 3, 4\%$

(Watts engine 1783 $\sim 5-7\%$)

Otto cycle driven by atomic collisions: [Q. Bouton, et al. Nat. Commun. 12, 2063 \(2021\)](#)



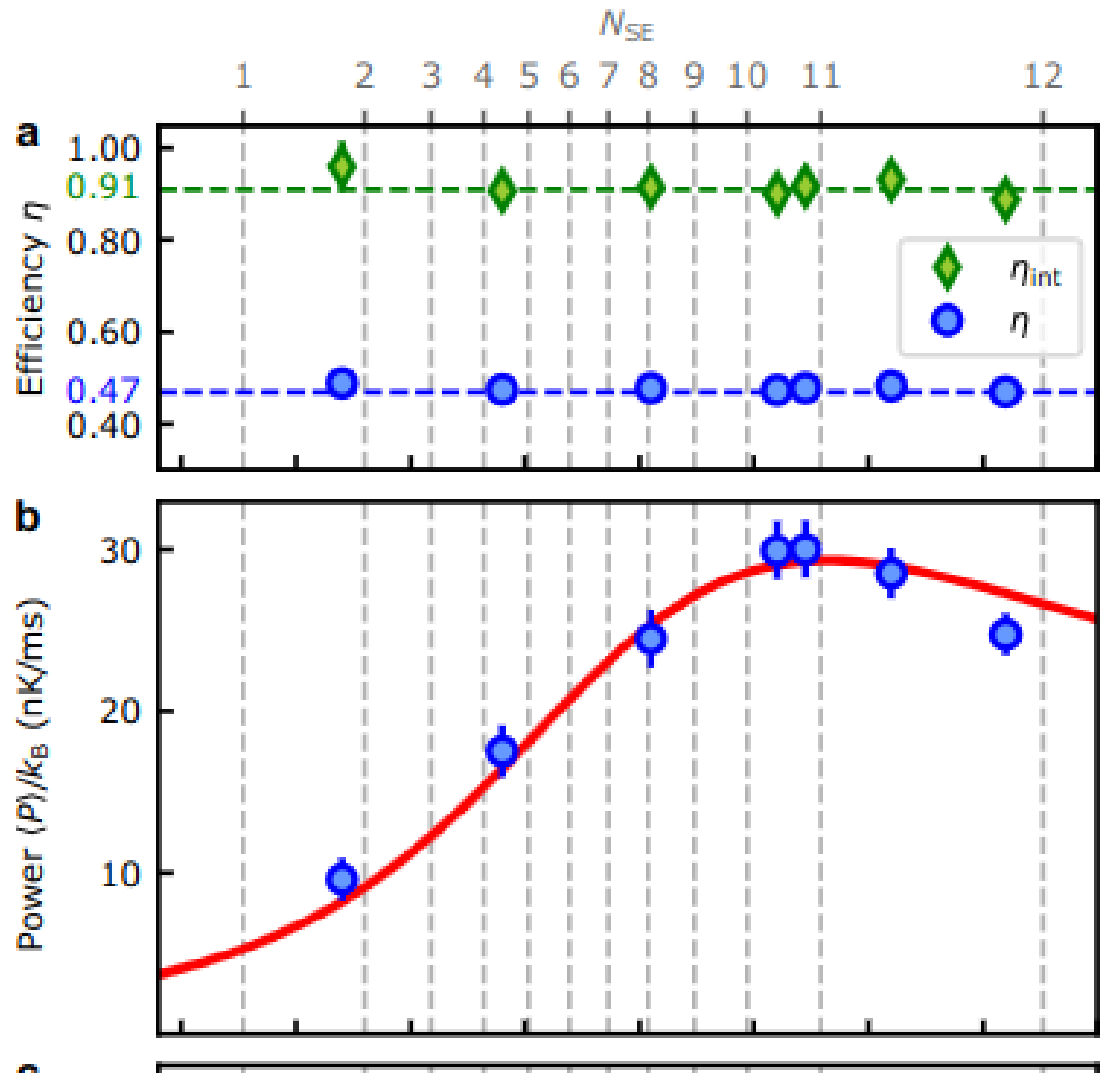
Cesium impurities in ultracold Rubidium cloud in optical trap \longrightarrow More realistic bath!

Magnetic field to implement the working substance (Cs impurity) adiabatic driving

$$E_n = n\lambda B \quad n = 0, 1, \dots, 7 \quad B_1 \rightarrow B_2$$

Microwaves to tune the temperature hot/cold of the Rb spins bath

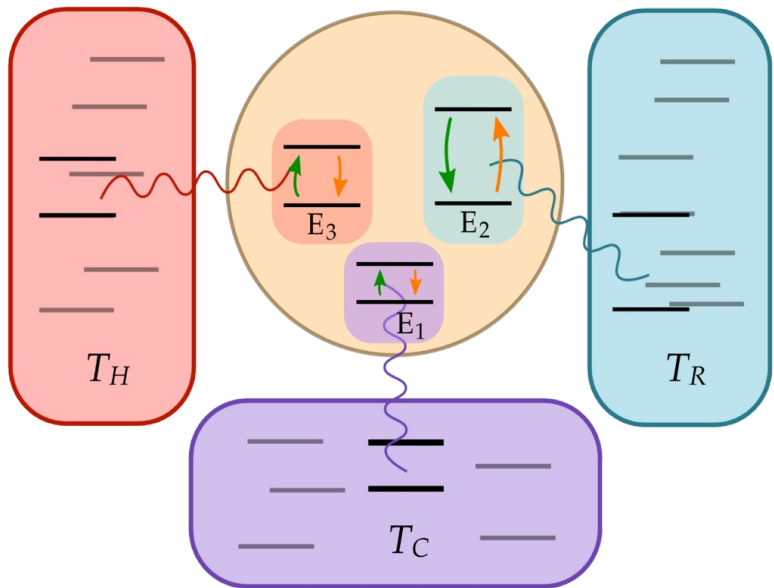
Otto cycle driven by atomic collisions: [Q. Bouton, et al. Nat. Commun. 12, 2063 \(2021\)](#)



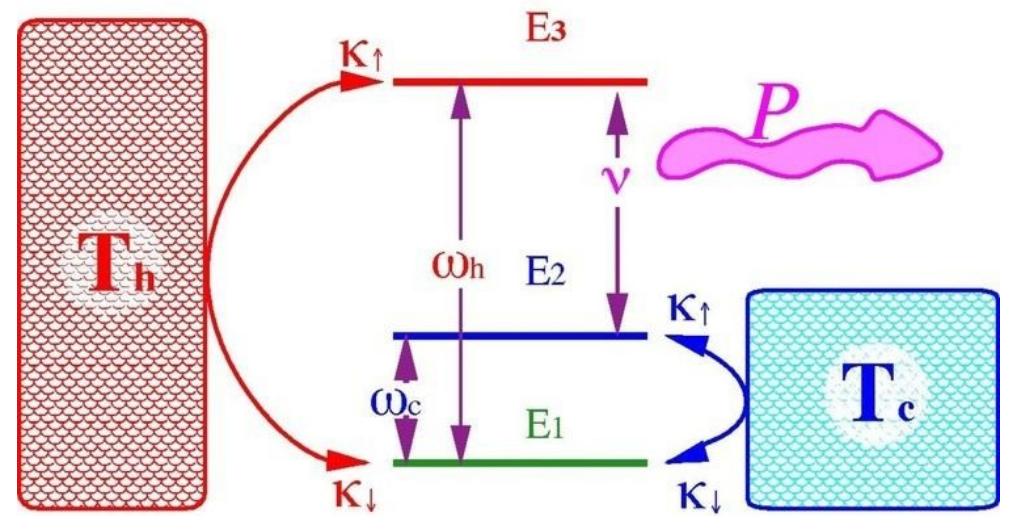
Much better efficiency!

Much less power than the single-atom engine

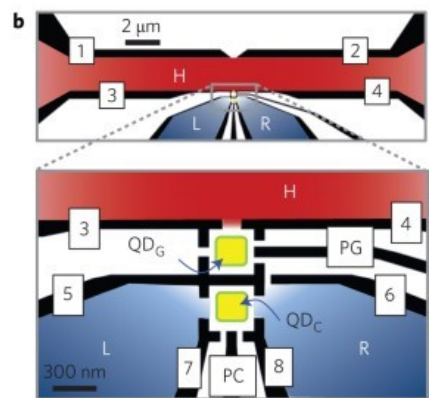
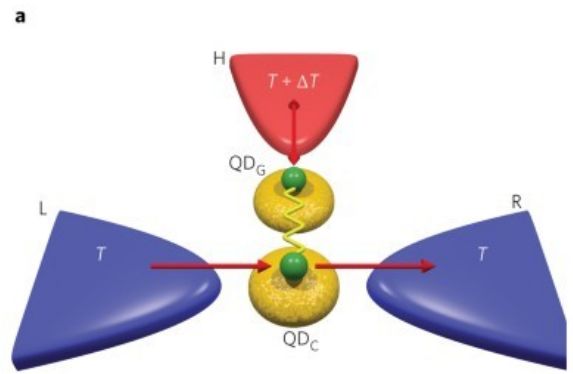
+ Work in non-equilibrium steady-state conditions



Small absorption refrigerators
Linden et al. PRL (2010)

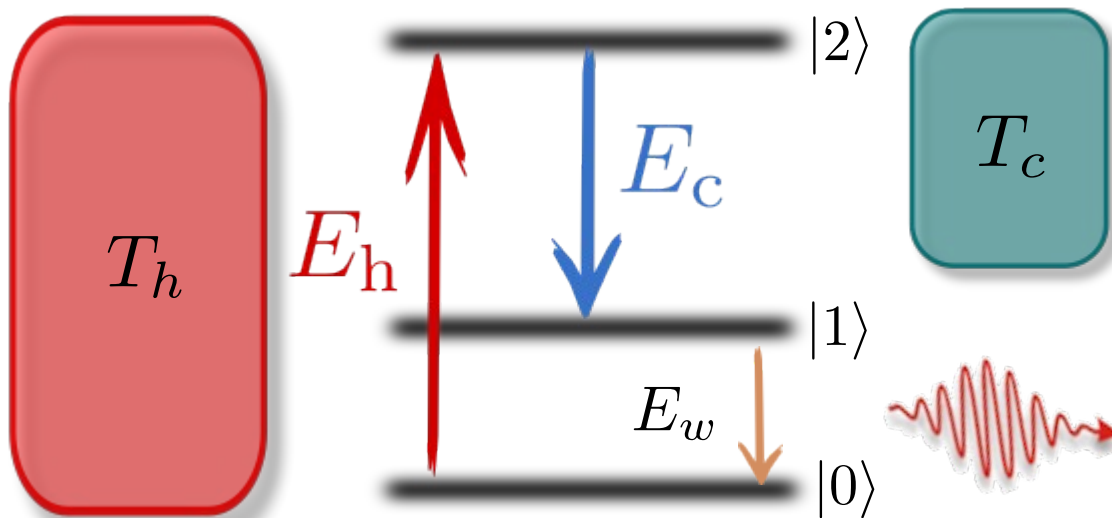


Three-level laser / amplifier
Kosloff et al, Annu. Rev. Phys. Chem. (2014)



Quantum-dot energy harvesters
Thierschmann et al. Nat. Nano (2015), Sanchez et al. PRB (2011)

Three-level laser / amplifier



Engine Hamiltonian:

$$H = E_h |2\rangle\langle 2| + E_w |1\rangle\langle 1|$$

$$E_h = E_w + E_c$$

External driving field (weak):

$$V = \epsilon |1\rangle\langle 0| e^{-iE_w t} + \text{h.c.}$$

Lindblad master equation (rotating frame):

$$\dot{\rho} = \underbrace{-i[V_R, \rho]}_{\text{driving}} + \sum_{i=h,c} \underbrace{\mathcal{D}_{\downarrow}^{(i)}[\rho] + \mathcal{D}_{\uparrow}^{(i)}[\rho]}_{\text{dissipation}}$$

Dissipators: $\mathcal{D}_{\uparrow\downarrow}^{(i)}[\rho] = L_{\uparrow\downarrow}^{(i)} \rho L_{\uparrow\downarrow}^{(i)\dagger} - \frac{1}{2} \{L_{\uparrow\downarrow}^{(i)\dagger} L_{\uparrow\downarrow}^{(i)}, \rho\}$

Local detailed balance: $\gamma_{\downarrow}^{(i)} = \gamma_{\uparrow}^{(i)} e^{\beta_i E_i}$

hot

$$L_{\downarrow}^{(h)} = \sqrt{\gamma_{\downarrow}^{(h)}} |0\rangle\langle 2|$$

$$L_{\uparrow}^{(h)} = \sqrt{\gamma_{\uparrow}^{(h)}} |2\rangle\langle 0|$$

cold

$$L_{\downarrow}^{(c)} = \sqrt{\gamma_{\downarrow}^{(c)}} |1\rangle\langle 2|$$

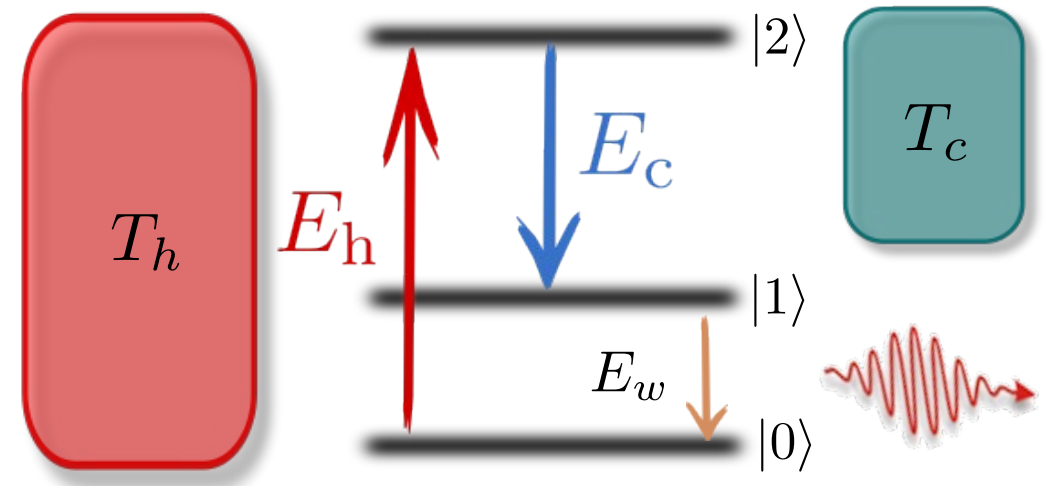
$$L_{\uparrow}^{(c)} = \sqrt{\gamma_{\uparrow}^{(c)}} |2\rangle\langle 1|$$

Steady-state:

$$\dot{\rho} \equiv 0 \rightarrow \pi$$

Solving as a matrix:

$$\vec{\dot{\pi}} = W \vec{\pi} \equiv 0$$



Heat currents
(into machine):

$$\dot{Q}_i = \text{Tr}[H(\mathcal{D}_{\downarrow}^{(i)}[\pi] + \mathcal{D}_{\uparrow}^{(i)}[\pi])] \quad \text{for } i = h, c$$

Hot: $\dot{Q}_h = E_h(\gamma_{\uparrow}^{(h)} \pi_0 - \gamma_{\downarrow}^{(h)} \pi_2)$

Cold: $\dot{Q}_c = E_c(\gamma_{\uparrow}^{(c)} \pi_1 - \gamma_{\downarrow}^{(c)} \pi_2)$

Driving (input) power: $\dot{W} = \text{Tr}[(\dot{V})_R \rho_{ss}] = \epsilon E_w i(c - c^*)$

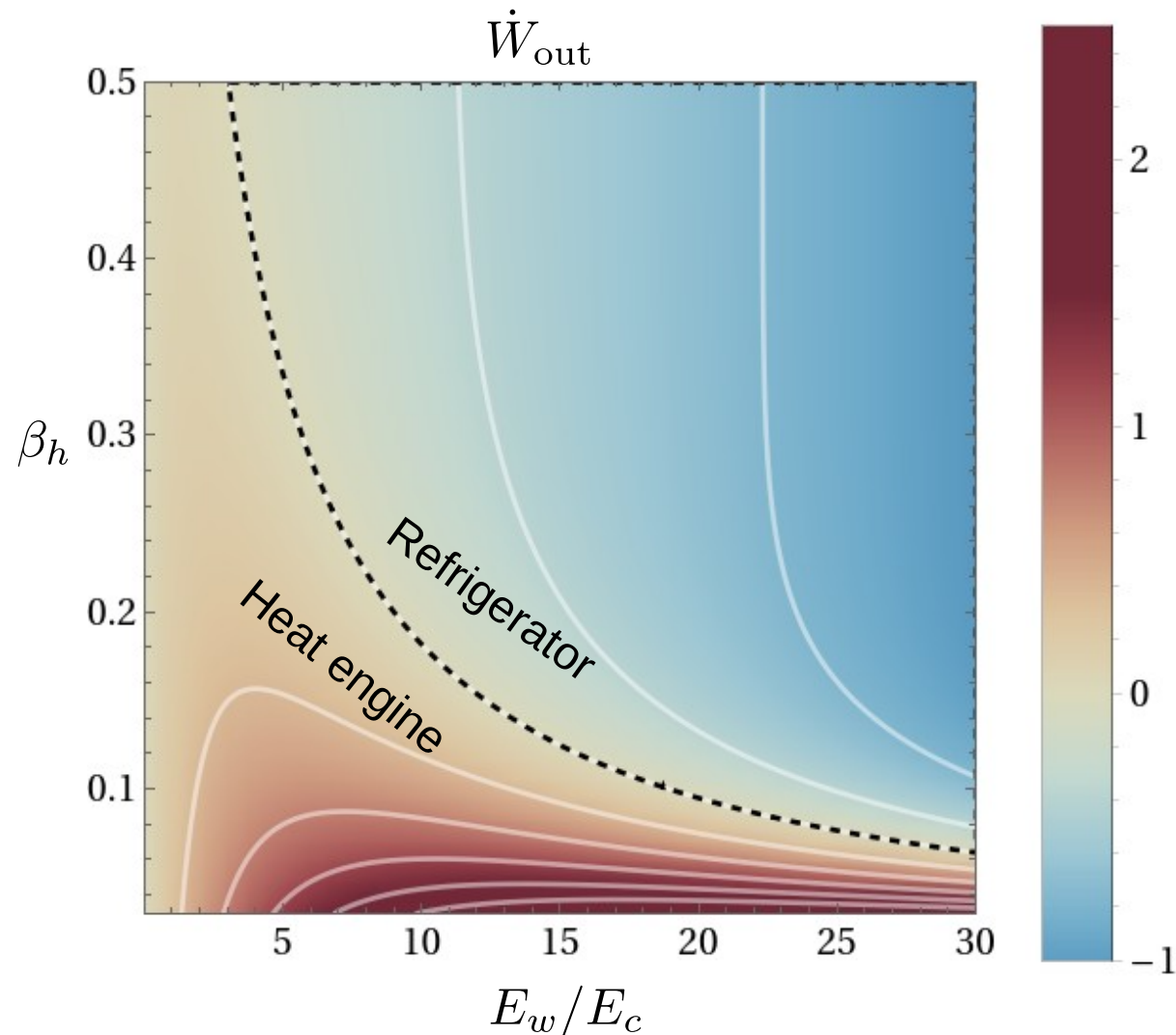
First law: $\dot{E} = \dot{Q}_c + \dot{Q}_h + \dot{W} = 0$

Second law: $\dot{S}_{\text{tot}} = -\beta_c \dot{Q}_c - \beta_h \dot{Q}_h \geq 0$

Efficiency: $\eta = \frac{\dot{W}_{\text{out}}}{\dot{Q}_h} = 1 - \frac{E_c}{E_h}$

As before: $\eta \leq \eta_C$

with output work: $\dot{W}_{\text{out}} = -\dot{W}$

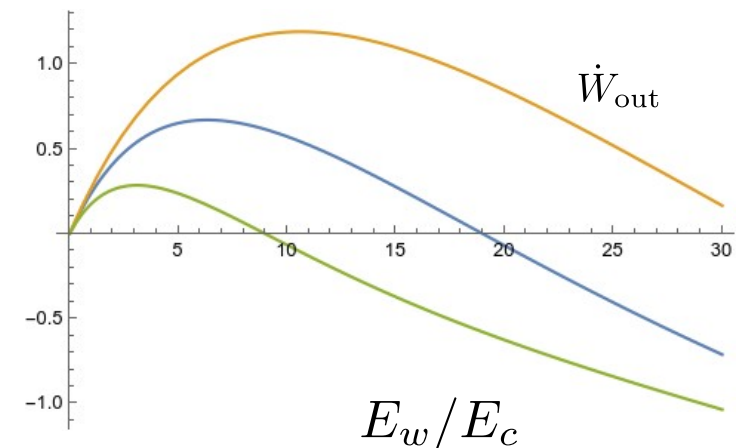


Heat engine regime:

$$\dot{W}_{\text{out}} \geq 0 \Leftrightarrow \beta_c E_c \geq \beta_h E_h$$

Refrigerator regime:

$$\dot{Q}_c \geq 0 \Leftrightarrow \beta_c E_c \leq \beta_h E_h$$



Many models of engines are **based on quantum effects** (e.g. tunneling) or even show an **intrinsic quantum dynamics**, leading e.g. to entanglement in multipartite systems, but...

Quantum-thermodynamic advantage?

+ Define and compare to classical analogs, introduce extra dephasing ...

R. Uzdin, et al. PRX (2015), L. Correa, et al. PRE (2019), ...

It can be ambiguous depending how one defines the “analog”...

+ Breaking of classical nonequilibrium inequalities such as TUR as a witness

→ *model independent*

Agarwalla and Segal PRB (2018), Ptaszyński PRB (2018), Kalae et al. PRE (2021)
G. Manzano and R. Lopez, PRR (in press), arXiv:2302.09414

Thermodynamic and Kinetic Uncertainty Relations

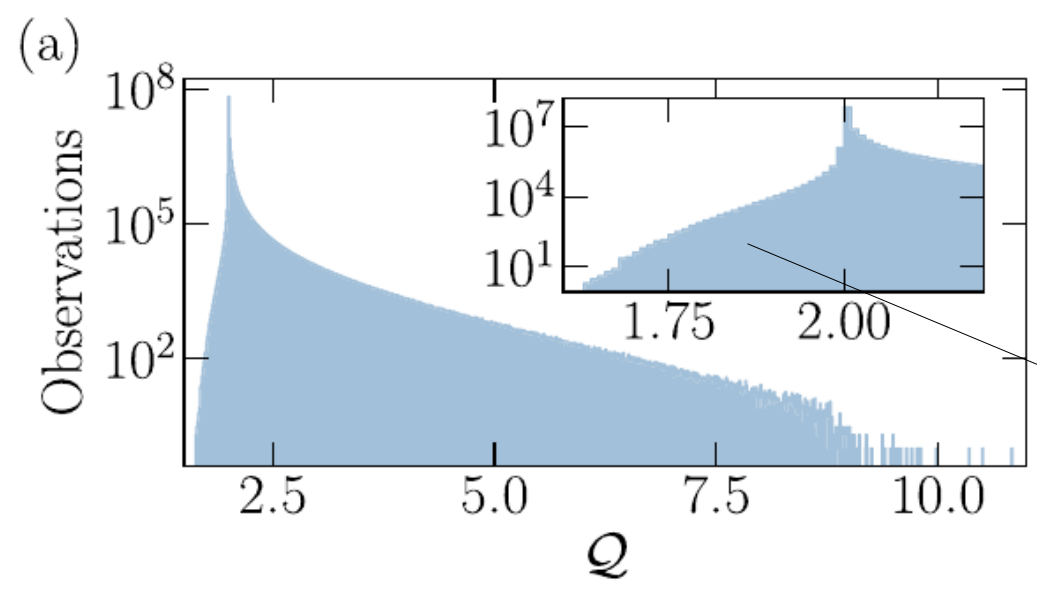
Classical Markovian processes in nonequilibrium steady states

TUR

$$\frac{\text{Var}[J(t)]}{\langle J(t) \rangle^2} \geq \frac{2k_B}{\dot{S}_{\text{tot}}}$$

Arbitrary current \rightarrow $J(t)$
 \dot{S}_{tot} \rightarrow Entropy production (EP) rate / dissipation

Barato and Seifert, PRL (2015), Gingrich *et al.* PRL (2016), ...



Or in other words, in classical engines:

$$Q \equiv \dot{S}_{\text{tot}} \frac{\text{Var}[\dot{W}]}{\dot{W}^2} \geq 2$$

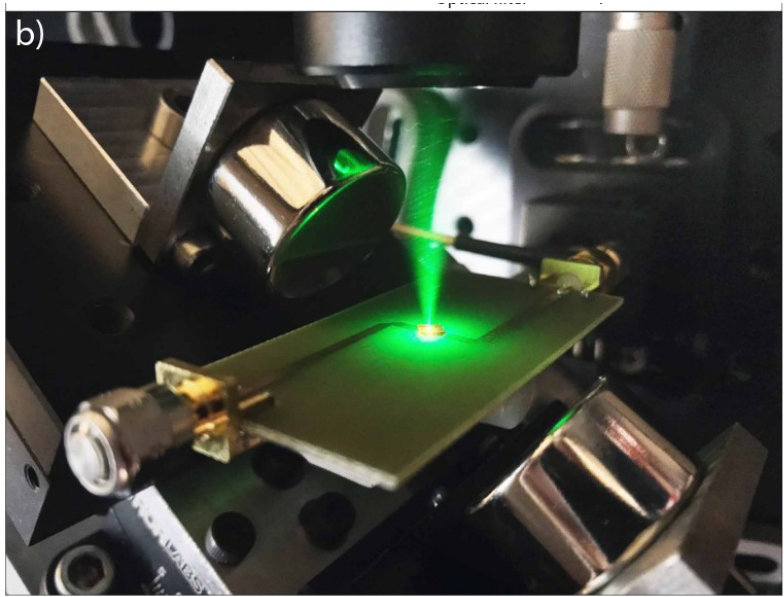
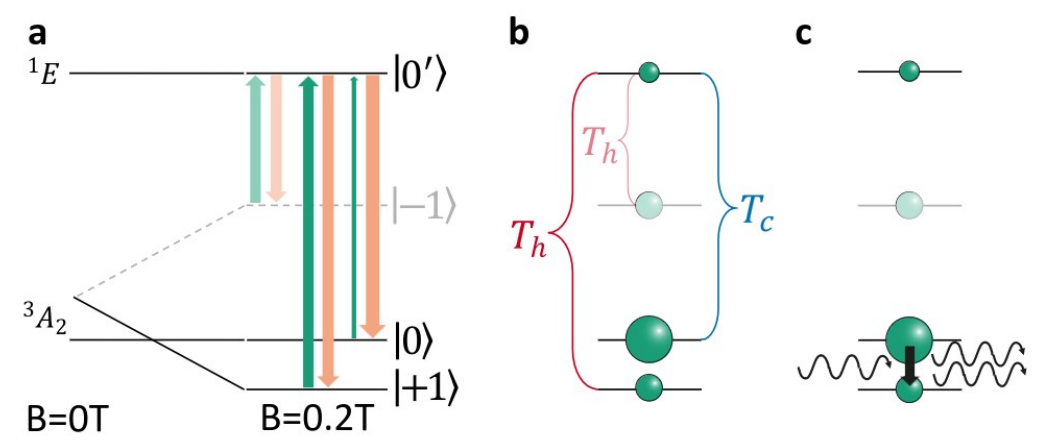
VIOLATION!

Quantum-thermodynamic advantage!

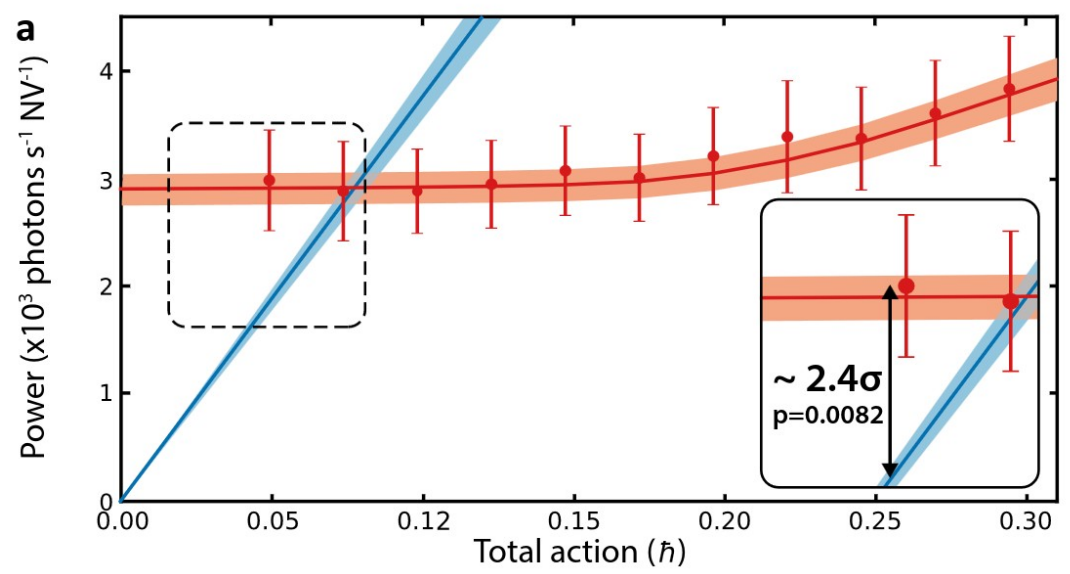
Kalae *et al.*, PRE **104** (2021)

NV three-level quantum heat engine: [Klatzow, et al. Phys. Rev. Lett, 122 \(2019\)](#)

- Nitrogen-vacancy centers in diamond
- Effective 3-level system
- Effective baths using optical pumping and decay by different mechanisms
- Driving with microwave field (work)



Focus is to demonstrate a quantum signature

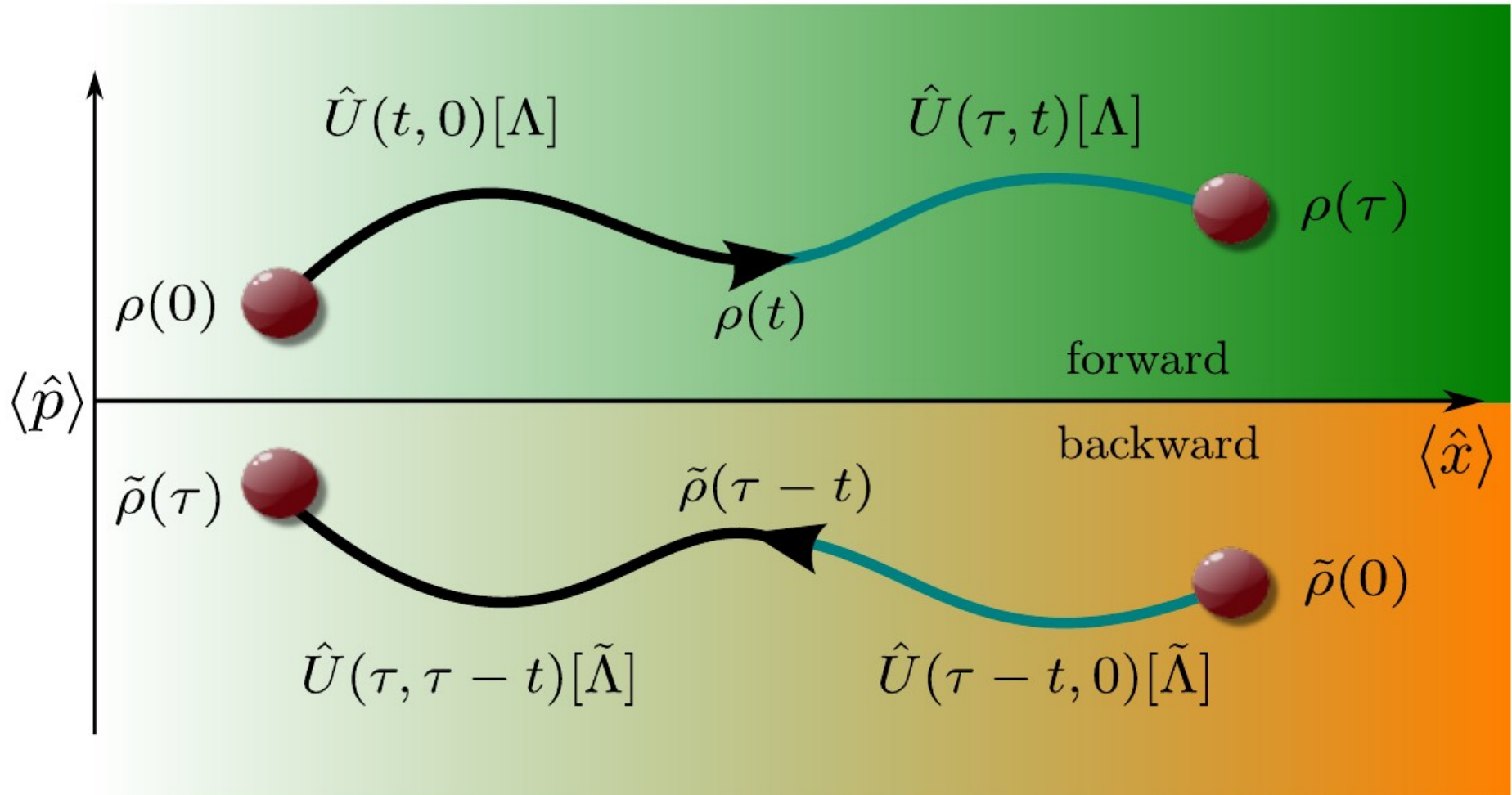




THANK YOU

for your attention

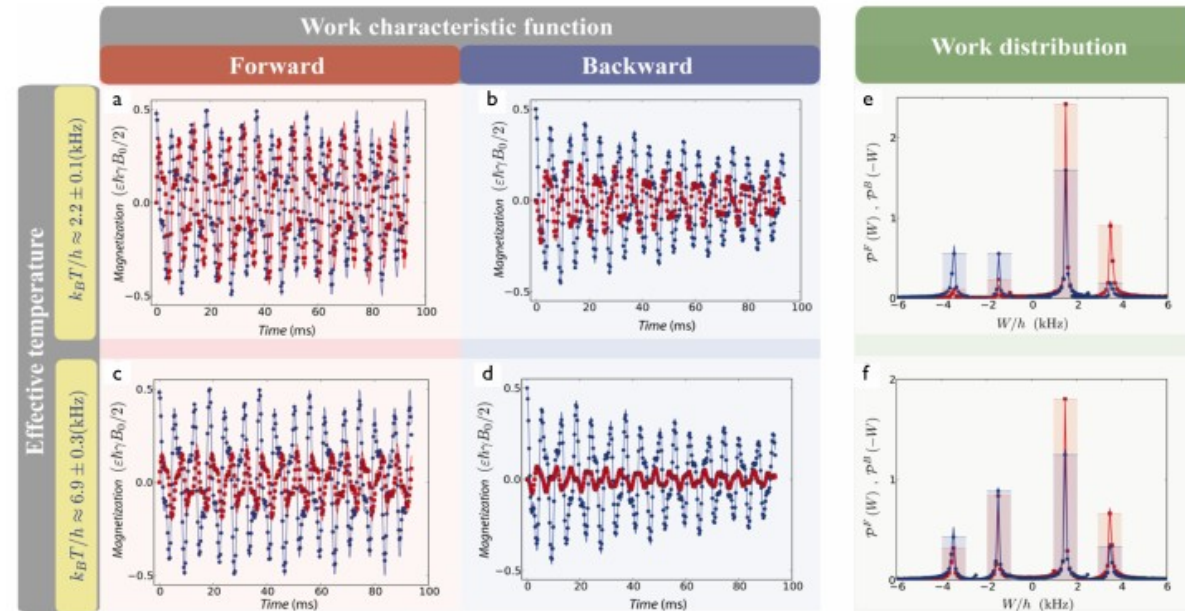
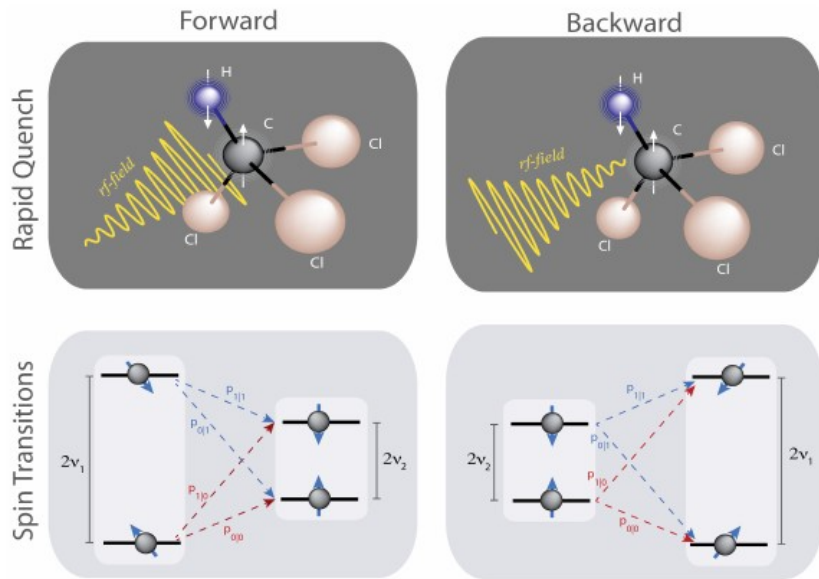
Micro-reversibility relation for non-autonomous systems:



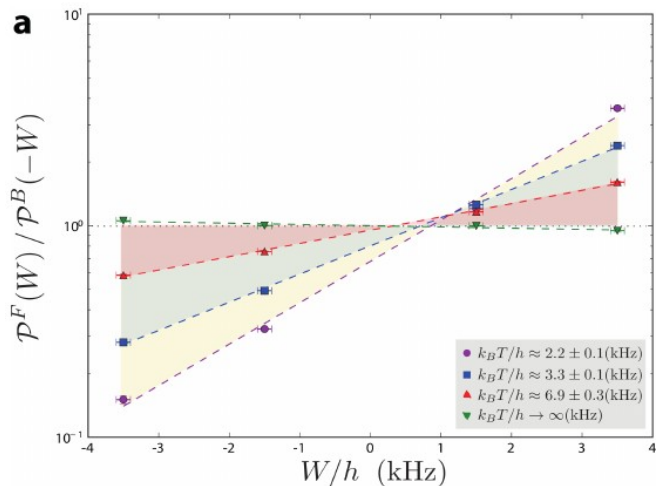
$$U^\dagger(\tau, t)[\Lambda] = \Theta^\dagger U(\tau - t, 0)[\tilde{\Lambda}]\Theta$$

Liquid-state NMR platform

T.B. Batalhao, *et al.* Phys. Rev. Lett, **113** (2014)

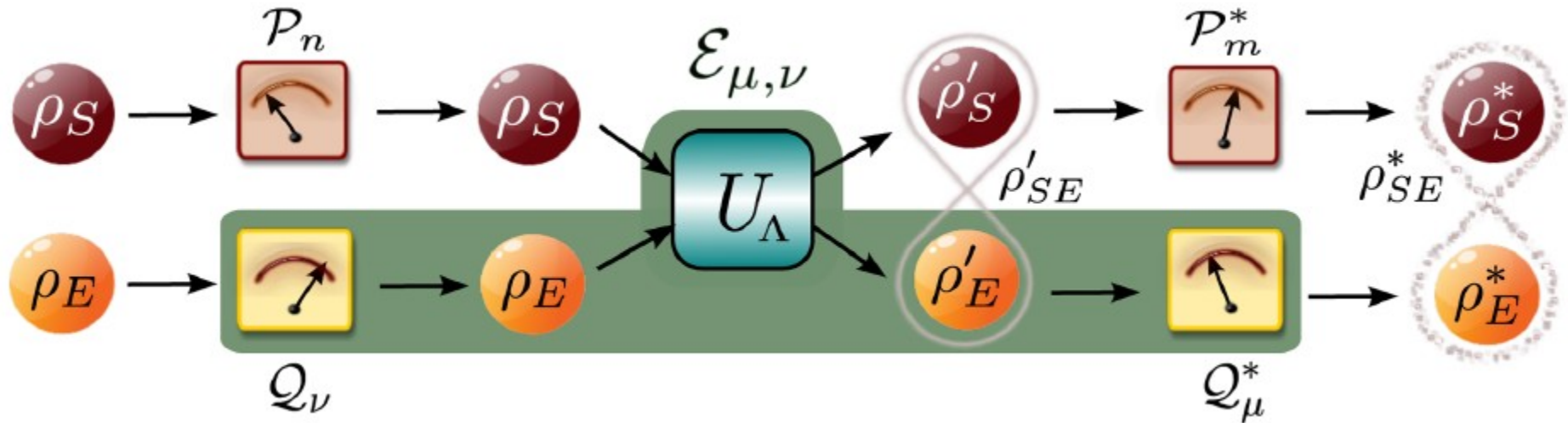


Testing Crooks fluctuation theorem (logarithm scale) and Jarzynski equality:



| $k_B T / h$ (kHz) | 2.2 ± 0.1 | 3.3 ± 0.1 | 6.9 ± 0.3 |
|-------------------------------------|-----------------|-----------------|-------------------|
| $\log \langle e^{-\beta W} \rangle$ | 0.38 ± 0.03 | 0.20 ± 0.02 | 0.06 ± 0.01 |
| $\beta \Delta F$ | 0.39 ± 0.06 | 0.22 ± 0.02 | 0.05 ± 0.01 |
| Theory | 0.43 ± 0.03 | 0.22 ± 0.01 | 0.053 ± 0.003 |

Fluctuation theorems for arbitrary environments setup: [G. Manzano, et al. PRX, 8 \(2018\)](#)



Initial state: $\rho_S = \sum_n p_n \mathcal{P}_n$, $\rho_E = \sum_\nu q_\nu \mathcal{Q}_\nu$,

Global evolution: $U_\Lambda \equiv \mathcal{T}_+ \exp \left(-\frac{i}{\hbar} \int_0^\tau dt H(\lambda_t) \right)$,

Evolved state: $\rho'_{SE} = U_\Lambda (\rho_S \otimes \rho_E) U_\Lambda^\dagger$,

Post-measurement state $\rho_{SE}^* = \sum (\mathcal{P}_m^* \otimes \mathcal{Q}_\mu^*) \rho'_{SE} (\mathcal{P}_m^* \otimes \mathcal{Q}_\mu^*)$