Lecture 2:
Discrete quantum heat engines

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Advanced School on Ubiquitous Quantum Physics:
The New Quantum Revolution

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The Abdus Salam International Centre for Theoretical Physics

THE FRITZ HABER RESEARCH CENTER FOR MOLECULAR DYNAMICS

How small a quantum engine can be

What is quantum in quantum heat devices

Inserting Dynamics into Thermodynamics

Open quantum system:

$$H = H_S + H_E + H_I$$

Markovian master equation

$$\frac{d\rho_s}{dt} = -i[H_s, \rho_s] + \mathcal{L}_D \rho_s \quad \longleftarrow \quad \frac{d\rho}{dt} = -i[H, \rho]$$

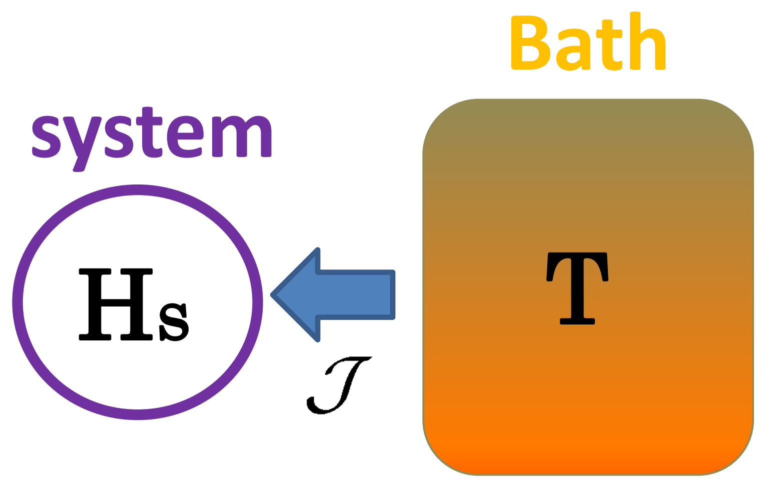
Reduced description

- weak coupling
- Low density

G. Lindblad

Generator of quantum dynamical semigroup (LGKS form)

$$\mathcal{L}\rho_s = \sum_k V_k^\dagger \rho_s V_k - \frac{1}{2}\left\{V_k V_k^\dagger, \rho_s\right\}$$



Inserting Dynamics into Thermodynamics

Power or efficiency?

$$\eta_{CA} = 1 - \sqrt{\frac{T_c}{T_h}}$$

Efficiency at maximum power

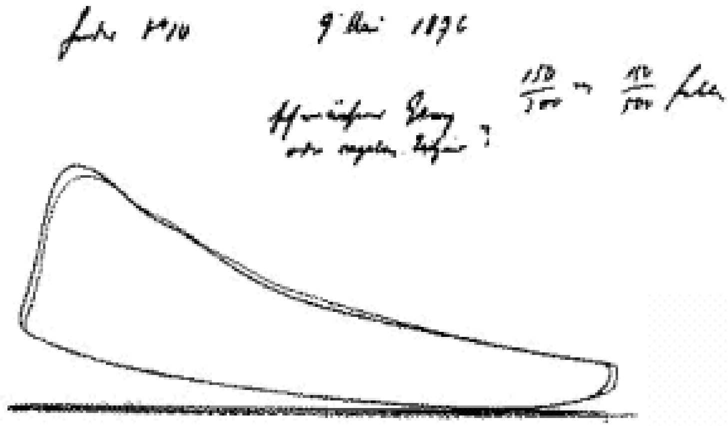
$$\Delta S^{o} > 0$$

$$\eta_{c} = 1 - \frac{T_c}{T_h}$$

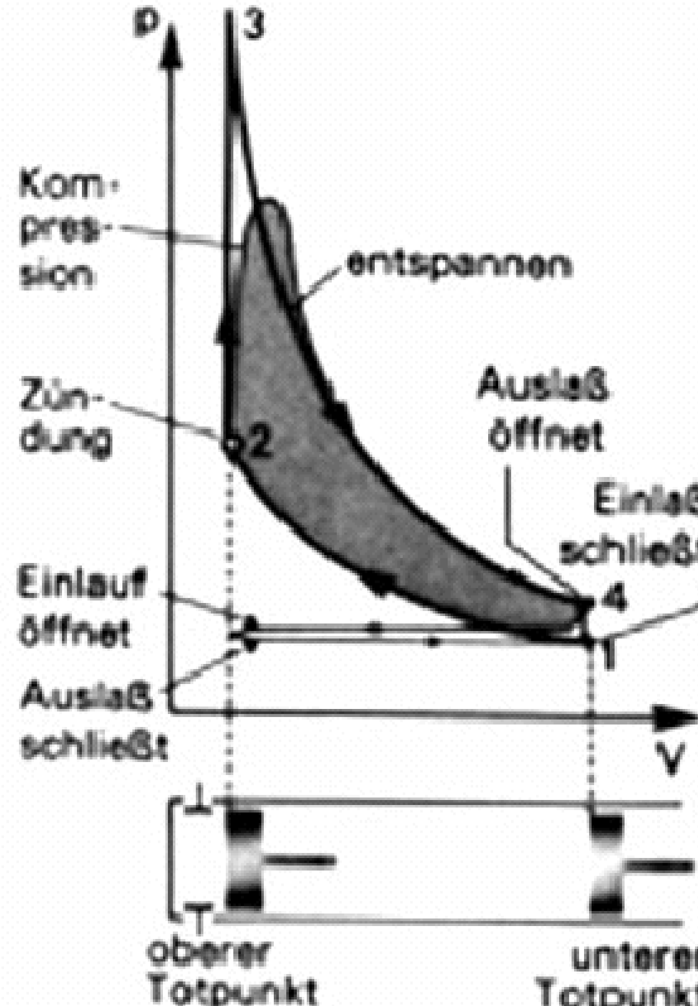
Maximum efficiency

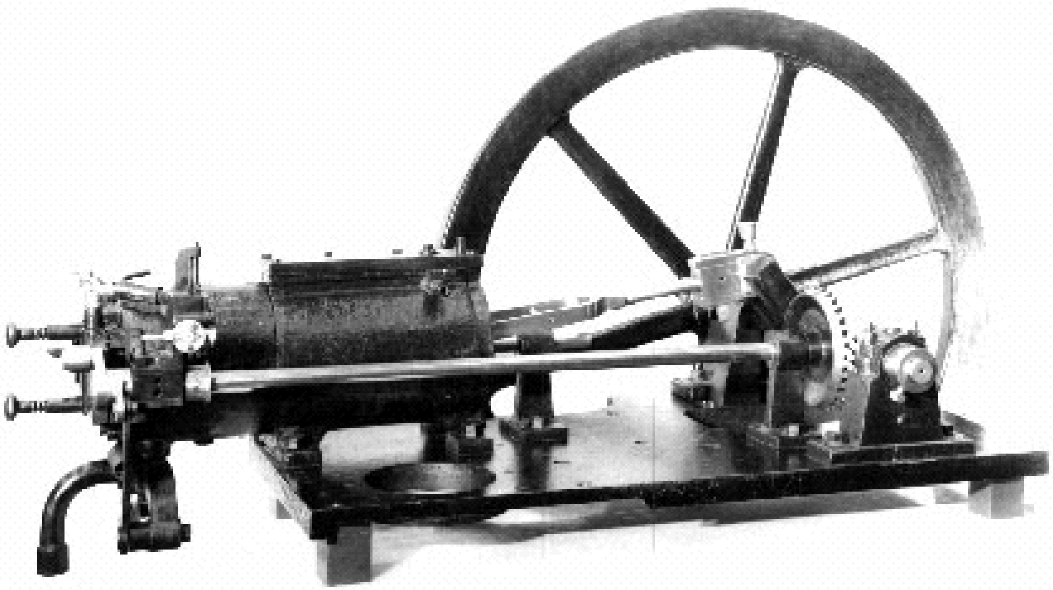
$$\Delta S^{o} = 0$$

Nicolaus August Otto



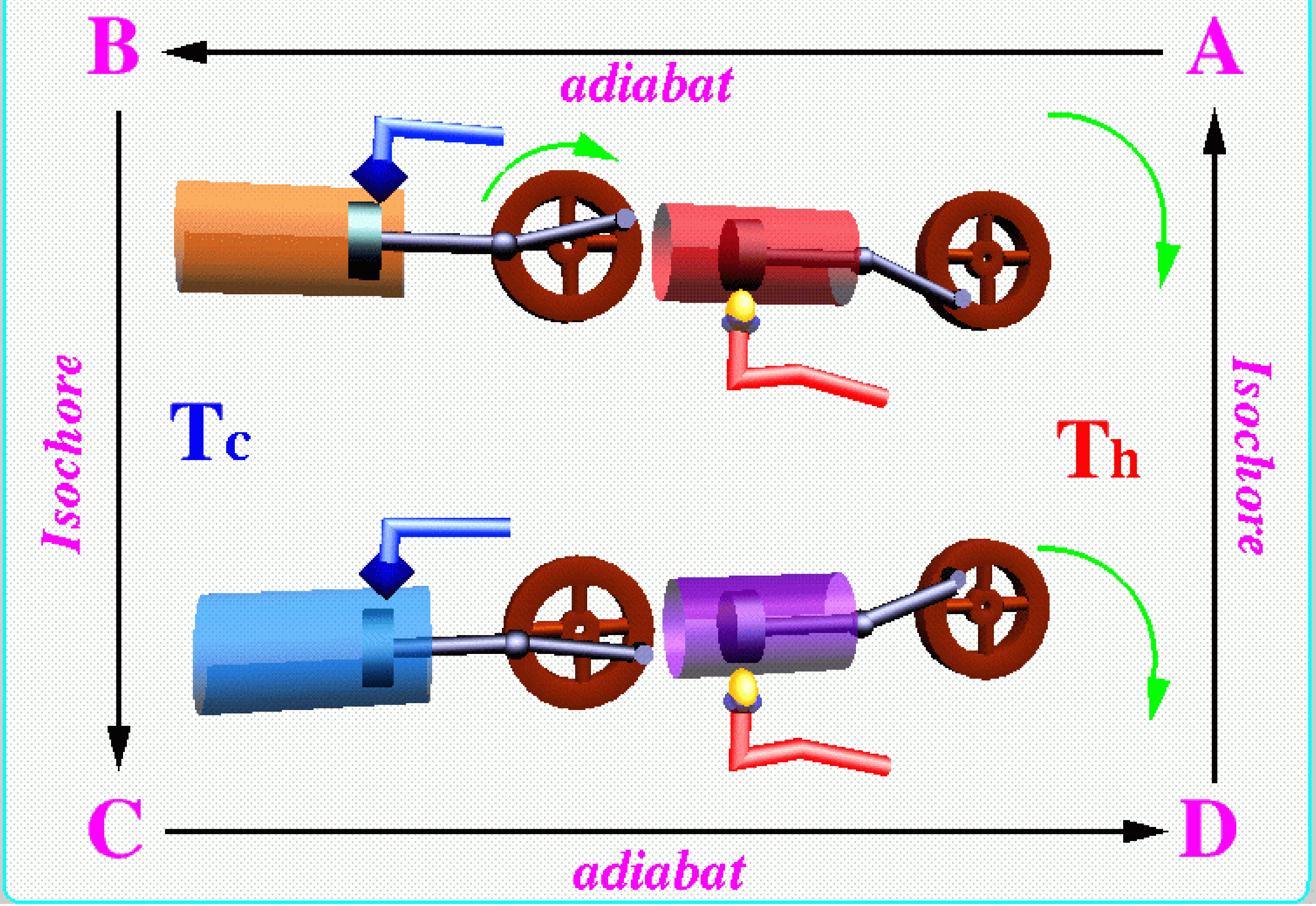
working diagram : 9th May 1876



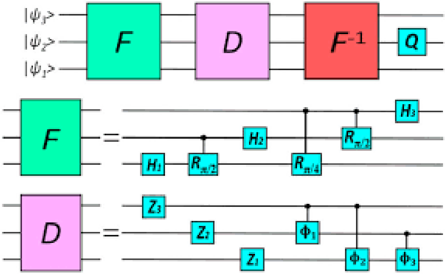


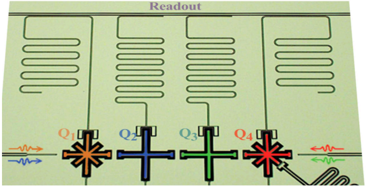
four–stroke cycle engine 1876

Otto Cycle



Reciprocating heat engines

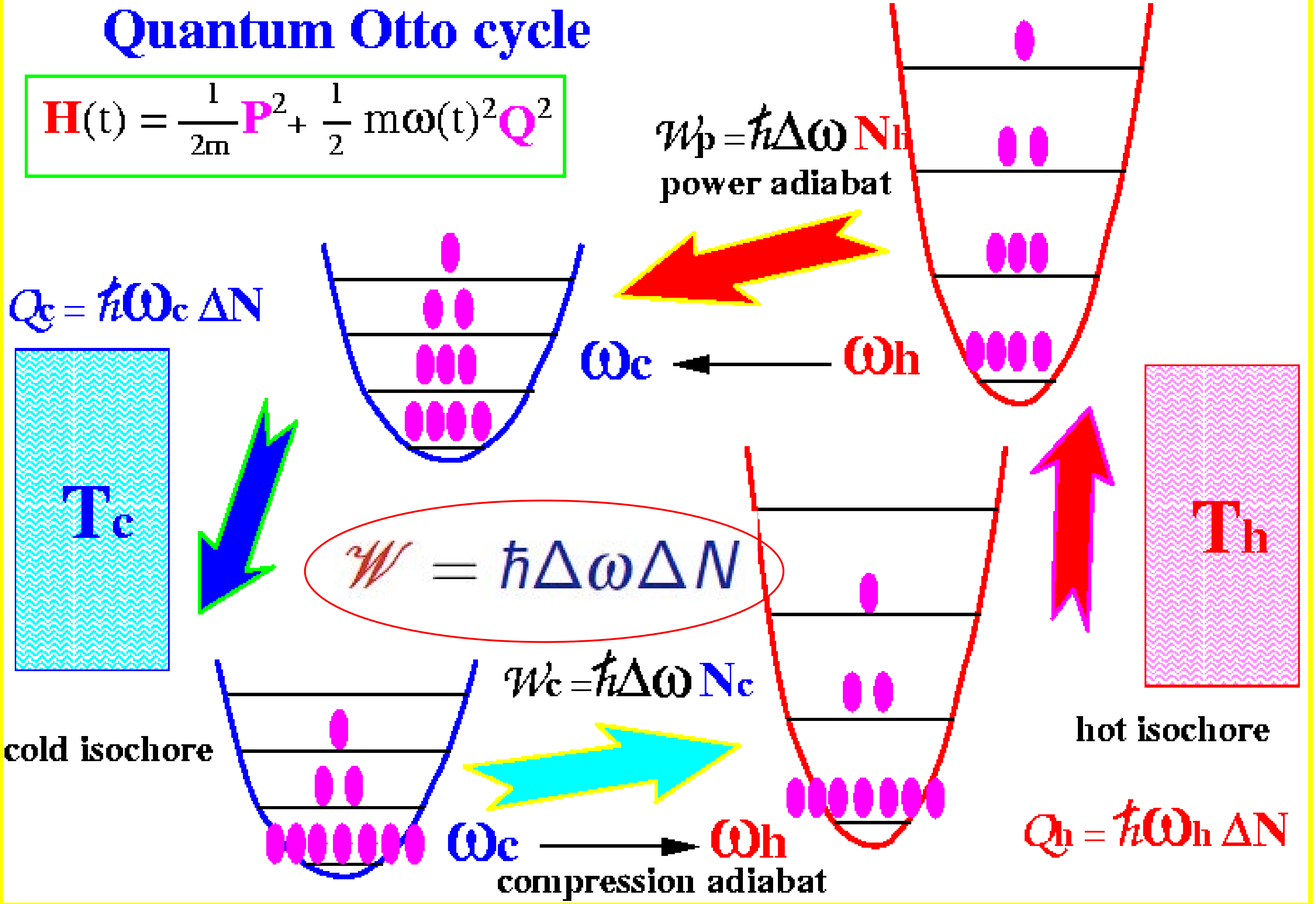




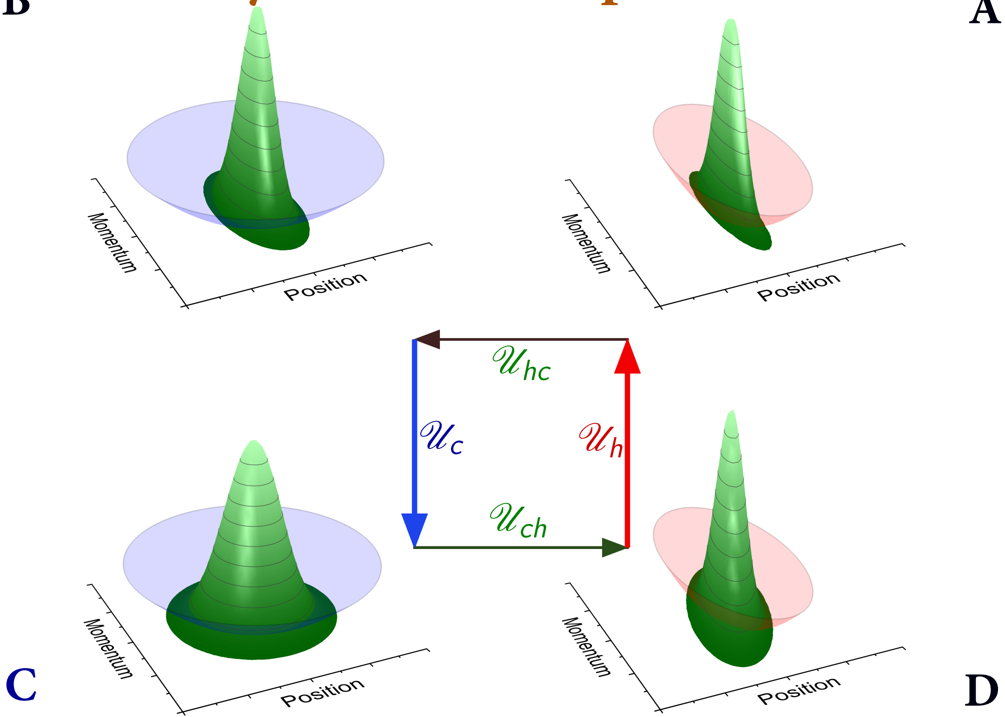
How far can we mintuaize?

Quantum Otto cycle

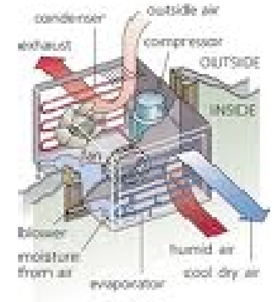
$$\mathbf{H}(t) = \frac{1}{2m}\mathbf{P}^2 + \frac{1}{2} m\omega(t)^2 \mathbf{Q}^2$$



Otto Cycle in Phase Space



The quantum Otto refrigeration cycle



Cycle Propagator: $\mathcal{U}_{cycle} = \mathcal{U}_h \mathcal{U}_{hc} \mathcal{U}_c \mathcal{U}_{ch}$

$\mathcal{U}_h$ **Hot Isochore (isomagnetic) A → B** $\omega = \omega_h$.

The working mediumis in contact with the hot bath of temperature T_h .

$\mathcal{U}_{hc}$ **Expansion adiabat (demagnetization) B → C**

The field changes from ω_h **to** ω_c

$\mathcal{U}_c$ **Cold Isochore (isomagnetic) C → D** $\omega = \omega_c$.

The working medium is in contact with the cold bath of temperature T_c .

$\mathcal{U}_{ch}$ **Compression adiabat (magnetization) D → A**

The field changes from ω_c **to** ω_h .

$$[\mathcal{U}_h \mathcal{U}_{hc}, \mathcal{U}_c \mathcal{U}_{ch}] \neq 0$$

limit cycle

$$\mathcal{U}_{cycle} Y = Y$$

Thermodynamic description of the engine.

- The Hamiltonian $\hat{\mathbf{H}}(t) = \frac{1}{2m}\hat{\mathbf{P}}^2 + \frac{1}{2}m\omega(t)^2\hat{\mathbf{Q}}^2$.
- The Lagrangian $\hat{\mathbf{L}}(t) = \frac{1}{2m}\hat{\mathbf{P}}^2 - \frac{1}{2}m\omega(t)^2\hat{\mathbf{Q}}^2$.
- The position momentum correlation $\hat{\mathbf{C}}(t) = \frac{1}{2}\omega(t)(\hat{\mathbf{Q}}\hat{\mathbf{P}} + \hat{\mathbf{P}}\hat{\mathbf{Q}})$

Maximum entropy state

$$\hat{\rho} = \frac{1}{Z}e^{-\beta'\hat{\mathbf{H}}+\eta\hat{\mathbf{L}}+\nu\hat{\mathbf{C}}} = \frac{1}{Z}e^{\gamma\hat{\mathbf{a}}^2}e^{-\beta\hat{\mathbf{H}}}e^{\gamma^*\hat{\mathbf{a}}^{\dagger 2}} \quad ,$$

This state $\hat{\rho}$ is defined by the parameters β, γ and γ^*:

Yair Rezek and Ronnie Kosloff
, Irreversible performance of a quantum harmonic heat engine
.(New J. Phys. 8, 83 2006

The dynamics on the isochores

The Heisenberg equations of motion for operator $\hat{\mathbf{X}}$:

$$\frac{d}{dt}\hat{\mathbf{X}} = \frac{i}{\hbar}[\hat{\mathbf{H}},\hat{\mathbf{X}}] + k_{\downarrow}(\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{X}}\hat{\mathbf{a}} - \frac{1}{2}\{\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}},\hat{\mathbf{X}}\}) + k_{\uparrow}(\hat{\mathbf{a}}\hat{\mathbf{X}}\hat{\mathbf{a}}^{\dagger} - \frac{1}{2}\{\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger},\hat{\mathbf{X}}\})$$

$$\frac{d}{dt}\begin{pmatrix}\hat{\mathbf{H}}\\ \hat{\mathbf{L}}\\ \hat{\mathbf{C}}\\ \hat{\mathbf{I}}\end{pmatrix}(t) = \begin{pmatrix} -\Gamma & 0 & 0 & \Gamma\langle\hat{\mathbf{H}}\rangle_{eq}\\ 0 & -\Gamma & -2\omega & 0\\ 0 & 2\omega & -\Gamma & 0\\ 0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\hat{\mathbf{H}}\\ \hat{\mathbf{L}}\\ \hat{\mathbf{C}}\\ \hat{\mathbf{I}}\end{pmatrix}(t)$$

The heat transport

$$\dot{Q} = \langle L_{D}(\mathbf{H})\rangle$$

$$\dot{Q} = -\Gamma\,(\langle\mathbf{H}\rangle - \langle\mathbf{H}\rangle_{eq})$$

The thermalization propagator:

$$\mathscr{U}_{h/c} = \begin{pmatrix} R & 0 & 0 & H_{eq}(1-R)\\ 0 & Rc & -Rs & 0\\ 0 & Rs & Rc & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$$

where $R = e^{-\Gamma t}$. $c = \cos(2\omega t)$, $s = \sin(2\omega t)$ and $H_{eq} = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}}-1}$.

The dynamics on the adiabats

$$P = \langle \frac{\partial \mathbf{H}}{\partial t} \rangle$$

The Heisenberg equations of motion:

$$\frac{d}{dt}\begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\mathbf{L}} \\ \hat{\mathbf{C}} \\ \hat{\mathbf{I}} \end{pmatrix}(t) = \omega(t)\begin{pmatrix} \mu & -\mu & 0 & 0 \\ -\mu & \mu & -2 & 0 \\ 0 & 2 & \mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\mathbf{L}} \\ \hat{\mathbf{C}} \\ \hat{\mathbf{I}} \end{pmatrix}(t) \ .$$

$\mu = \frac{\dot{\omega}}{\omega^2}$ is a dimensionless adiabatic parameter.

$$P = \omega\mu \left(\langle \mathbf{H} \rangle - \langle \mathbf{L} \rangle\right)$$

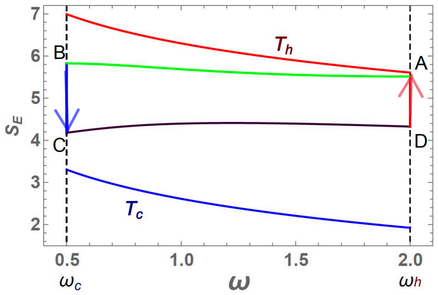
$$\begin{cases} P_{\text{ext}} = \omega\mu \langle \mathbf{H} \rangle & \textbf{useful work} \\ P_{\text{fric}} = \omega\mu \langle \mathbf{L} \rangle & \textbf{work against friction} \end{cases}$$

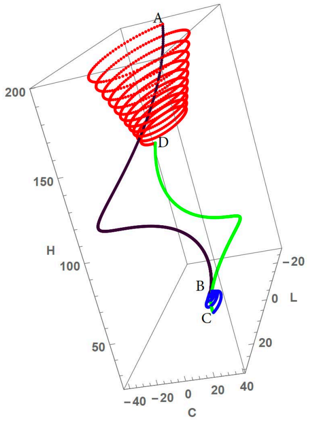
The adiabatic propagator:

$$\mathscr{U}_a = \frac{\omega(t)}{\omega(0)} \frac{1}{\Omega^2}\begin{pmatrix} 4-\mu^2 c & -\mu\Omega s & -2\mu(c-1) & 0 \\ -\mu\Omega s & \Omega^2 c & -2\Omega s & 0 \\ 2\mu(c-1) & 2\Omega s & 4c-\mu^2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$\Omega = \sqrt{4-\mu^2}$, $c = \cos(\Omega\theta(t))$, $s = \sin(\Omega\theta(t))$, $\theta(t) = -\frac{1}{\mu}\log(\frac{\omega(t)}{\omega(0)})$.

Engine cycle $[\hat{\mathbf{H}}(t), \hat{\mathbf{H}}(t')] \neq 0$





Adiabatic efficiency $\eta = 1 - \frac{\omega_c}{\omega_h} \leq 1 - \frac{T_c}{T_h}$

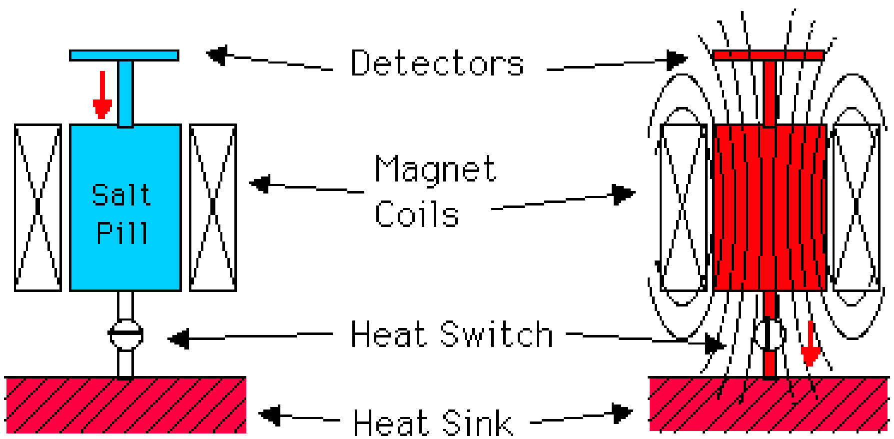
Quantum friction is the inability to stay on the energy shell

Shortcuts to adiabaticity use coherence to reach frictionless conditions.

At high temperature the efficiency at maximum power becomes: $\eta_{CA} = 1 - \sqrt{\frac{T_c}{T_h}}$

Adiabatic Demagnetization Refrigerator ADR

The ADR Cycle: a Simple Schematic



Operating

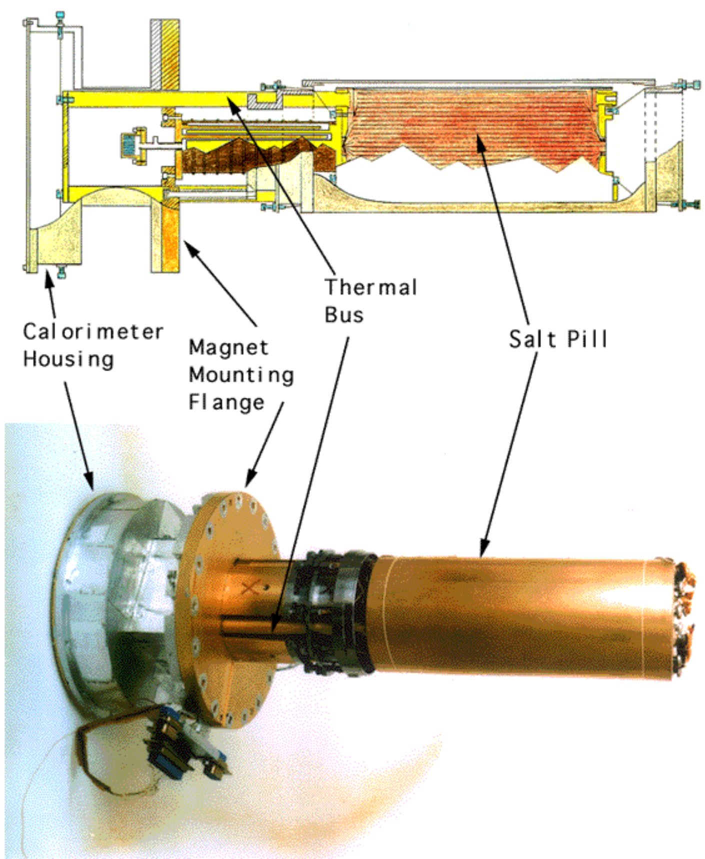
Magnetic Field: Low
Heat Switch: Off
Salt Pill: Cold

Recycling

Magnetic Field: High
Heat Switch: On
Salt Pill: Warm

Red arrow shows direction of heat flow.

ADR
Drawing and Photo Compared

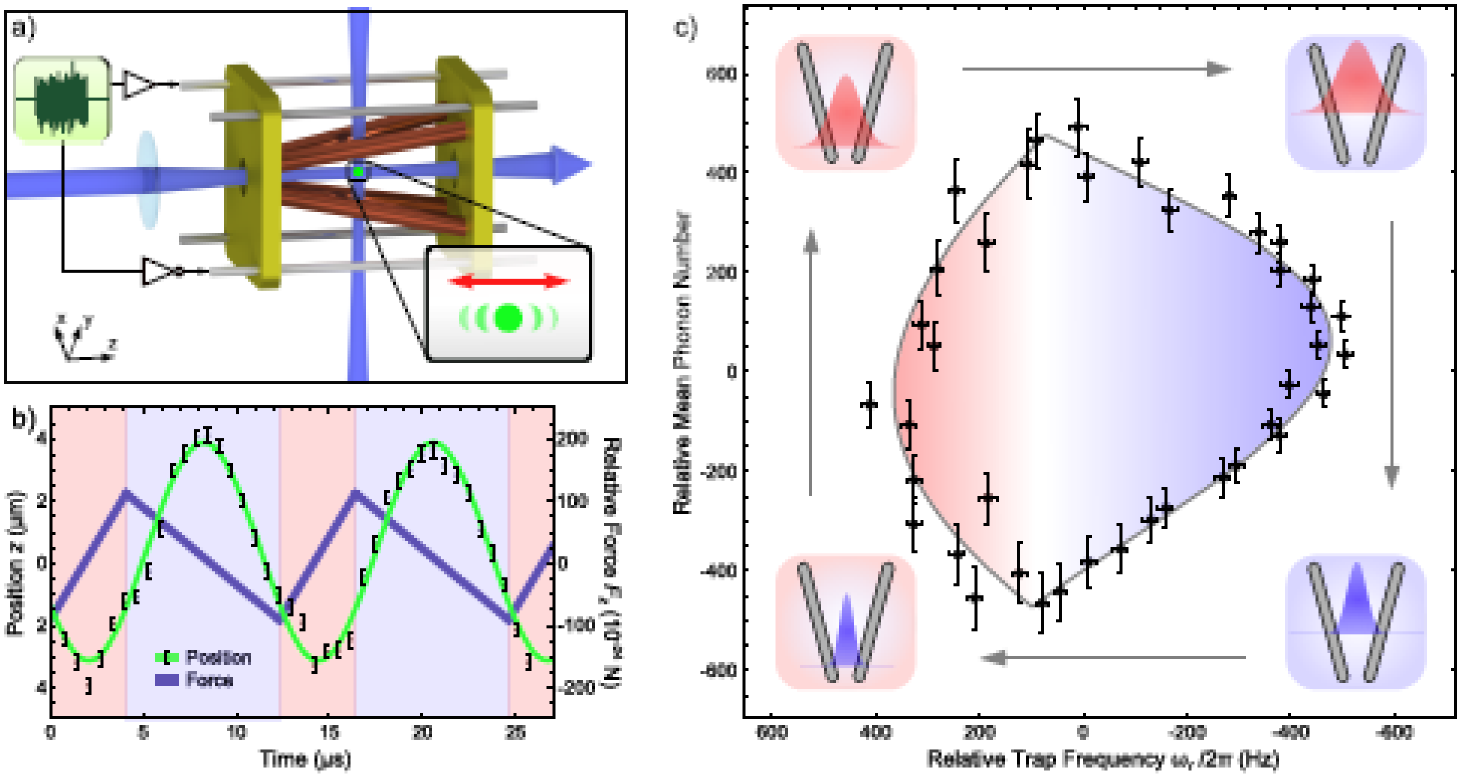


Realizations 2016

Science 352 , 325 (2016)

A single-atom heat engine

Johannes Roßnagel,[1,*] Samuel Thomas Dawkins,[1] Karl Nicolas Tolazzi,[1]
Obinna Abah,[2] Eric Lutz,[2] Ferdinand Schmidt-Kaler,[1] and Kilian Singer[1,3]



A quantum-mechanical heat engine operating in finite time. A model consisting of spin-1/2 systems as the working fluid

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(Received 28 August 1991; accepted 21 October 1991)

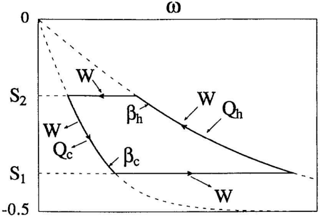


FIG. 1. The reversible Carnot cycle (solid line) in the (ω,S) plane (ω is the field and S the polarization). The cycle is composed of two reversible isotherms corresponding to the temperatures β_h and β_c $(\beta_c > \beta_h)$ and of two adiabats corresponding to the polarizations S_1 and S_2 $(S_1 < S_2; S_1, S_2 < 0)$. Positive net work production is obtained by going anticlockwise. The directions of work and heat flows along each branch are indicated.

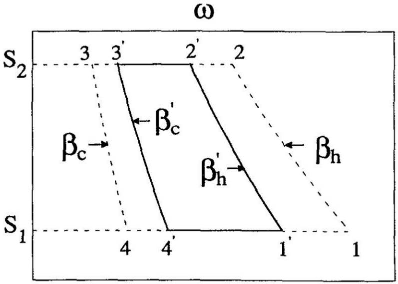


FIG. 5. The cycle $1' \to 2' \to 3' \to 4' \to 1'$ is of the Curzon–Ahlborn

Heisenberg picture, reads as follows:

$$\dot{\mathbf{X}} = i[\mathbf{H},\mathbf{X}] + \frac{\partial \mathbf{X}}{\partial t} + \mathcal{L}_D(\mathbf{X}),$$

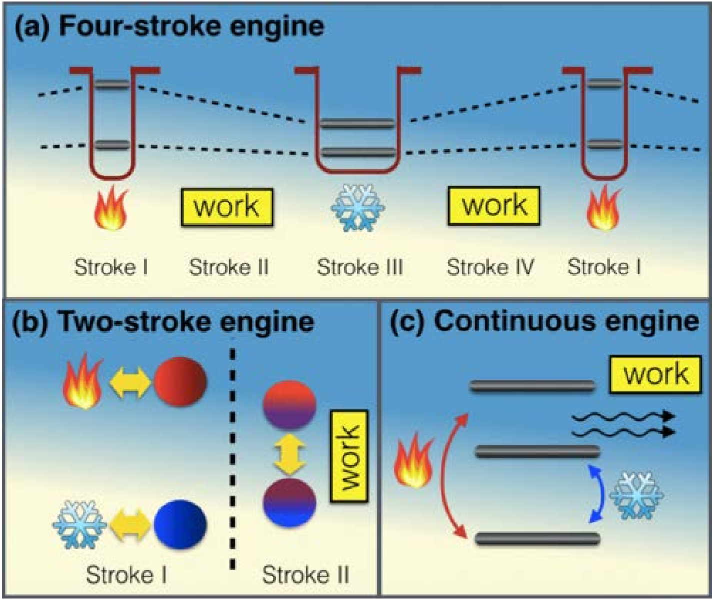
$$\mathcal{L}_D(\mathbf{X}) = \sum_\alpha \gamma_\alpha (\mathbf{V}_\alpha^\dagger [\mathbf{X},\mathbf{V}_\alpha] + [\mathbf{V}_\alpha^\dagger,\mathbf{X}]\mathbf{V}_\alpha).$$

J. Chem. Phys., Vol. 96, No. 4, 15 February 1992

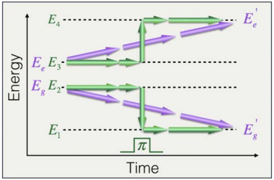
Quantum equivalence

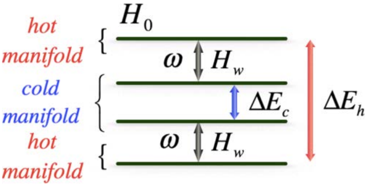
Uzdin, Raam, Amikam Levy, and Ronnie Kosloff. "Equivalence of Quantum Heat Machines, and Quantum-Thermodynamic Signatures." Physical Review X 5, no. 3 (2015): 031044.

Three types of engines

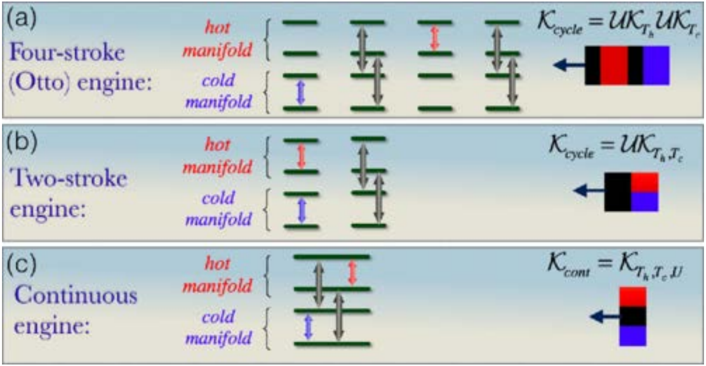


Multilevel embedding





Quantum equivalence



Quantum eqivalence

The propagator: $\mathscr{U} = e^{\mathscr{L} t}$

Four stroke cycle propagator:

$$\mathscr{U}_{cyc} = \mathscr{U}_c \mathscr{U}_{hc} \mathscr{U}_h \mathscr{U}_{ch} = e^{\mathscr{L}_c t} e^{\mathscr{L}_{hc} t} e^{\mathscr{L}_h t} e^{\mathscr{L}_{ch} t}$$

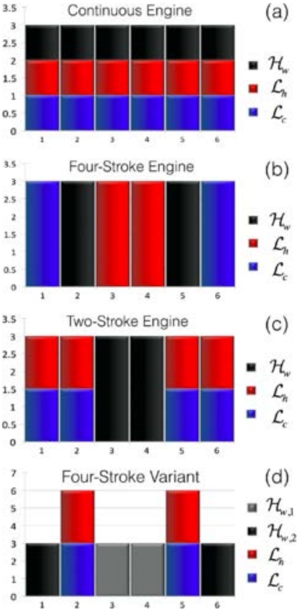
In the limit of small action: $s = ||\mathscr{L} t|| \ll \hbar$

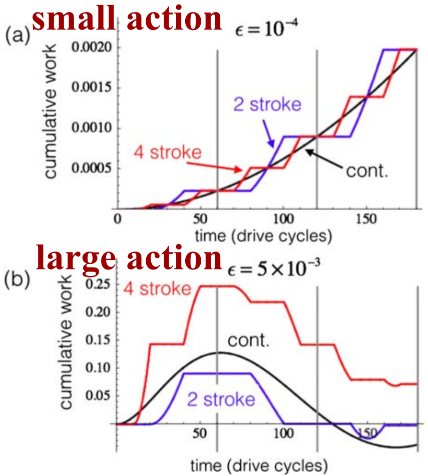
$$\mathscr{U}_{cyc} = e^{\mathscr{L}_c t/2} e^{\mathscr{L}_{hc} t} e^{\mathscr{L}_h t} e^{\mathscr{L}_{ch} t} e^{\mathscr{L}_c t/2}$$

$$\mathscr{U}_{cyc} \approx e^{(\mathscr{L}_c + \mathscr{L}_{hc} + \mathscr{L}_h + \mathscr{L}_{ch}) t} + O(s^3)$$

Raam Uzdin, Amikam Levy, and Ronnie Kosloff
Equivalence of Quantum Heat Machines, and Quantum-Thermodynamic
.(Phys. Rev. X 5, 031044 2015

Quantum equivalence



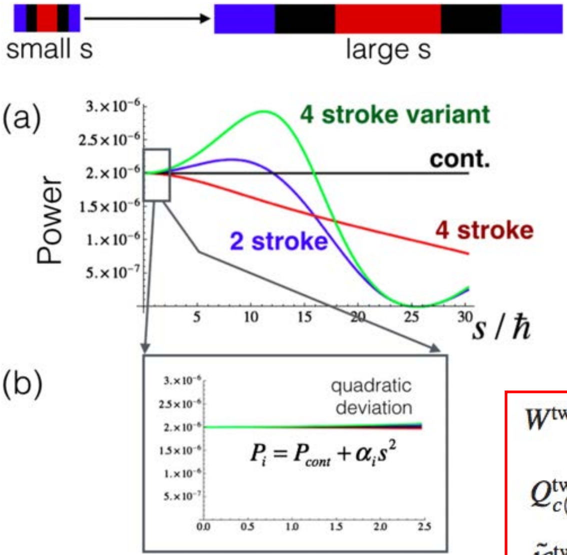


$$W^{\text{two stroke}} \cong W^{\text{four stroke}} \cong W^{\text{cont}},$$

$$Q_{c(h)}^{\text{two stroke}} \cong Q_{c(h)}^{\text{four stroke}} \cong Q_{c(h)}^{\text{cont}},$$

$$\tilde{\mathcal{K}}^{\text{two stroke}} \cong \tilde{\mathcal{K}}^{\text{four stroke}} \cong \tilde{\mathcal{K}}^{\text{cont}}.$$

Quantum equivalence



At large action:
Work extracted from
population differences.

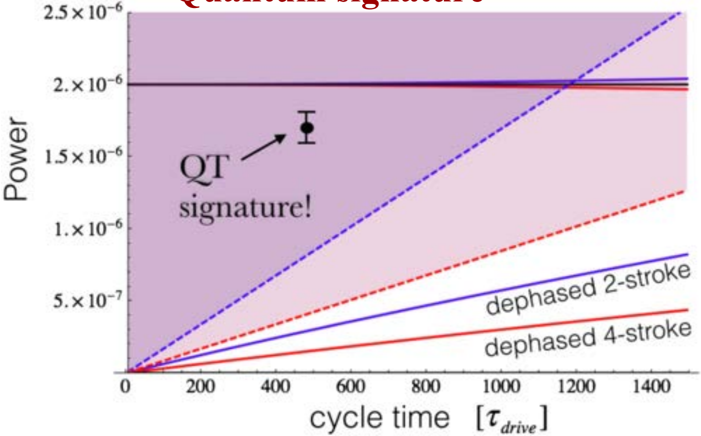
At small action:
Work can only be
extracted from coherence

$$W^{\text{two stroke}} \cong W^{\text{four stroke}} \cong W^{\text{cont}},$$

$$Q_{c(h)}^{\text{two stroke}} \cong Q_{c(h)}^{\text{four stroke}} \cong Q_{c(h)}^{\text{cont}},$$

$$\tilde{\mathcal{K}}^{\text{two stroke}} \cong \tilde{\mathcal{K}}^{\text{four stroke}} \cong \tilde{\mathcal{K}}^{\text{cont}}.$$

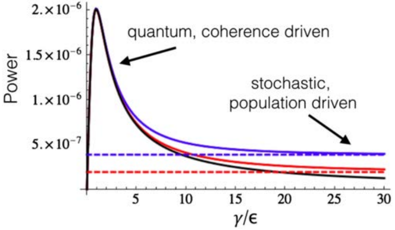
Quantum signature



$$P_{\text{stoch}} \leq \frac{z}{8\hbar^2}\sqrt{tr(H_0^2) - tr(H_0)^2}\,\Delta_w^2 d^2 \tau_{\text{cyc}},$$

$$z = 1 \text{ two-stroke,}$$

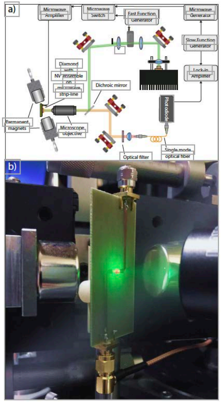
$$z = 1/2 \text{ four-stroke,}$$



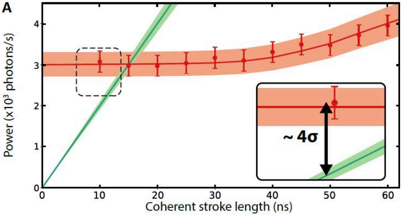
Realization 2017

Experimental demonstration of quantum effects in the operation of microscopic heat engines

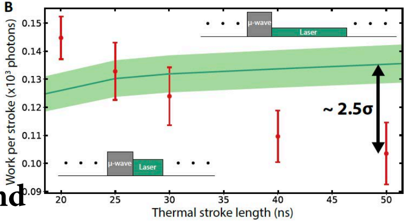
J. Klatzow,[1] C. Weinzetl,[1] P. M. Ledingham,[1] J. N. Becker,[1] D. J. Saunders,[1] J. Nunn,[1] I. A. Walmsley,[1] R. Uzdin,[2] and E. Poem[1,3,*]



NV center in Diamond

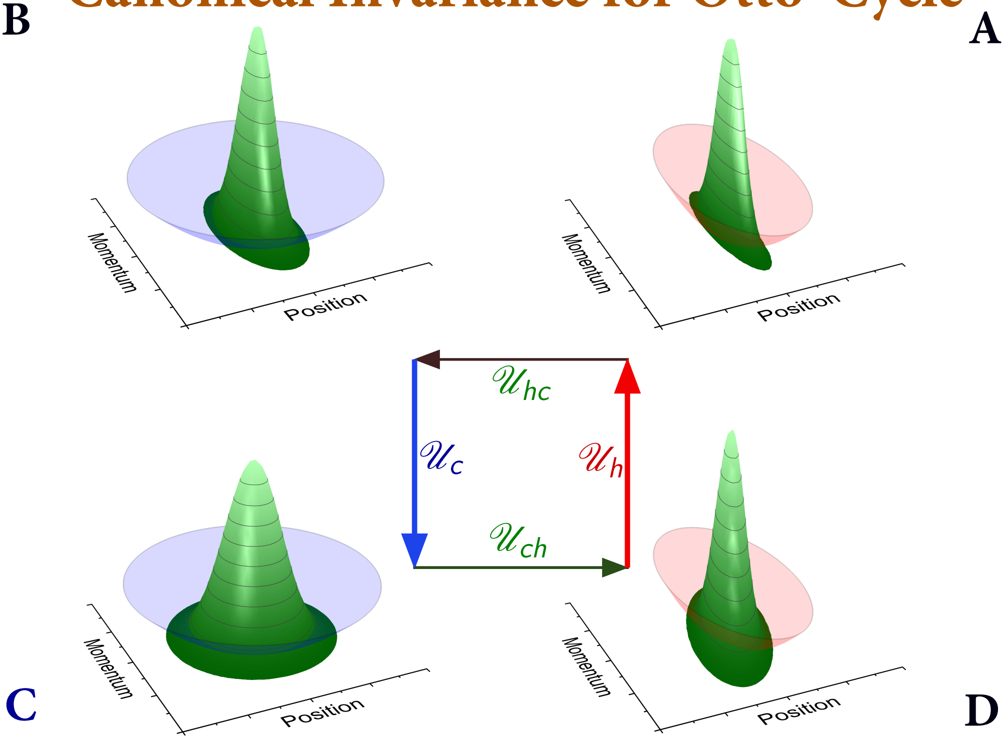


quantum signature



dephasing

Canonical Invariance for Otto Cycle



The end

Thank you