

# Thermodynamic Geometry for Quantum Thermal Machines

Perspectives on Non-Equilibrium Statistical Mechanics:  
The 45<sup>th</sup> Anniversary Symposium of Yamada Science Foundation

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Kay Brandner

School of Physics and Astronomy, University of Nottingham

KB, K. Saito; Phys. Rev. Lett. **124**, 040602 (2020)

J. Eglinton, KB; Phys. Rev. E **105**, L052102 (2022)

J. Eglinton, T. Pyhäranta, K. Saito, KB; New J. Phys. **25** 043014 (2023)



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Nottingham  
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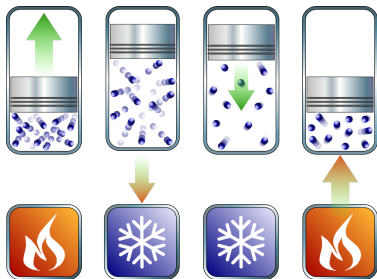
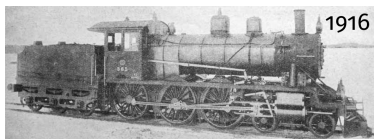
UK Research  
and Innovation

## **From Horsepowers to Zeptowatts**

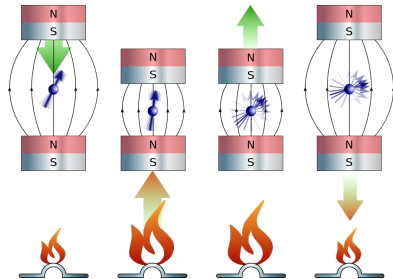
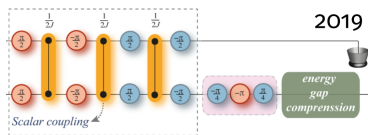
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# From Horsepowers to Zeptowatts

## Macroscopic Engine

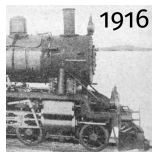


## Microscopic Engine



# From Horsepowers to Zeptowatts

## Macro Engine

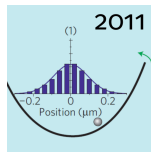


$$d \sim 10^0 \text{m}$$

$$P \sim 10^3 \text{W}$$

$$\eta \simeq 7\% | 0.3\eta_C$$

## Micro Engine



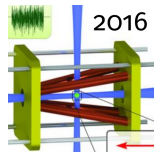
$$d \sim 10^{-6} \text{m}$$

$$P \sim 10^{-22} \text{W}$$

$$\eta \simeq 14\% | 0.9\eta_C$$

➔ V. Blickle, C. Bechinger;  
Nat. Phys. **8**, 143 (2011).

## Pico Engine



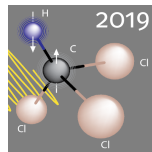
$$d \sim 10^{-10} \text{m}$$

$$P \sim 10^{-22} \text{W}$$

$$\eta \simeq 0.3\% | 0.07\eta_C$$

➔ J. Roßnagel et al.;  
Science **352**, 325 (2016).

## Quantum Engine



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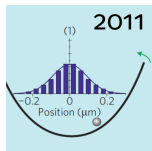
$$P \sim 10^{-28} \text{W}$$

$$\eta \simeq 42\% | 0.5\eta_C$$

➔ J. Peterson et al.;  
PRL **123**, 240601 (2019).

# From Horsepowers to Zeptowatts

## Micro Engine



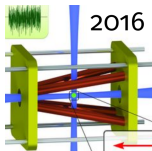
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## Pico Engine



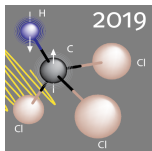
$$d \sim 10^{-10} \text{ m}$$

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➔ J. Roßnagel et al.;  
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## Quantum Engine



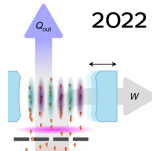
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$$P \sim 10^{-28} \text{ W}$$

$$\eta \simeq 42\% | 0.5\eta_C$$

➔ J. Peterson et al.;  
PRL **123**, 240601 (2019).

## Collective QE



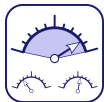
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$$P \sim 10^{-28} \text{ W}$$

$$\eta \simeq 95\% | 0.97\eta_C$$

➔ J. Kim et al.;  
Nat. Phot. **16**, 707 (2022).

## Why going small?



### Fundamental Limits

Are there universal constraints on thermodynamic figures of merit?



### Micro Engineering

Can we systematically develop optimal design and control strategies?



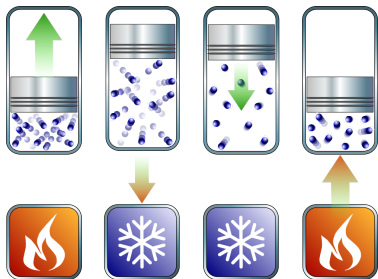
### Quantum World

How can we describe the role of quantum effects and exploit them to improve performance?

# Classical Thermodynamics

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# Classical Thermodynamics

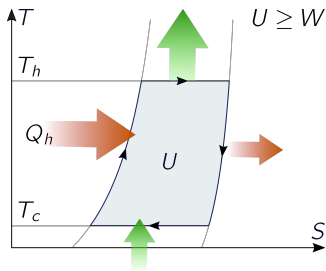
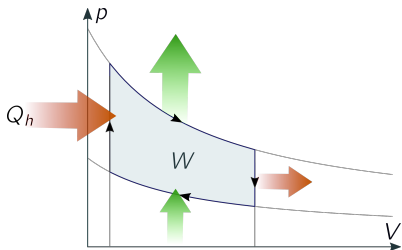


Efficiency:

$$\eta_{\text{th}} \equiv W/Q_h \leq 1 - T_c/T_h \equiv \eta_c$$

Power:

$$P = W/T$$

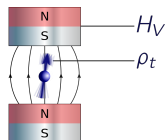




# **Thermodynamic Geometry of Microscopic Heat Engines**

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# Thermodynamic Geometry of Microscopic Heat Engines



Driving protocol:

$$\mathbf{\Lambda} \equiv (T, V) \equiv (\Lambda^u, \Lambda^w)$$

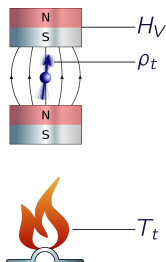
$$\gamma : \mathbf{\Lambda} \mapsto \mathbf{\Lambda}_t$$

Generalized forces:

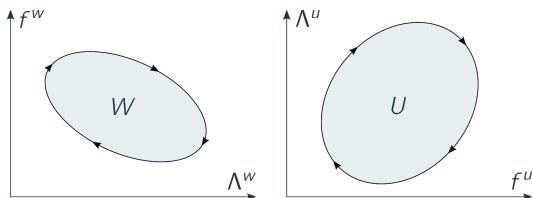
$$f_t^u \equiv S_t \equiv -\text{Tr}[\rho_t \ln \rho_t]$$

$$f_t^w \equiv p_t \equiv -\text{Tr}[\rho_t \partial_{V_t} H_{V_t}]$$

# Thermodynamic Geometry of Microscopic Heat Engines



Generalized  $p - V$  and  $T - S$  diagrams:



Driving protocol:

$$\mathbf{\Lambda} \equiv (T, V) \equiv (\Lambda^u, \Lambda^w)$$

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Generalized forces:

$$f_t^u \equiv S_t \equiv -\text{Tr}[\rho_t \ln \rho_t]$$

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Output and input:

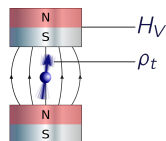
$$W = \oint_{\gamma} p dV = \int_0^{\mathcal{T}} dt f_t^w \dot{\Lambda}_t^w \quad U = \oint_{\gamma} T dS = - \int_0^{\mathcal{T}} dt f_t^u \dot{\Lambda}_t^u$$

Dissipated availability:

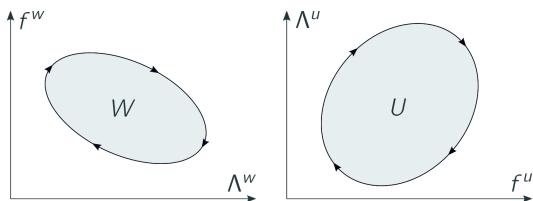
$$A \equiv W - U = \int_0^{\mathcal{T}} dt f_t^w \dot{\Lambda}_t^w = \int_0^{\mathcal{T}} dt T_t \Sigma_t \geq 0$$

$$\Sigma_t \equiv \dot{S}_t - \dot{Q}_t/T_t$$

# Thermodynamic Geometry of Microscopic Heat Engines



Generalized  $p - V$  and  $T - S$  diagrams:



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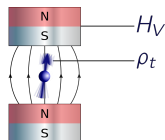
Dissipated availability:

$$A \equiv W - U = \int_0^{\mathcal{T}} dt f_t^\mu \dot{\Lambda}_t^\mu = \int_0^{\mathcal{T}} dt T_t \Sigma_t \geq 0$$

Generalized efficiency:

$$\eta \equiv W/U \leq 1 \quad (\eta \leq \eta_{\text{th}}/\eta_{\text{c}})$$

# Thermodynamic Geometry of Microscopic Heat Engines



Output and input:

$$W = \oint_{\gamma} p dV = \int_0^{\mathcal{T}} dt f_t^w \dot{\Lambda}_t^w \quad U = \oint_{\gamma} T dS = - \int_0^{\mathcal{T}} dt f_t^u \dot{\Lambda}_t^u$$

Generalized efficiency:

$$\eta \equiv W/U \leq 1 \quad (\eta \leq \eta_{\text{th}}/\eta_{\text{C}})$$

Driving protocol:

$$\mathbf{\Lambda} \equiv (T, V) \equiv (\Lambda^u, \Lambda^w)$$

$$\gamma : \mathbf{\Lambda} \mapsto \mathbf{\Lambda}_t$$

**Quasi-static Limit**

$$\rho_t = \rho_{\Lambda_t}$$

$$f_t^{\mu} = \mathcal{F}_{\Lambda_t}^{\mu}$$

$$\eta = \eta_{\text{th}}/\eta_{\text{C}} = 1$$

$$\rho_{\Lambda} \equiv \exp[-(H_V - \mathcal{F}_{\Lambda})/T]$$

$$\mathcal{F}_{\Lambda}^{\mu} \equiv -\partial_{\mu} \mathcal{F}_{\Lambda}$$

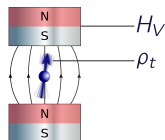
$$P = W/\mathcal{T} = A = 0$$

Generalized forces:

$$f_t^u \equiv S_t \equiv -\text{Tr}[\rho_t \ln \rho_t]$$

$$f_t^w \equiv p_t \equiv -\text{Tr}[\rho_t \partial_{V_t} H_{V_t}]$$

# Thermodynamic Geometry of Microscopic Heat Engines



Driving protocol:

$$\mathbf{\Lambda} \equiv (T, V) \equiv (\Lambda^u, \Lambda^w)$$

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## Adiabatic Response

$$f_t^\mu \equiv \mathcal{F}_{\Lambda_t}^\mu + R_{\Lambda_t}^{\mu\nu} \dot{\Lambda}_t^\nu \quad P \equiv \mathcal{W}/\mathcal{T} \quad \eta \equiv 1 - A/\mathcal{W}$$

Geometric work and dissipated availability:

$$\mathcal{W} \equiv \oint_\gamma \mathcal{A}_\Lambda^\mu d\Lambda^\mu \quad \mathcal{A}_\Lambda^\mu \equiv \partial_\mu \mathcal{F}_\Lambda^w \Lambda^w$$

$$A \equiv \int_0^{\mathcal{T}} dt g_{\Lambda_t}^{\mu\nu} \dot{\Lambda}_t^\mu \dot{\Lambda}_t^\nu \geq 0 \quad g_{\Lambda}^{\mu\nu} \equiv -(R_{\Lambda}^{\mu\nu} + R_{\Lambda}^{\nu\mu})/2 \succeq 0$$

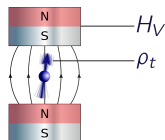
Thermodynamic length:

$$A \geq \mathcal{L}^2/\mathcal{T} \quad \mathcal{L} \equiv \oint_\gamma \sqrt{g_{\Lambda}^{\mu\nu} d\Lambda^\mu d\Lambda^\nu}$$

Trade-off relation between power and efficiency:

$$(1 - \eta)(\mathcal{W}/\mathcal{L})^2 \geq P$$

# Thermodynamic Geometry of Microscopic Heat Engines



Driving protocol:

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**Adiabatic Response**

$$f_t^\mu \equiv \mathcal{F}_{\Lambda_t}^\mu + R_{\Lambda_t}^{\mu\nu} \dot{\Lambda}_t^\nu \quad P \equiv \mathcal{W}/\mathcal{T} \quad \eta \equiv 1 - A/\mathcal{W}$$

Geometric work and thermodynamic length:

$$\mathcal{W} \equiv \oint_\gamma \mathcal{A}_\Lambda^\mu d\Lambda^\mu \quad \mathcal{A}_\Lambda^\mu \equiv \partial_\mu \mathcal{F}_\Lambda^w \Lambda^w$$

$$A \equiv \int_0^{\mathcal{T}} dt g_{\Lambda_t}^{\mu\nu} \dot{\Lambda}_t^\mu \dot{\Lambda}_t^\nu \geq \mathcal{L}^2/\mathcal{T} \quad \mathcal{L} \equiv \oint_\gamma \sqrt{g_{\Lambda}^{\mu\nu} d\Lambda^\mu d\Lambda^\nu}$$

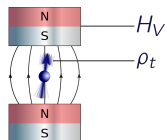
Optimization principle:

$$t \rightarrow \phi_t \quad t \equiv \mathcal{T} \int_0^{\phi_t} ds \sqrt{g_{\Lambda_s}^{\mu\nu} \dot{\Lambda}_s^\mu \dot{\Lambda}_s^\nu} / \mathcal{L}$$

Optimal efficiency:

$$(1 - \eta^*)(\mathcal{W}/\mathcal{L})^2 = P \quad \eta^* = 1 - \mathcal{L}^2/\mathcal{W}\mathcal{T}$$

# Thermodynamic Geometry of Microscopic Heat Engines



Driving protocol:

$$\mathbf{\Lambda} \equiv (T, V) \equiv (\Lambda^u, \Lambda^w)$$

$$\gamma : \mathbf{\Lambda} \mapsto \mathbf{\Lambda}_t$$

Generalized forces:

$$f_t^u \equiv S_t \equiv -\text{Tr}[\rho_t \ln \rho_t]$$

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**Adiabatic Response**

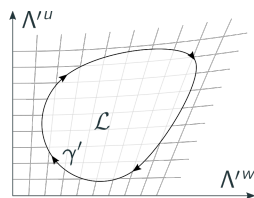
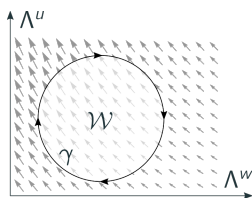
$$f_t^\mu \equiv \mathcal{F}_{\Lambda_t}^\mu + R_{\Lambda_t}^{\mu\nu} \dot{\Lambda}_t^\nu \quad P \equiv \mathcal{W}/\mathcal{T} \quad \eta \equiv 1 - A/\mathcal{W}$$

Geometric work and thermodynamic length:

$$\mathcal{W} \equiv \oint_\gamma \mathcal{A}_\Lambda^\mu d\Lambda^\mu \quad \mathcal{A}_\Lambda^\mu \equiv \partial_\mu \mathcal{F}_\Lambda^w \Lambda^w$$

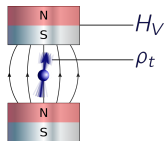
$$A \equiv \int_0^{\mathcal{T}} dt g_{\Lambda_t}^{\mu\nu} \dot{\Lambda}_t^\mu \dot{\Lambda}_t^\nu \geq \mathcal{L}^2/\mathcal{T} \quad \mathcal{L} \equiv \oint_\gamma \sqrt{g_{\Lambda}^{\mu\nu}} d\Lambda^\mu d\Lambda^\nu$$

Graphical interpretation:





# Example: Two-Level Engine



Driving protocols:

$$T_t = \hbar\Omega(1 + \sin^2[\pi\Omega t])$$

$$V_t = 1 + \sin^2[\pi\Omega t + \pi/4]$$

Hamiltonian:

$$H_V = -\frac{\hbar\Omega}{2}(\varepsilon\sigma_x + \Delta_V\sigma_z)$$

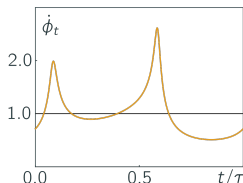
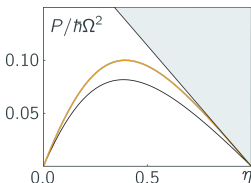
$$\Delta_V \equiv \sqrt{V^2 - \varepsilon^2}$$

Dynamics:

$$\dot{\rho}_t = -\frac{i}{\hbar}[H_{V_t}, \rho_t] + \sum_{\sigma=\pm} \left( [L_{\Lambda_t}^{\sigma} \rho_t, L_{\Lambda_t}^{\sigma\dagger}] + [L_{\Lambda_t}^{\sigma}, \rho_t L_{\Lambda_t}^{\sigma\dagger}] \right)$$

$$[H_V, L_{\Lambda}^{\pm}] = \pm\hbar\Omega V L_{\Lambda}^{\pm} \quad \text{Tr}[L_{\Lambda}^{\pm} L_{\Lambda}^{\pm\dagger}] = \frac{\pm\Gamma\Omega V}{1 - \exp[\mp\hbar\Omega V/T]}$$

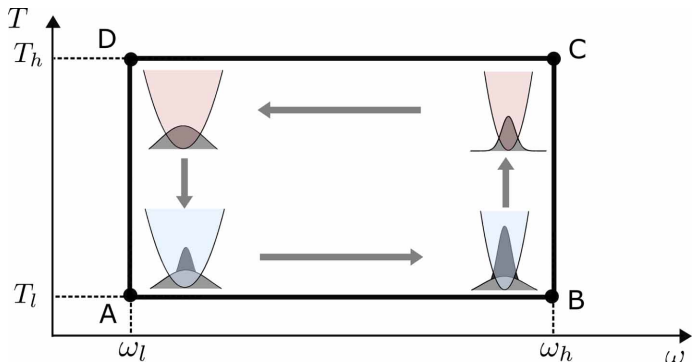
Results:



$$(1 - \eta)(W/L)^2 \geq P \quad t = \mathcal{T} \int_0^{\phi_t} ds \sqrt{g_{\Lambda_s}^{\mu\nu} \dot{\Lambda}_s^{\mu} \dot{\Lambda}_s^{\nu}} / \mathcal{L}$$

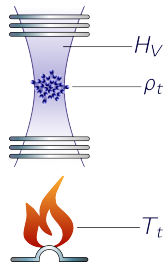
# **Thermodynamic Geometry of Many-Body Quantum Engines**

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➔ N. M. Myers, F. J. Peña, O. Negrete, P. Vargas, G. D. Chiara, S. Deffner; *New J. Phys.* **24**, 025001 (2022).

# Thermodynamic Geometry of Many-Body Quantum Engines



## Grand Canonical Adiabatic Response

$$\hat{f}_t^\mu = \hat{\mathcal{F}}_{\Lambda_t}^\mu + \hat{R}_{\Lambda_t}^{\mu\nu} \dot{\lambda}_t^\nu \quad \hat{\mathcal{F}}_{\Lambda}^\mu = -\partial_\mu \Phi_{\Lambda}$$

Fix  $\Lambda_t^z = \mu_t$  by fixing mean particle number:

$$\mathcal{N}_t = \hat{f}_t^z = \hat{\mathcal{F}}_{\Lambda_t}^z + \hat{R}_{\Lambda_t}^{z\nu} \dot{\lambda}_t^\nu \stackrel{!}{=} N$$

$$\Lambda_t^z = \Lambda_{\lambda_t}^{z0} + \Lambda_{\lambda_t}^{za} \dot{\lambda}_t^a \quad \lambda \equiv (T, V) \equiv (\lambda^u, \lambda^w)$$

Driving protocol:

$$\Lambda \equiv (T, V, \mu) \\ \equiv (\Lambda^u, \Lambda^w, \Lambda^z)$$

$$\gamma : \Lambda \mapsto \Lambda_t$$

Generalized forces:

$$\hat{f}_t^u \equiv S_t = -\text{Tr}[\rho_t \ln \rho_t]$$

$$\hat{f}_t^w \equiv p_t = -\text{Tr}[\rho_t \partial_{V_t} H_{V_t}]$$

$$\hat{f}_t^z \equiv \mathcal{N}_t = \text{Tr}[\rho_t N_t]$$

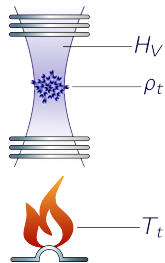
## Effective Canonical Adiabatic Response

$$f_t^a = \mathcal{F}_{\lambda_t}^a + R_{\lambda_t}^{ab} \dot{\lambda}_t^b \quad a, b = u, w$$

$$g_{\lambda}^{ab} \equiv -(R_{\lambda}^{ab} + R_{\lambda}^{ba})/2 \succeq 0$$

Optimal efficiency:

$$(1 - \eta^*)(\mathcal{W}/\mathcal{L})^2 \equiv (1 - \eta^*)\Psi = P \quad \eta^* = 1 - \mathcal{L}^2/\mathcal{W}\mathcal{T}$$



Driving protocol:

$$\lambda \equiv (T, \omega) \equiv (\lambda^u, \lambda^w)$$

$$\gamma : \Lambda \mapsto \Lambda_t$$

Generalized forces:

$$f_t^u \equiv S_t = -\text{Tr}[\rho_t \ln \rho_t]$$

$$f_t^w \equiv p_t = -\text{Tr}[\rho_t \partial_{\omega_t} H_{\omega_t}]$$

Hamiltonian

$$H_{\omega} = \sum_{\mathbf{n}} E_{\mathbf{n}} A_{\mathbf{n}}^{\dagger} A_{\mathbf{n}} \quad \mathbf{n} = (n_x, n_y) \quad E_{\mathbf{n}} = \hbar\omega(n_x + n_y + 1)$$

Dynamics:

$$\begin{aligned} \dot{\rho}_t = -\frac{i}{\hbar} [H, \rho_t] + \kappa \sum_{\mathbf{n}} (n_{\mathbf{n}} + 1) & \left( A_{\mathbf{n}} \rho_t A_{\mathbf{n}}^{\dagger} - \frac{1}{2} \{ \rho_t, A_{\mathbf{n}}^{\dagger} A_{\mathbf{n}} \} \right) \\ & + n_{\mathbf{n}} \left( A_{\mathbf{n}}^{\dagger} \rho_t A_{\mathbf{n}} - \frac{1}{2} \{ \rho_t, A_{\mathbf{n}} A_{\mathbf{n}}^{\dagger} \} \right) \end{aligned}$$

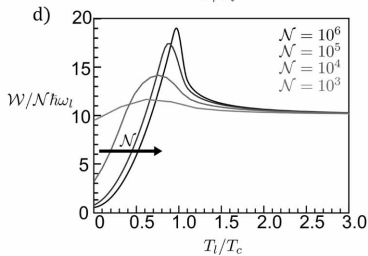
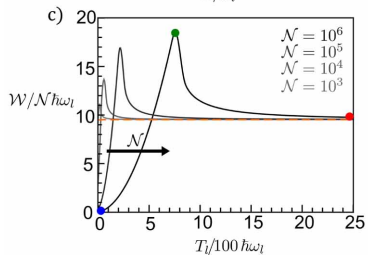
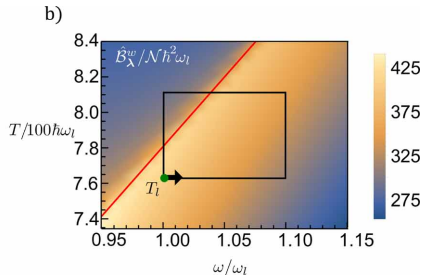
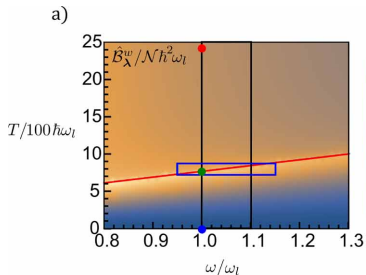
Thermodynamic quantities:

$$\mathcal{W} = \oint_{\gamma} \mathcal{A}_{\lambda}^a d\lambda^a \equiv \iint_{\Gamma} \mathcal{B}_{\lambda}^w d\lambda^u d\lambda^w$$

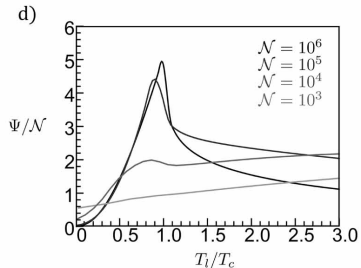
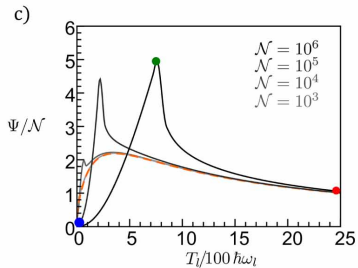
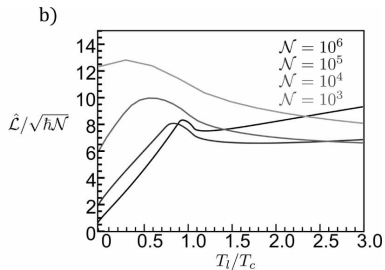
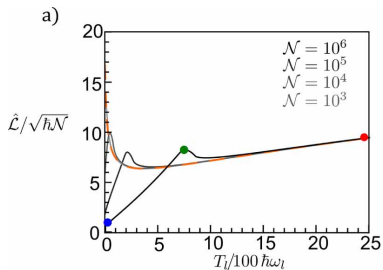
$$\mathcal{L} = \oint_{\gamma} \sqrt{g_{\lambda}^{ab} d\lambda^a d\lambda^b}$$

$$\Psi \equiv (\mathcal{W}/\mathcal{L})^2$$

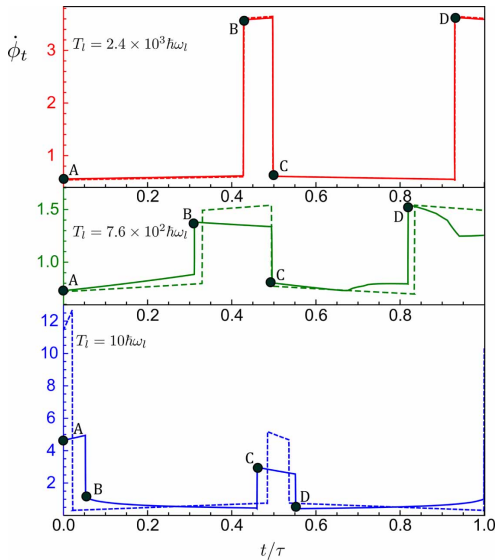
# BEC Engine Revisited: Geometric Work



# BEC Engine Revisited: Thermodynamic Length



# BEC Engine Revisited: Optimal Speed Function

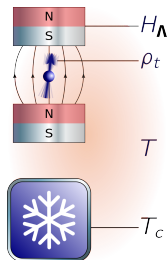




## **Thermodynamic Geometry of Microscopic Refrigerators**

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# Thermodynamic Geometry of Microscopic Refrigerators



Output and input:

$$Q = \int_0^{\mathcal{T}} dt j_t \quad W = - \oint_{\gamma} p^{\alpha} d\Lambda^{\alpha} = - \int_0^{\mathcal{T}} dt f_t^{\alpha} \dot{\Lambda}_t^{\alpha}$$

Efficiency:

$$\varepsilon \equiv Q/W \leq \varepsilon_C \equiv T_c/(T - T_c)$$

Driving:

$$\mathbf{\Lambda} \equiv (\Lambda^1, \Lambda^2)$$

$$\gamma : \mathbf{\Lambda} \mapsto \mathbf{\Lambda}_t$$

$$F_q \equiv 1/T - 1/T_c$$

Generalized forces:

$$j_t \equiv \text{Tr}[\dot{\rho}_t H_{\Lambda_t}]$$

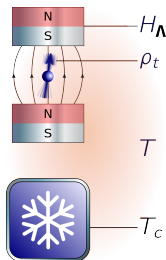
$$f_t^{\alpha} \equiv p_t^{\alpha} \equiv -\text{Tr}[\rho_t \partial_{\Lambda_t^{\alpha}} H_{\Lambda_t}]$$

**Adiabatic Response**

$$j_t = R_{\Lambda_t}^{qq} F_q + R_{\Lambda_t}^{q\alpha} \dot{\Lambda}_t^{\alpha} / T + R_{\Lambda_t}^{qq\alpha} \dot{\Lambda}_t^{\alpha} F / T$$

$$f_t^{\alpha} = \mathcal{F}_{\Lambda_t}^{\alpha} - R_{\Lambda_t}^{\alpha q} F_q - R_{\Lambda_t}^{\alpha\beta} \dot{\Lambda}_t^{\beta} / T - R_{\Lambda_t}^{\mu qq} F_q^2$$

# Thermodynamic Geometry of Microscopic Refrigerators



## Adiabatic Response

$$j_t = R_{\Lambda_t}^{qq} F_q + R_{\Lambda_t}^{q\alpha} \dot{\Lambda}_t^\alpha / T + R_{\Lambda_t}^{qq\alpha} \dot{\Lambda}_t^\alpha F / T$$

$$f_t^\alpha = \mathcal{F}_{\Lambda_t}^\alpha - R_{\Lambda_t}^{\alpha q} F_q - R_{\Lambda_t}^{\alpha\beta} \dot{\Lambda}_t^\beta / T - R_{\Lambda_t}^{\mu qq} F_q^2$$

Power-efficiency trade-off relation ( $R_{\Lambda}^{qq} = 0$ ):

$$\mathcal{Z}(\varepsilon_c - \varepsilon)^2 / \varepsilon_c^2 \geq J_q \equiv Q/T$$

Driving:

$$\Lambda \equiv (\Lambda^1, \Lambda^2)$$

$$\gamma : \Lambda \mapsto \Lambda_t$$

$$F_q \equiv 1/T - 1/T_c$$

Generalized forces:

$$j_t \equiv \text{Tr}[\dot{\rho}_t H_{\Lambda_t}]$$

$$f_t^\alpha \equiv \rho_t^\alpha \equiv -\text{Tr}[\rho_t \partial_{\Lambda_t^\alpha} H_{\Lambda_t}]$$

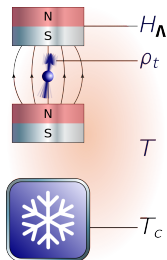
Optimization principle:

$$t = \mathcal{T} \int_0^{\phi_t} ds \sqrt{g_{\Lambda_s}^{\alpha\beta} \dot{\Lambda}_s^\alpha \dot{\Lambda}_s^\beta} / \mathcal{L} \quad A_q = -\sqrt{z/T}$$

$$\mathcal{Z} \equiv L_{qw}^3 / 4(L_{wq}^q + L_{qw}^q) \mathcal{L}^2 \quad z \equiv \mathcal{L}^2 / (L_{wq}^q + L_{qw}^q) \mathcal{T}$$

$$\begin{bmatrix} L_{wq} & L_{qw} \\ L_{wq}^q & L_{qw}^q \end{bmatrix} = - \oint_\gamma \Lambda^\beta \partial_\alpha \begin{bmatrix} R_{\Lambda}^{\beta q} & R_{\Lambda}^{q\beta} \\ R_{\Lambda}^{\beta qq} & R_{\Lambda}^{qq\beta} \end{bmatrix} d\Lambda^\alpha$$

# Thermodynamic Geometry of Microscopic Refrigerators



## Adiabatic Response

$$j_t = R_{\Lambda_t}^{qq} F_q + R_{\Lambda_t}^{q\alpha} \dot{\Lambda}_t^\alpha / T + R_{\Lambda_t}^{qq\alpha} \dot{\Lambda}_t^\alpha F / T$$

$$f_t^\alpha = \mathcal{F}_{\Lambda_t}^\alpha - R_{\Lambda_t}^{\alpha q} F_q - R_{\Lambda_t}^{\alpha\beta} \dot{\Lambda}_t^\beta / T - R_{\Lambda_t}^{\mu qq} F_q^2$$

Power-efficiency trade-off relation ( $R_{\Lambda}^{qq} = 0$ ):

$$\mathcal{Z}(\varepsilon_c - \varepsilon)^2 / \varepsilon_c^2 \geq J_q \equiv Q / \mathcal{T}$$

Driving:

$$\Lambda \equiv (\Lambda^1, \Lambda^2)$$

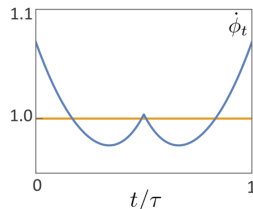
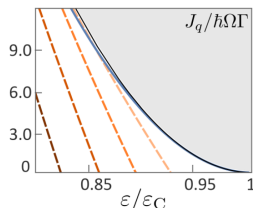
$$\gamma : \Lambda \mapsto \Lambda_t$$

$$F_q \equiv 1/T - 1/T_c$$

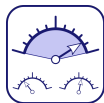
Generalized forces:

$$j_t \equiv \text{Tr}[\dot{\rho}_t H_{\Lambda_t}]$$

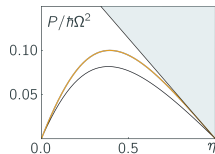
$$f_t^\alpha \equiv p_t^\alpha \equiv -\text{Tr}[\rho_t \partial_{\Lambda_t^\alpha} H_{\Lambda_t}]$$



## Why going small?



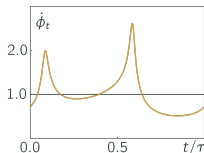
### Fundamental Limits



Power-efficiency  
trade-off



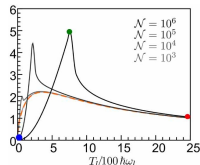
### Micro Engineering



Optimal speed  
functions



### Quantum World



BEC-enhanced  
performance