

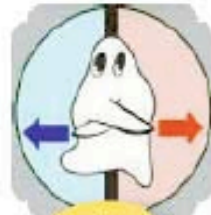




# Optimization At a Small Scale

UCSD • July 20-21 • 2009

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## Sponsors

European Science Foundation

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UCSD funds: Kurt Shuler, Misha Galperin,

Katja Lindenberg

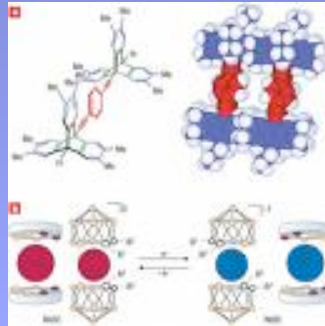
Patricia Edwins



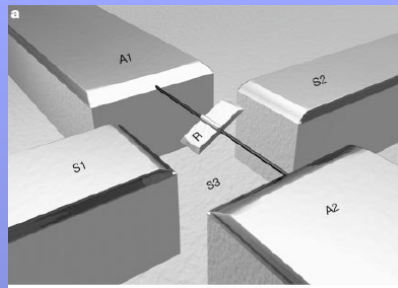


# Exploring The Physics of Small Devices

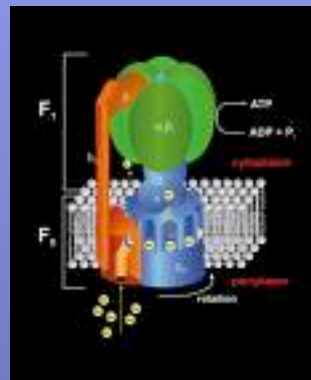
- Chemical



- Physical



- Bio-physical



Austria

Belgium Flemish

Belgium Walloon

Czech Republic

Finland

Germany

Ireland

Norway

Spain

Sweden

Switzerland

C. Dellago

C. Van den Broeck

P. Gaspard

E. Hulcius

J. Pekola

U. Seifert

J. Gleeson

A. Hansen

JMR Parrondo

Hongqi Xu

MO Hongler

Tuesday night 6:30



El Torito (Mexican Restaurant)



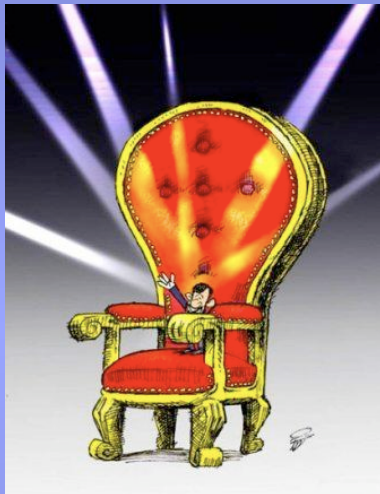
Marriott  
Residence  
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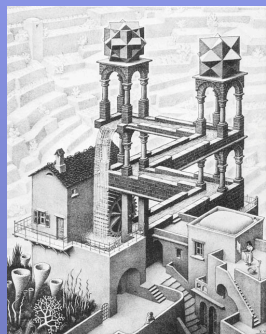
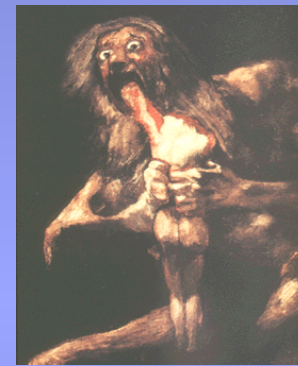
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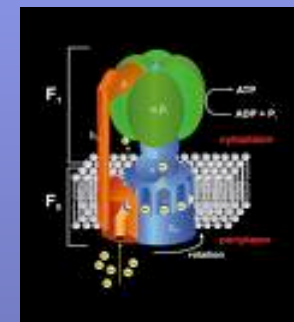
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# Universality of Efficiency At Maximum Power

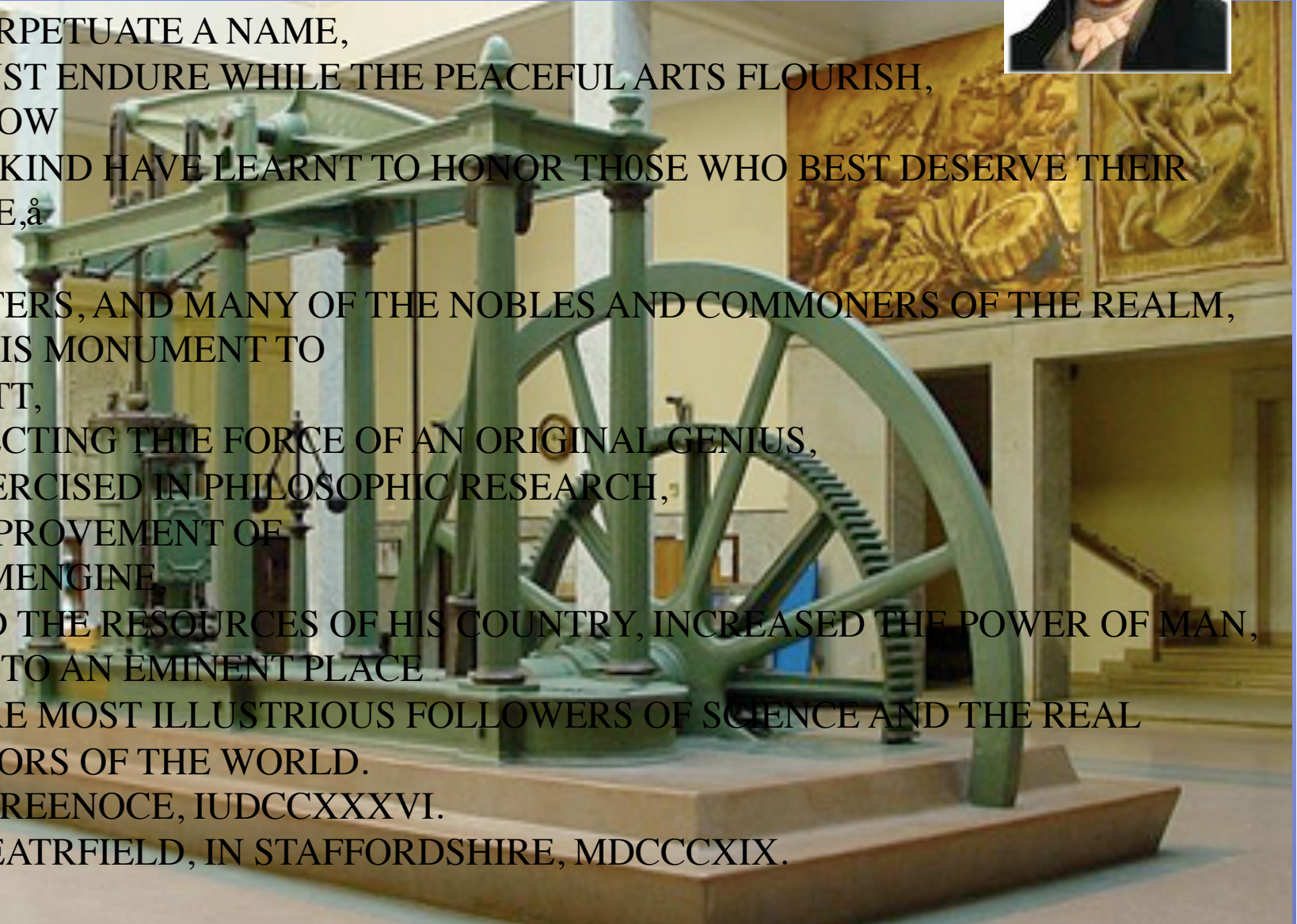


**Christian Van den Broeck**  
Universiteit Hasselt  
christian.vandenbroeck@uhasselt.be

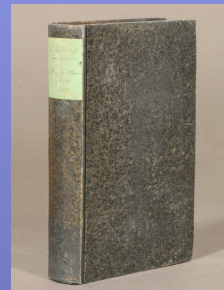
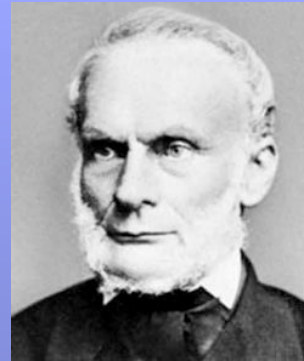
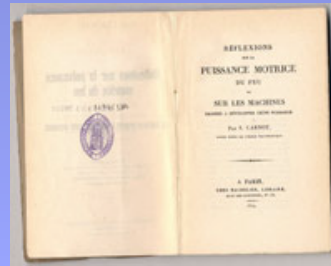
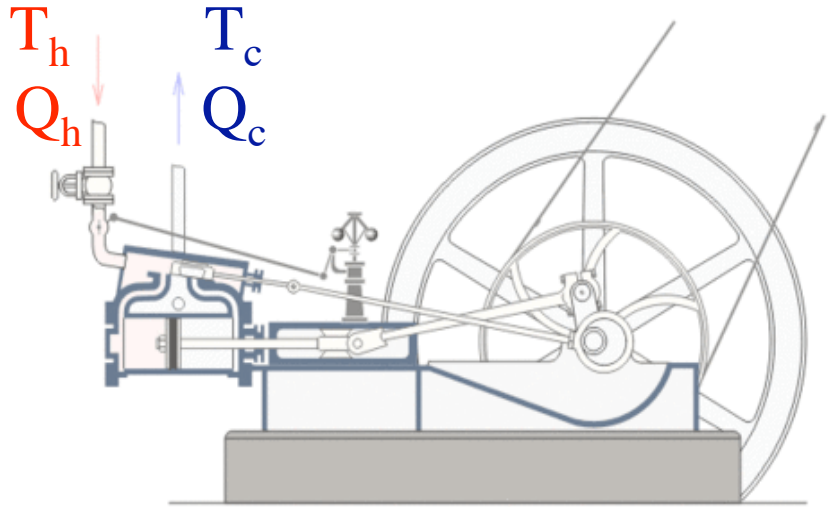




NOT TO PERPETUATE A NAME,  
WHICH MUST ENDURE WHILE THE PEACEFUL ARTS FLOURISH,  
BUT TO SHOW  
THAT MANKIND HAVE LEARNT TO HONOR THOSE WHO BEST DESERVE THEIR  
GRATITUDE, &  
THE KING  
HIS MINISTERS, AND MANY OF THE NOBLES AND COMMONERS OF THE REALM,  
RAISED THIS MONUMENT TO  
JAMES WATT,  
WHO, DIRECTING THE FORCE OF AN ORIGINAL GENIUS,  
EARLY EXERCISED IN PHILOSOPHIC RESEARCH,  
TO THE IMPROVEMENT OF  
THE STEAMENGINE,  
ENLARGED THE RESOURCES OF HIS COUNTRY, INCREASED THE POWER OF MAN,  
AND ROSE TO AN EMINENT PLACE  
AMONG THE MOST ILLUSTRIOUS FOLLOWERS OF SCIENCE AND THE REAL  
BENEFACTORS OF THE WORLD.  
BORN AT GREENOCE, IUDCCXXXVI.  
DIED AT BEATRFIELD, IN STAFFORDSHIRE, MDCCCXIX.







$$\frac{W}{Q_h} \leq \eta_c$$

$$\eta_c = 1 - \frac{T_c}{T_h}$$

$$W = Q_h - Q_c$$

$$\Delta S = \frac{Q_h}{T_h} + \frac{Q_c}{T_c} \geq 0$$

$$\Delta S = \int_{rev} \frac{dQ}{T} \geq 0$$

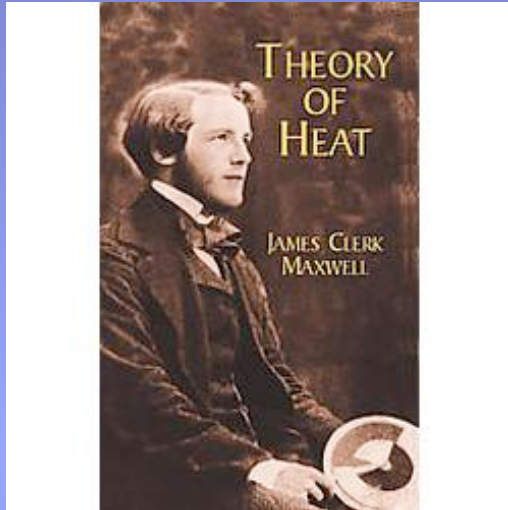
Réflexions sur la puissance motrice du feu et sur les machines propres à développer cette puissance.

## Second law

Equality Sign:  
Reversible Process

Ueber die bewegende Kraft der Wärme und die Gesetze, welche sich daraus für die Wärme selbst ableiten lassen

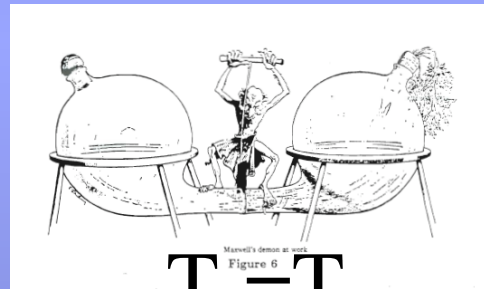
# Exceed Carnot at Small Scale?



$$\eta = \frac{W}{Q_h} \leq 1 - \frac{T_c}{T_h}$$



Yes?

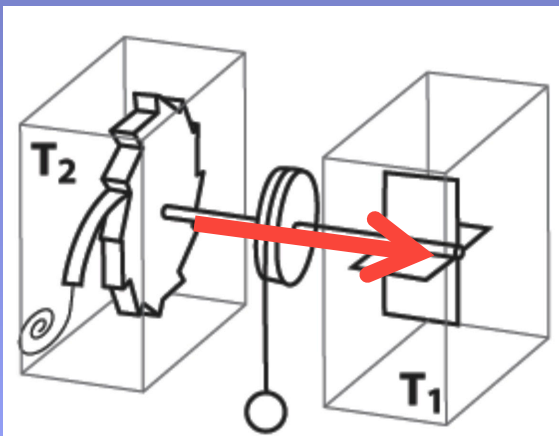


$$T_c = T_h$$

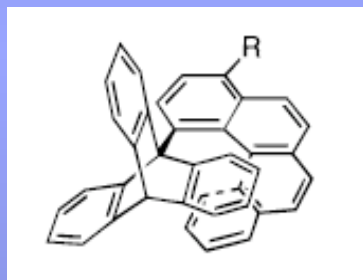
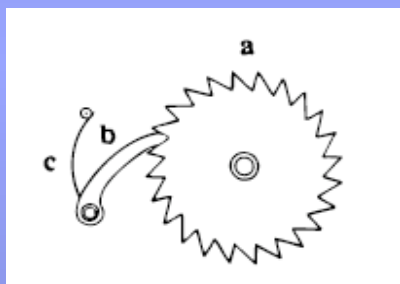
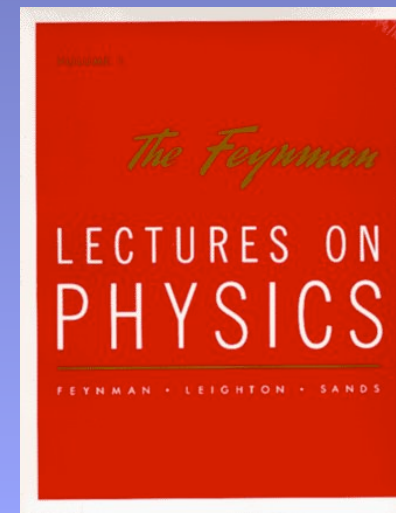
No!



Erase 1 bit:  $\Delta S = k_B \ln 2$



$$\eta = \frac{W}{Q_h} \leq 1 - \frac{T_c}{T_h}$$



*J. Org. Chem.* **1998**, *63*, 3655–3665

**New Molecular Devices: In Search of a Molecular Ratchet**

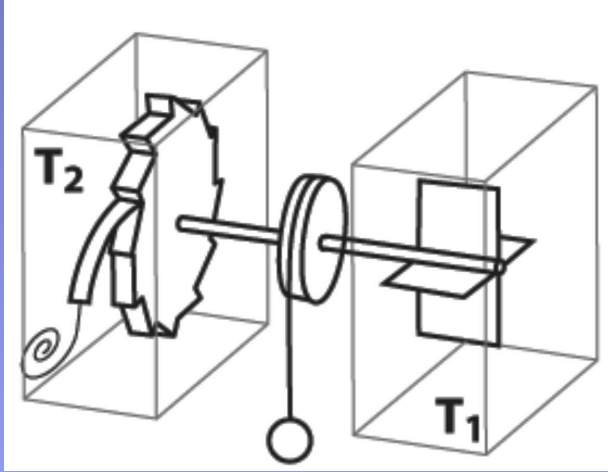
T. Ross Kelly,\* José Pérez Sestelo,† and Imanol Tellitu‡

**Irreversible  
Heat Flux**



**Below Carnot at  
Small Scale?  
Under Steady State  
Conditions?**

J. Parrondo P. Espagnol, *Am J Phys* **64**, 1125 (1996)  
C. Van den Broeck, R. Kawai, and P. Meurs,  
*PRL*.**93**, 090601 (2004)



Thermal  $X_1 = \Delta T/T^2$     Mechanical  $X_2 = F/T$   
 Heat flux  $J_1$                       Rotation Speed  $J_2$

$$J_1 = L_{11}X_1 + L_{12}X_2$$

$$J_2 = L_{21}X_1 + L_{22}X_2.$$



$$L_{11} \geq 0 \quad L_{22} \geq 0$$

$$L_{11}L_{22} - L_{12}L_{21} \geq 0.$$

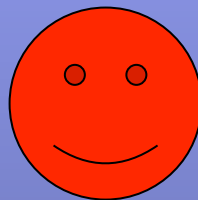
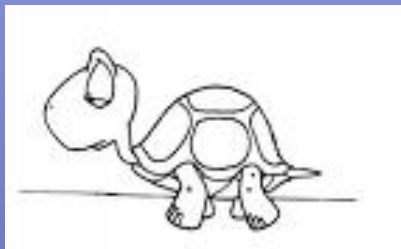
$$d_i S/dt = J_1 X_1 + J_2 X_2 \geq 0.$$

## Carnot efficiency?

C. Van den Broeck, Adv Chem Phys  
 135, 189 (2007)

**Reversible:  $d_i S/dt=0$  hence  $\eta=\eta_c$ . If  $J_1=J_2=0$  for  $X_1$  and  $X_2$  nonzero.  
 Only possible if determinant of matrix  $L$  is zero:  $L_{11}L_{22}=(L_{12})^2$**

## Carnot efficiency



Architectural constraint of strong  
 coupling  $J_2/J_1 = L_{21}/L_{11}$  .

$$L_{11}L_{22}=(L_{12})^2$$

# Thermodynamic efficiency at maximum power

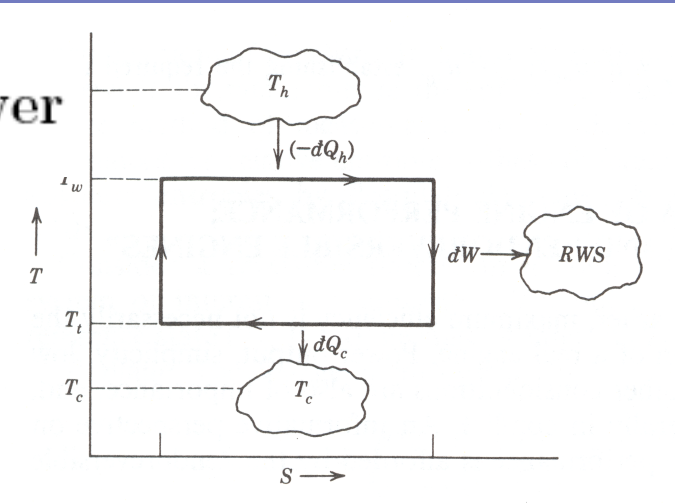
**FL Curzon B Ahlborn**

Am. J. Phys. 43, 22 (1975)

## Efficiency at maximum power

$$\eta = \frac{W}{Q_h} \quad \begin{array}{l} \text{endoreversible} \\ \text{approximation} \end{array} = 1 - \sqrt{\frac{T_c}{T_h}}$$

$$1 - \eta_C = \frac{T_c}{T_h}$$



Plant	$T_h$ (K)	$T_c$ (K)	$\eta_{obs}$	$\eta_{CA}$	$\eta_{opt}$	$\eta_{opt} (I = 0.8-0.9)$
Doel 4 (nuclear PWR, Belgium) <sup>a</sup>	566	283	0.350	0.293	0.405	0.297-0.357
Almaraz II (nuclear PWR, Spain) <sup>b</sup>	600	290	0.345	0.305	0.420	0.315-0.373
Sizewell B (nuclear PWR, UK) <sup>c</sup>	581	288	0.363	0.296	0.410	0.302-0.361
Cofrentes (nuclear BWR, Spain) <sup>b</sup>	562	289	0.340	0.283	0.393	0.282-0.343
Heysham (nuclear AGR, UK) <sup>c</sup>	727	288	0.4	0.371	0.501	0.410-0.460

Exact in linear approx. for :  $L_{11}L_{22}=(L_{12})^2$   
 C. Van den Broeck, Phys Rev Lett 95,  
 190602 (2005)

$$\eta = \eta_C / 2 + \eta_C^2 / 8 + 6\eta_C^3 / 96$$

Thermal  $X_1 = \Delta T / T^2$

Heat flux  $J_1$

Mechanical  $X_2 = F / T$

Motion  $J_2$

$$\eta = \frac{W}{Q} = \frac{\dot{W}}{\dot{Q}} = -\frac{FJ_2}{J_1} = -\frac{\Delta T}{T} \frac{X_2 J_2}{X_1 J_1} = -\eta_C \frac{X_2 J_2}{X_1 J_1}$$

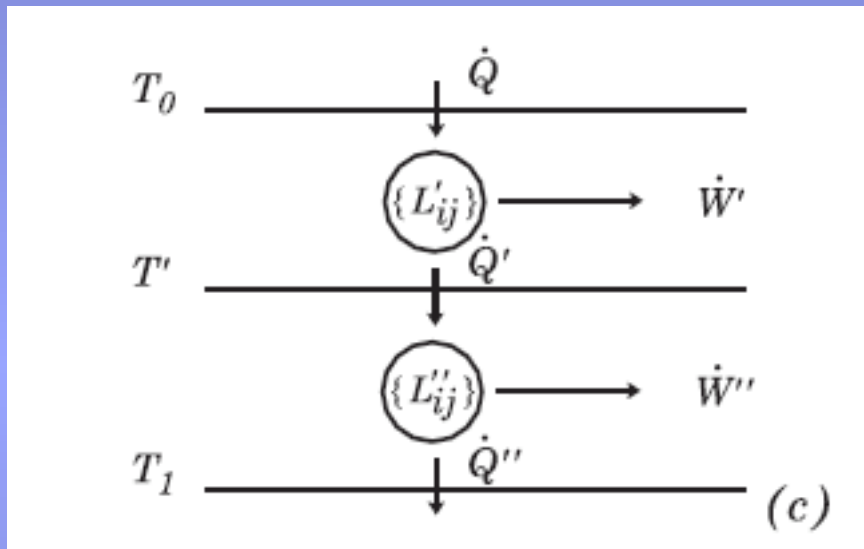
$$\stackrel{\text{strong}}{=} -\eta_C \frac{X_2 L_{21}}{X_1 L_{11}} \stackrel{\text{max power}}{=} \frac{1}{2} \eta_C$$

$$\stackrel{\text{max power}}{?} X_2 (L_{21} X_1 + L_{22} X_2) \stackrel{\text{max for}}{=} \frac{X_2}{X_1} = -\frac{L_{21}}{2L_{22}}$$

# Concatination property

suppose *efficiency*  $\eta = \frac{\dot{W}}{\dot{Q}} = \eta\left(\frac{T_1}{T_0}\right)$

is unchanged upon inserting heat bath



$$\eta\left(\frac{T_1}{T_0}\right) = \frac{\dot{W}' + \dot{W}''}{\dot{Q}} = \frac{\eta\left(\frac{T'}{T_0}\right)\dot{Q} + \eta\left(\frac{T_1}{T'}\right)\dot{Q}'}{\dot{Q}}$$

$$= \frac{\eta\left(\frac{T'}{T_0}\right)\dot{Q} + \eta\left(\frac{T_1}{T'}\right)(\dot{Q} - \eta\left(\frac{T'}{T_0}\right)\dot{Q})}{\dot{Q}}$$

$$t = \frac{T_1}{T_0} \quad x = \frac{T_1}{T'}$$

$$\eta(t) = \eta(t/x) + \eta(x)(1 - \eta(t/x)) \quad \forall x \quad T_0/T_1 < x < 1$$

implies:

$$\Rightarrow \eta(t) = 1 - t^\alpha$$

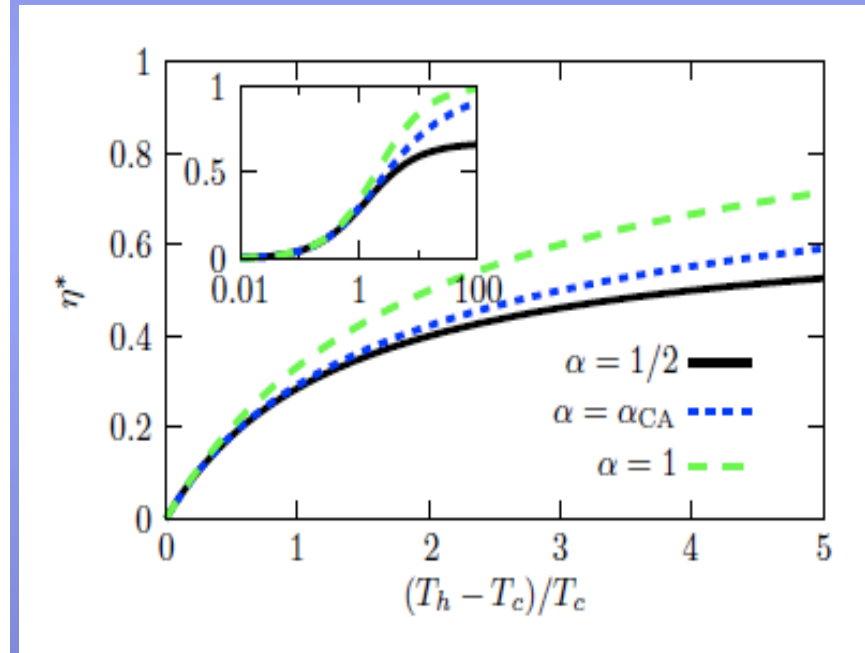
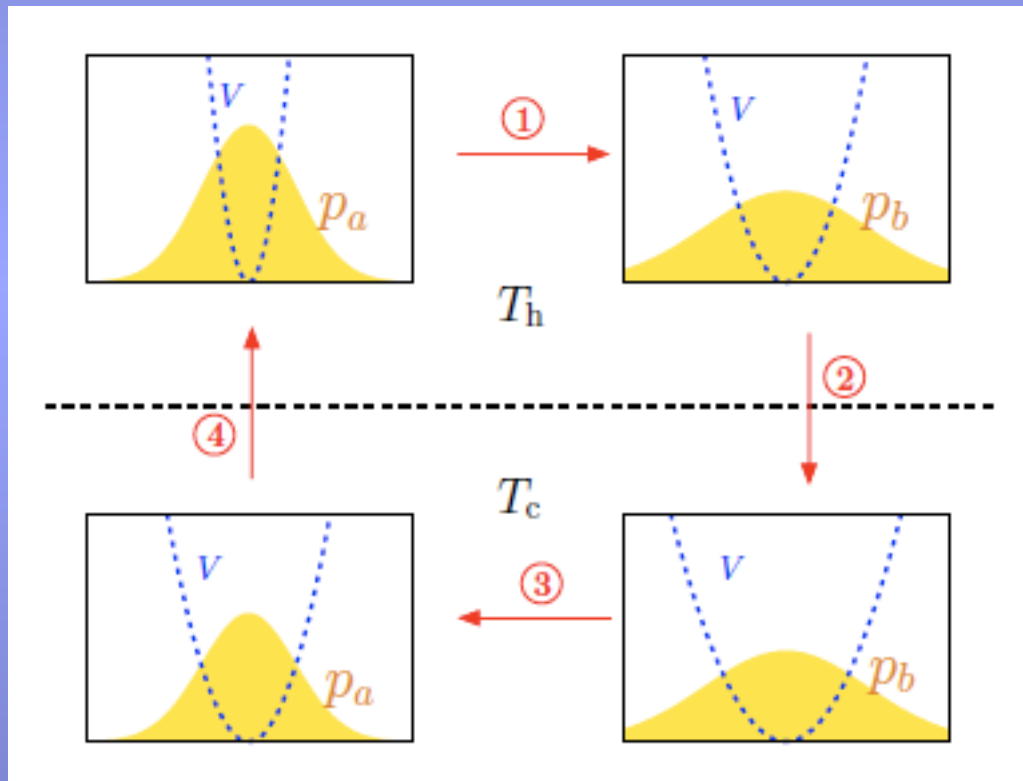
$\alpha = 1$     *Carnot*

$\alpha = 1/2$     *Curzon Ahlborn*

# Carnot Cycle for Brownian particle

$$\eta = \eta_C / 2 + \eta_C^2 / 8 + 3\eta_C^3 / 96$$

T. Schmiedl U. Seifert, EPL 81, 20003 (2008)



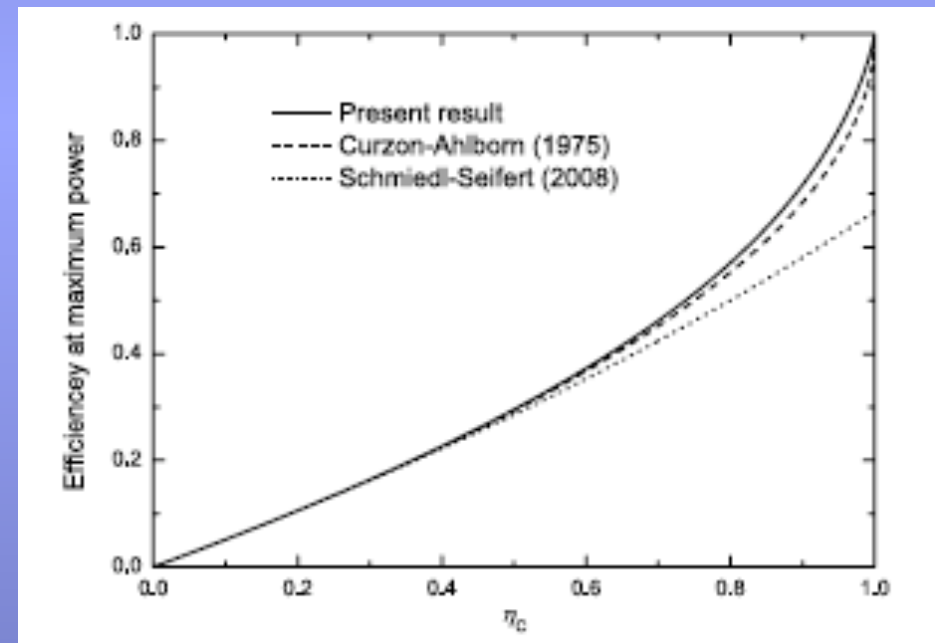
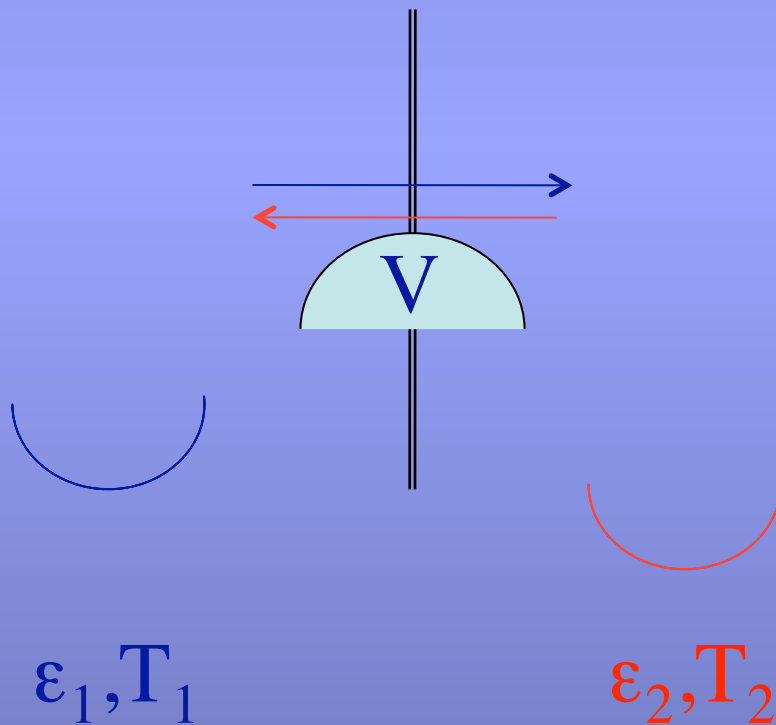
# Thermal Engine via Kramer's Escape

$$\eta = \eta_c / 2 + \eta_c^2 / 8 + 7\eta_c^3 / 96$$

Z.C. Tu, J Phys 41, 312003 (2008)

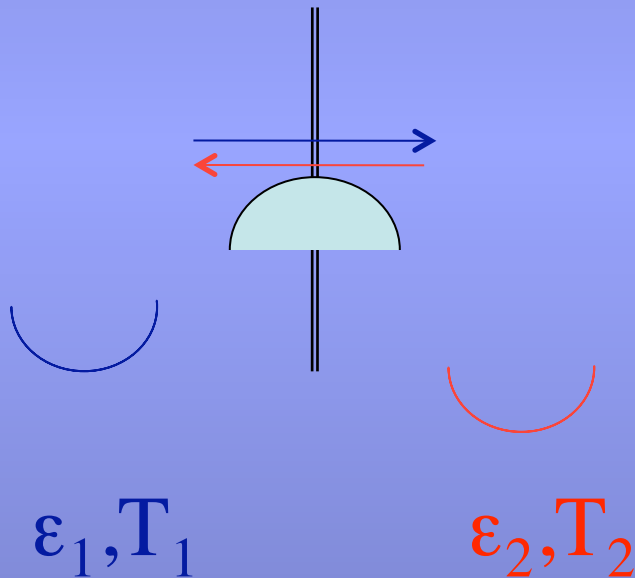
*classical particle*

$$W = a e^{-(V-\varepsilon)/T}$$





$$W = a e^{-(V-\varepsilon)/T}$$



$$W_{\rightarrow} = a e^{-x_1} \quad x_1 = (V - \varepsilon_1)/T$$

$$W_{\leftarrow} = a e^{-x_2} \quad x_2 = (V - \varepsilon_2)/T$$

$$P = \dot{W} = a(e^{-x_2} - e^{-x_1})(\varepsilon_1 - \varepsilon_2) = aT_2(e^{-x_2} - e^{-x_1})[x_2 - (1 - \eta_c)x_1]$$

$$\dot{Q} = a(e^{-x_2} - e^{-x_1})(V - \varepsilon_2) = a(e^{-x_2} - e^{-x_1})T_2x_2$$

$$\eta = \frac{\dot{W}}{\dot{Q}} = 1 - (1 - \eta_c) \frac{x_1}{x_2}$$

$$\frac{\partial P}{\partial x_2} = 0 \Rightarrow (e^{-x_2} - e^{-x_1}) = e^{-x_2} [x_2 - (1 - \eta_c)x_1]$$

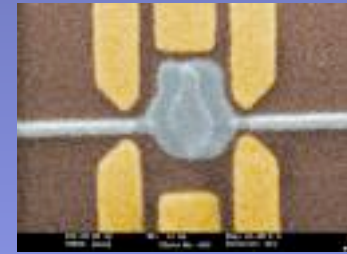
$$\frac{\partial P}{\partial x_1} = 0 \Rightarrow (e^{-x_2} - e^{-x_1})(1 - \eta_c) = e^{-x_1} [x_2 - (1 - \eta_c)x_1]$$

$$x_1 = 1 - \frac{1}{\eta_c} \ln(1 - \eta_c) \quad x_2 = 1 - \frac{1 - \eta_c}{\eta_c} \ln(1 - \eta_c)$$

$$\eta = \frac{(\eta_c)^2}{\eta_c - (1 - \eta_c) \ln(1 - \eta_c)} \approx \frac{\eta_c}{2} + \frac{(\eta_c)^2}{8} + \frac{3(\eta_c)^3}{96}$$

# Thermo-electric quantum dot

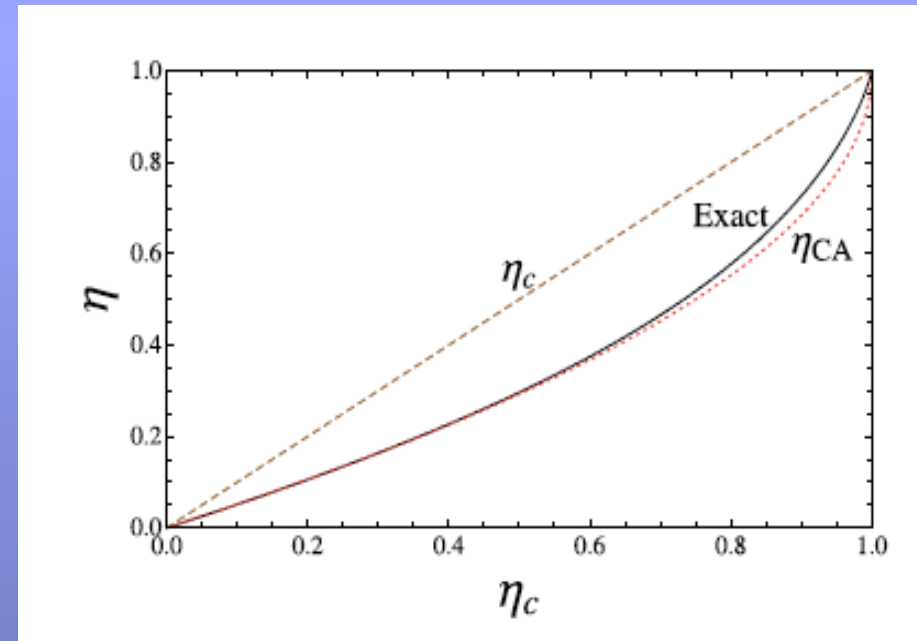
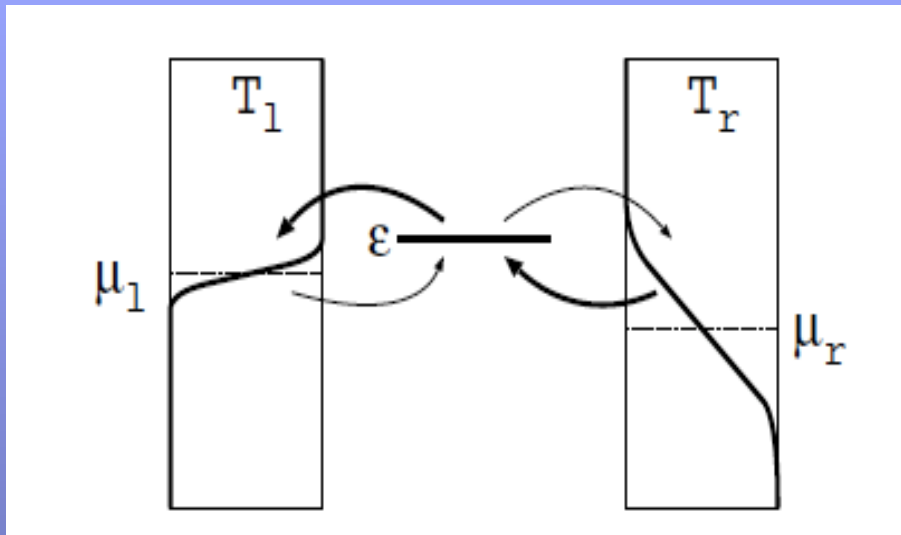
M. Esposito K. Lindenberg C. Van den Broeck  
EPL 85, 60010 (2009)



$$\eta = \eta_c / 2 + \eta_c^2 / 8 + (7 + a)\eta_c^3 / 96$$

*fermions*

$$W_{in} = af \quad W_{out} = a(1-f) \quad f = \frac{1}{e^{(\varepsilon-\mu)/T} + 1}$$



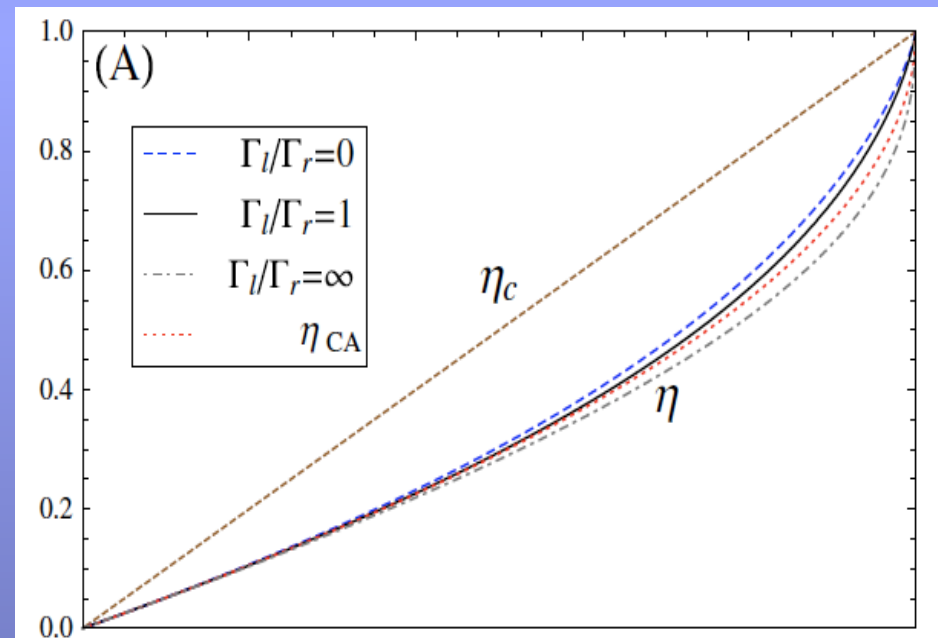
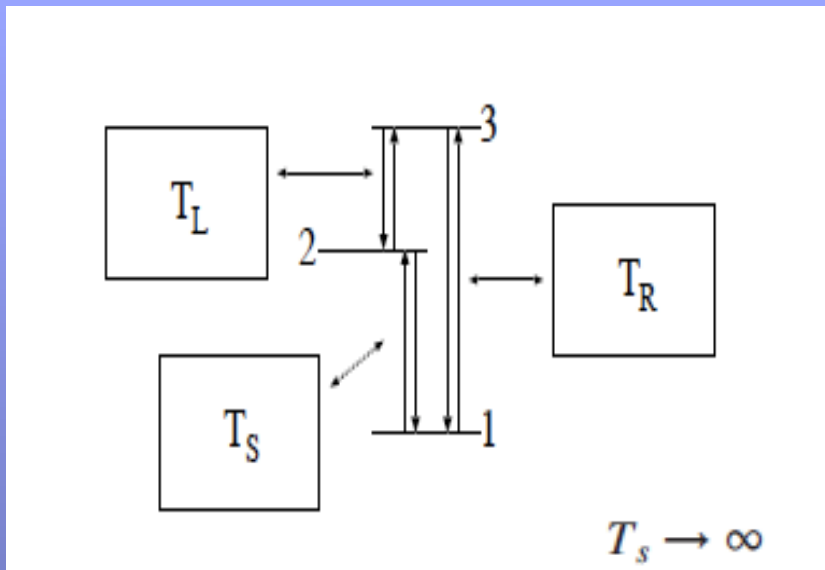
# Maser

M. Esposito K. Lindenberg C. Van den Broeck  
 PRL 102,130602 (2009)



$$\eta = \frac{\eta_c}{2} + \left(1 - \frac{3(\Gamma_l - \Gamma_r)}{(\Gamma_l + \Gamma_r)(3 \cosh \alpha + \sinh \alpha)}\right) \frac{\eta_c^2}{8} + \mathcal{O}(\eta_c^3)$$

*bosons*  $W_{abs} = \Gamma n$   $W_{emis} = \Gamma(1 + n)$   $n = \frac{1}{e^{h\nu/T} - 1}$



# Stochastic Thermodynamics: General Proof of 1/8

M. Esposito K. Lindenberg C. Van den Broeck PRL 102,130602 (2009)

$$\eta = \eta_c / 2 + \eta_c^2 / 8 + \dots$$

$\mu_1, T_1$



$\epsilon_i, N_i$

$\epsilon_j, N_i$

$\mu_2, T_2$

$$\dot{p}_i(t) = \sum_j W_{ij} p_j(t).$$

$$\frac{W_{ji}^{(\nu)}}{W_{ij}^{(\nu)}} = \exp \left\{ \beta_\nu [(\epsilon_i - \epsilon_j) - \mu_\nu (N_i - N_j)] \right\}.$$

$$\dot{S}_i(t) = \sum_{i,j,\nu} W_{ij}^{(\nu)} p_j(t) \ln \frac{W_{ij}^{(\nu)} p_j(t)}{W_{ji}^{(\nu)} p_i(t)} \geq 0.$$

$$\eta = \frac{\eta_c}{2} + \left(1 + \frac{M}{\partial_{x_l} L}\right) \frac{\eta_c^2}{4} + \mathcal{O}(\eta_c^3).$$

$$\mathcal{I} = L\mathcal{F} + M\mathcal{F}^2 + \mathcal{O}(\mathcal{F}^3)$$

$$\mathcal{I}(x_r, x_l) = -\mathcal{I}(x_l, x_r).$$

# Conclusion

*Time-reversibility in linear regime*

Symmetry Onsager matrix

Prigogine minimum entropy production

Efficiency at max power  $\eta = \eta_c / 2$



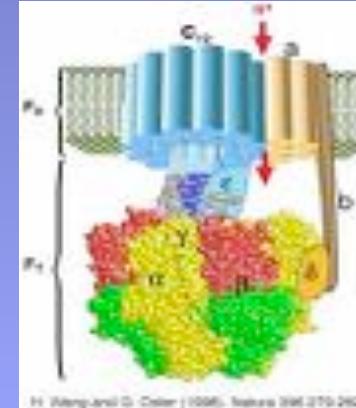
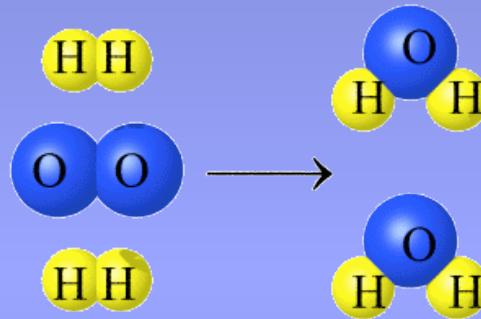
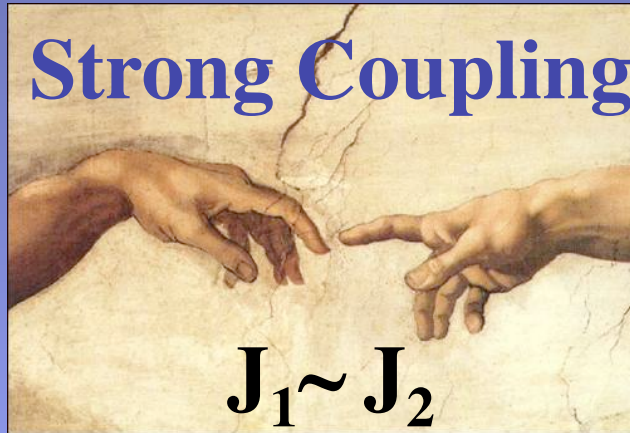
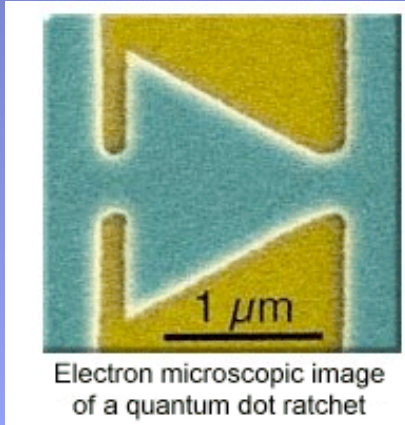
*Time-reversibility in nonlinear regime*

Efficiency at max power  $\eta = \eta_c / 2 + \eta_c^2 / 8$

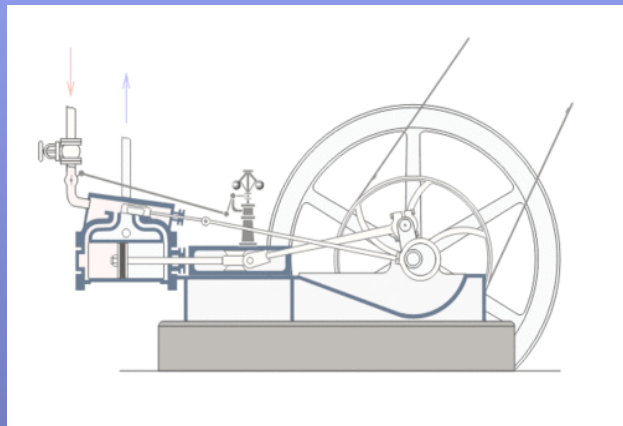
(strong coupling, spatial symmetry)



# Strong Coupling



## Thermal



## Chemical Machines



## Entropic





I want to be important  
**NOW**