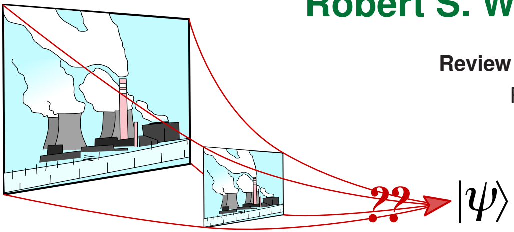
Laboratoire de Physique et Modélisation des Milieux Condensés
Univ. Grenoble Alpes & CNRS, Grenoble, France

CLOSED questions in heat transport and conversion at the nanoscale

Robert S. Whitney



Review – Benenti, Casati, Saito, R.W.
Physics Reports **694**, 1 (2017)

Marseille – Nov 2018

OVERVIEW

(I) Laws of thermodynamics same in quantum

- where does entropy come from?

  Schrodinger Eq. = Reversible

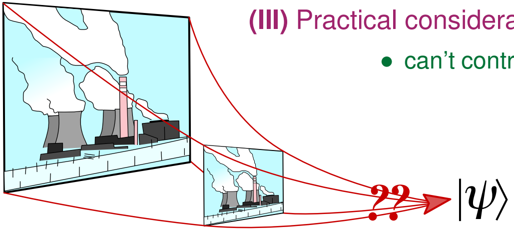
- Carnot efficiency

(II) Extra constraints from quantum

- quantized heat flow

(III) Practical considerations

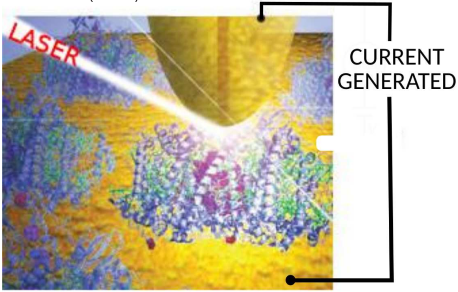
- can't control heat!



NANOSCALE MACHINES

Photosynthetic molecule (experiment)

Gerster et al (2012)



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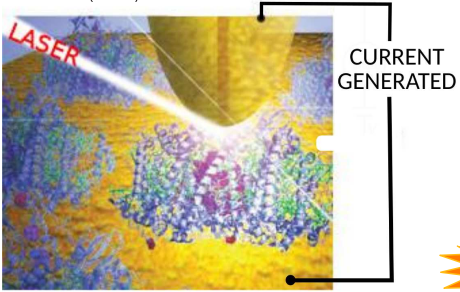
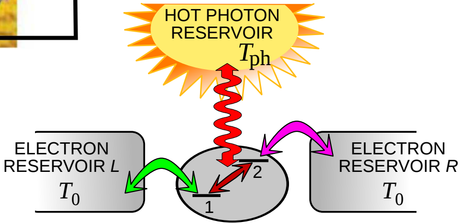


SIMPLE MODEL



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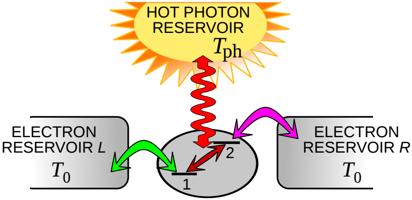


FOR THIS TALK, I ASSUME:

♣ Nanoscale/quantum system between *macroscopic* reservoirs

- Long times (steady state) ⇒"macroscopic" work output

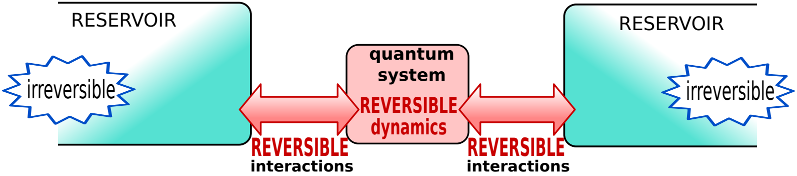
cf. fluctuation theorems

♣ Thermal reservoir states:

- No squeezed reservoir states — cf. J. Roßnagel,et al PRL (2014)
- No non-equil. reservoir states

cf. Sanchez, Splettstoesser & Whitney "Demon preprint" (2018)

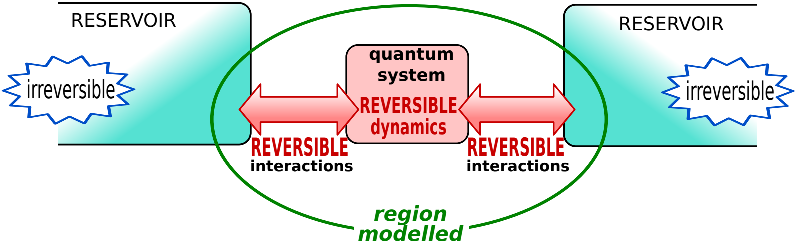
REVERSIBLE OR NOT



REVERSIBLE or NOT?

- Where is *entropy produced*?
- 2nd law of thermodynamics?

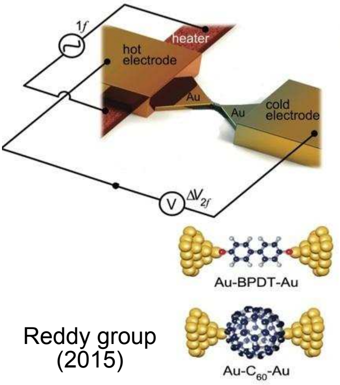
REVERSIBLE OR NOT



REVERSIBLE or NOT?

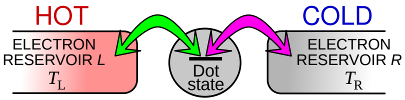
- Where is *entropy produced?*
- 2nd law of thermodynamics*?*

SIMPLER – NANOSCALE THERMOELECTRIC



Reddy group (2015)

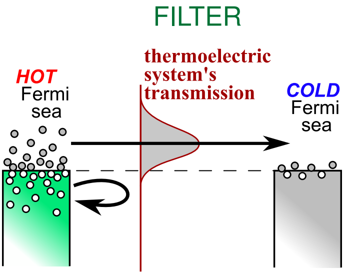
SIMPLE MODEL



SIMPLER – NANOSCALE THERMOELECTRIC

Acts as Energy FILTER

different dynamics *above* and *below* Fermi surface



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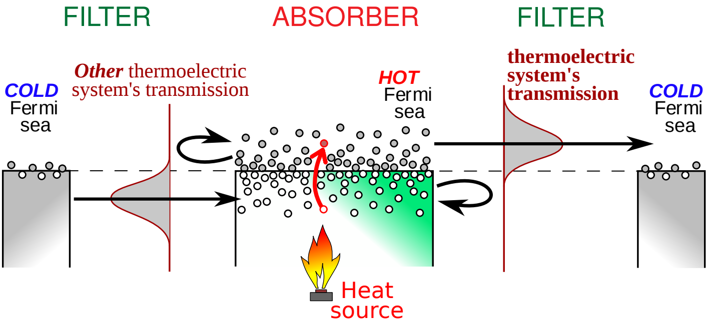

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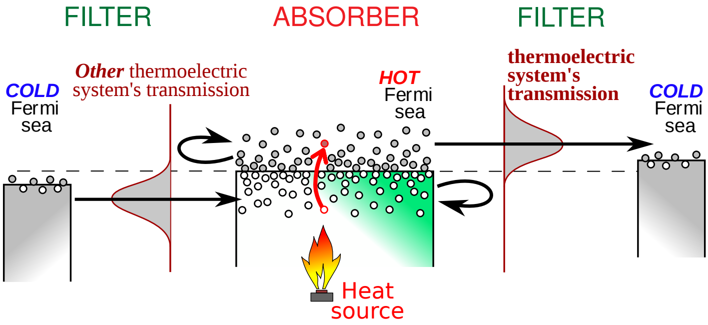
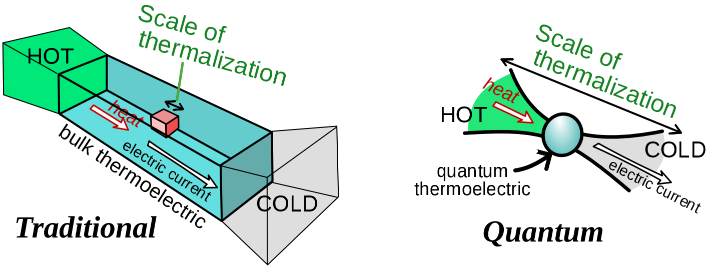


TRADITIONAL versus QUANTUM



(1) Filters $\ll$ scale of thermalisation $\Rightarrow$ Quantum thermoelectric

(2) Central region (absorber) also $\ll$ scale of thermalisation

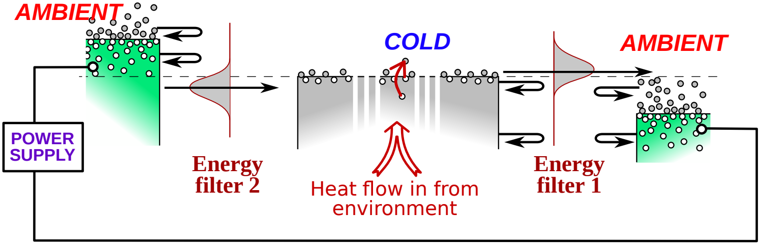
$\Rightarrow$ Quantum thermocouple

- Often filters-absorber *combined* in in quantum thermocouples

cf. simple model of photosynthetic molecule

QUANTUM THERMOELECTRICS FOR REFRIGERATOR

PELTIER FRIDGE



EFFICIENCIES AND ZT

HEAT-ENGINE efficiency

$$\eta_{\text{engine}} = \frac{\text{work done}}{\text{heat used}}$$

Carnot limit

$$\eta_{\text{engine}}^{\text{Carnot}} = 1 - T_{\text{cold}}/T_{\text{hot}}$$

LINEAR RESPONSE:

$$\eta_{\text{engine}} = \eta_{\text{engine}}^{\text{Carnot}} \times \frac{\sqrt{ZT+1}-1}{\sqrt{ZT+1}+1}$$

$$ZT = \frac{\text{(Electric Conductance) (Seebeck)}^2\, T}{\text{Thermal Conductance}}$$

$$\begin{cases} \text{ZT} = \infty \Rightarrow \text{Carnot} \\ \text{ZT} = 3 \Rightarrow \text{Carnot/3} \\ \text{ZT} = 1 \Rightarrow \text{Carnot/6} \end{cases}$$

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FRIDGE efficiency

$$\eta_{\rm fridge} = \frac{\text{heat removed}}{\text{work used}}$$

Carnot limit

$$\eta_{\rm fridge}^{\rm Carnot} = T_{\rm cold}/(T_{\rm ambient} - T_{\rm cold})$$

"LINEAR" RESPONSE: Max T difference : $\dfrac{\Delta T}{T} \leq \frac{1}{2} ZT$

MODELLING METHODS

- Landauer scattering theory $\Longleftarrow$ *No e-e Interactions*

  see chapters 4-6 of Benenti *et al*, Physics Reports **694**, 1 (2017)

- Rate Equations $\Longleftarrow$ *Weak Coupling*

  see chapters 8-9 of Benenti *et al*, Physics Reports **694**, 1 (2017)

- Keldysh field theory $\Longleftarrow$ *"everything"* often need approx similar to above

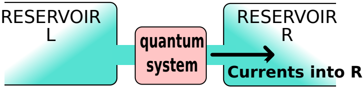
  OPEN questions ask Rosa & David, or Fabienne & Adeline ...

- Schrodinger eq. for system+environment

LANDAUER SCATTERING THEORY

LANDAUER SCATTERING THEORY

(TWO TERMINALS)



Particle current into R $\equiv \frac{\mathrm{d}}{\mathrm{d}t} N_R = \int \mathrm{d}E \quad \mathcal{T}(E) \left[f\left(\frac{E-\mu_L}{T_L}\right) - f\left(\frac{E-\mu_R}{T_R}\right) \right]$

Energy current into R $\equiv \frac{\mathrm{d}}{\mathrm{d}t} E_R = \int \mathrm{d}E \; E \; \mathcal{T}(E) \left[f\left(\frac{E-\mu_L}{T_L}\right) - f\left(\frac{E-\mu_R}{T_R}\right) \right]$

UNITS: $\hbar = k_{\mathrm{B}} = 1$

LANDAUER SCATTERING THEORY

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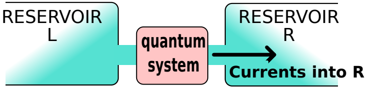

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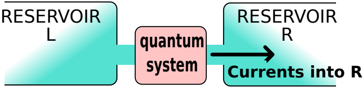
UNITS: $\hbar = k_{\mathrm{B}} = 1$

- Electric current into R $= e \, \frac{\mathrm{d}}{\mathrm{d}t} N_R$
- Work into R$= \mu_R \frac{\mathrm{d}}{\mathrm{d}t} N_R$ $\Longrightarrow$ power generated $=$ sum L & R $= (\mu_R - \mu_L) \frac{\mathrm{d}}{\mathrm{d}t} N_R$
- Heat current into R $= \frac{\mathrm{d}}{\mathrm{d}t} E_R - \mu_R \frac{\mathrm{d}}{\mathrm{d}t} N_R$
- Entropy current into R $=$ Heat current$\big/ T_R$ $\Leftarrow$ CLAUSIUS LAW (1855)

LANDAUER SCATTERING THEORY

(TWO TERMINALS)



see section 6.4 of Phys. Rep. **694**, 1 (2017)

- Rate of change of entropy $\frac{\mathrm{d}}{\mathrm{d}t}S$

  = (Entropy current into L) + (Entropy current into R) ≥ 0

  $\Rightarrow$ 2nd law proven for all $\mathcal{T}(E)$, T_L, T_R, ...

  Nenciu (2007) = proof for N reservoirs

- Carnot efficient system : reversible $\frac{\mathrm{d}}{\mathrm{d}t}S = 0$

  requires transmission is only non-zero at $\frac{E-\mu_L}{T_L} = \frac{E-\mu_R}{T_R}$

  Humphrey, Newbury, Taylor, Linke (2002)

Quantum bound on heat flow

Maximum HEAT FLOW per transverse mode $\Rightarrow$ maximum ENTROPY CHANGE

Bekenstein, Phys. Rev. Lett. (1981)
Pendry, J. Phys. A (1983)

Heat current out of hot reservoir

$$J_{\rm hot} \leq N \frac{\pi^2 k_{\rm B}^2}{6h}\left(T_{\rm hot}^2 - T_{\rm cold}^2\right)$$

with "quantum" $N \sim \frac{\text{cross-section}}{\text{wavelength}}$

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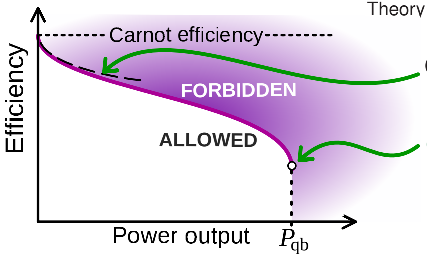
Quantum bound on power output

Theory: RW (2013) – Experiment: Chen et al (2018)



Carnot $\times \left(1 - \alpha_1 \sqrt{P/P_{\rm qb}} + \cdots\right)$

Quantum bound (qb)

$$P_{\rm qb} \propto N\,(T_{\rm hot} - T_{\rm cold})^2$$

...do better with B-field/interactions cf. Brandner et al 2015, Lao et al 2018

Is quantum bound relevant for REAL applications?

Cross-section for $100W$ of power ?

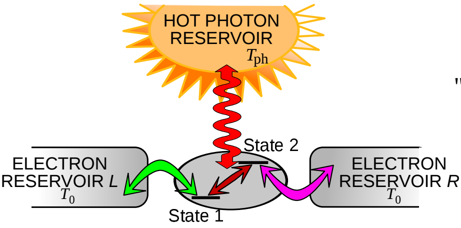
with wavelength $\lambda_{\rm F} \sim 10^{-8}{\rm m}$

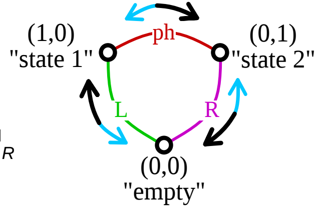
$\diamondsuit$ Minimal cross-section $\sim 4{\rm mm}^2$

$\diamondsuit$ 90% of Carnot requires $> 0.4{\rm cm}^2$

RATE EQUATIONS

RATE EQUATIONS





Set of coupled equations for system evolution:

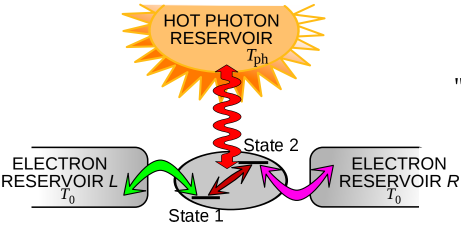
$$\frac{\mathrm{d}}{\mathrm{d}t} P_b(t) \;=\; \sum_a \Big(\Gamma_{b\leftarrow a}\, P_a(t) \;-\; \Gamma_{a\leftarrow b}\, P_b(t) \Big)$$

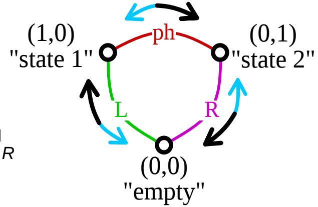
where P_b = prob. system is in state b

& $\Gamma_{b\leftarrow a}$ = rate $a \rightarrow b$

Current into R $= \Gamma_{(0,0)\leftarrow(0,1)}\, P_{(0,1)} \;-\; \Gamma_{(0,1)\leftarrow(0,0)}\, P_{(0,0)}$

RATE EQUATIONS



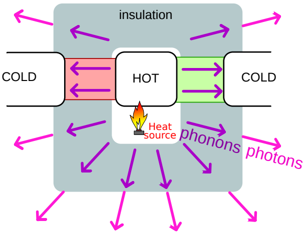


USEFUL TRICKS – look at loops:

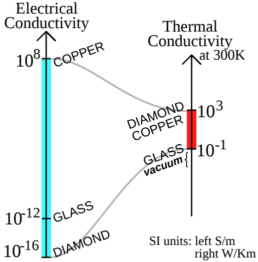
- only Carnot efficient if no loop generates entropy
- if single-loop system $\Rightarrow \eta_{\text{engine}} = \dfrac{\text{Work in one cycle}}{\text{Heat in one cycle}}$

CAN'T CONTROL HEAT !!

(a)



(b)



Heat engine efficiency

$$\eta_{\text{engine}} = \frac{\text{work done}}{\text{heat used} + \text{heat lost}}$$

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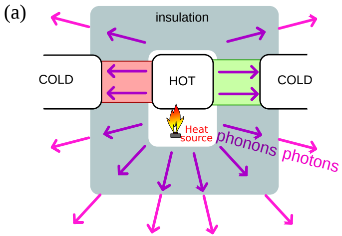

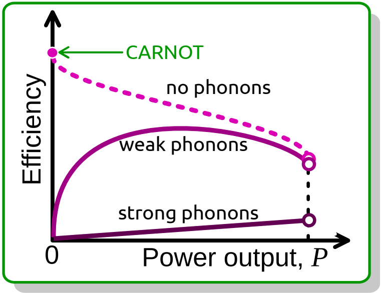

Heat engine efficiency $$\eta_{\text{engine}} = \frac{\text{work done}}{\text{heat used} + \text{heat lost}}$$

CONCLUSION: CLOSED† QUESTIONS

†*closed* for theories simple enough to treat

≡ (a) Landauer & (b) Rate eqs.

(I) Laws of thermodynamics same at nanoscale

if reservoirs are macroscopic & internal equlibrium

- Entropy produced
- Carnot efficiency (in principle) $\Leftarrow$ vanishing power

(II) Extra constraints from quantum

- quantized heat flow

(III) Practical considerations

- can't control heat!