



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

***The best quantum thermoelectric
at finite power output***

Robert S. Whitney

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OVERVIEW

Ioffe (1958)
Inst. Semicond.
Leningrad

2 Watts
(80-90 Volts)



Kerosene Radio Made in Moscow for use in rural areas, this all-wave radio is reportedly powered by the kerosene lamp hanging above it. A group of thermocouples is heated internally to 570 degrees by the flame. Fins cool the outside to about 90 degrees. The temperature differential generates enough current to operate the low-drain receiver. Regular listeners may want fur-lined union suits, though: It works best in a room with open windows.

$$T_{\text{HOT}} = 572 \text{ K}$$

$$T_{\text{COLD}} = 305 \text{ K}$$

www.neazoi.com/technology/thermocouple.htm

MY QUESTION:
What is MAX. efficiency
at GIVEN power output?

- ♣ Quantum thermoelectric
- ♣ Nonlinear Landauer-Büttiker
- ◇ *parasitic* heat flows
— phonons & photons
- ◇ *inelastic / relaxation*
in quantum system

CENTRAL RESULTS

Heat-engine efficiency:

$$\eta_{\text{eng}} = P/J$$

Output : power = $P = VI$

Input : heat-current = J

Refrigerator efficiency

≡ coeff. of performance (COP):

$$\eta_{\text{fri}} = J/P$$

Output : J

Input : P

[1] ABSOLUTE upper bound on Power Output: $P \leq P_{\text{qb}}$

♣ P_{qb} is *quantum-bound* (ill-defined in classical thermodyn)

[2] MAX. efficiency, $\eta_{\text{eng}}(P)$, at given power P

♣ function of P/P_{qb} \Leftarrow *Quantum*

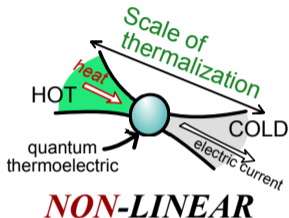
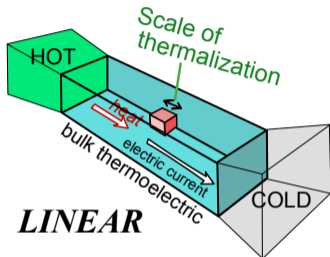
unlike Carnot efficiency = classical

Example low power : $\eta_{\text{eng}}(P) \leq \eta_{\text{eng}}^{\text{Carnot}} \left(1 - \alpha_1 \sqrt{P/P_{\text{qb}}} + \dots \right)$

INTRODUCTION

Bulk versus Quantum : for LARGE ΔT

Linearity requires temp. drop to be *small on scale of thermalization*



Nonlinear regime : efficiency η is meaningful, but ZT is **NOT**.

Muralidharan-Grifoni (2012), Whitney (2013), Meier-Jacquod (2013), Michelini's poster

Linear formula

$$\eta/\eta_{\text{Carnot}} = \frac{\sqrt{ZT+1}-1}{\sqrt{ZT+1}+1}$$

Dictionary (for linear people)

$$ZT = \infty \iff \eta = \eta_{\text{Carnot}}$$

$$ZT = 3 \iff \eta = \frac{1}{3}\eta_{\text{Carnot}}$$

$$ZT = 0 \iff \eta = 0$$

METHOD: scattering theory beyond linear response

Heat current: $J_L = \int_{-\infty}^{\infty} \frac{d\epsilon}{h} \epsilon \mathcal{T}_{RL}(\epsilon) \left(f \left[\frac{\epsilon - eV_L}{k_B T_L} \right] - f \left[\frac{\epsilon - eV_R}{k_B T_R} \right] \right)$

◇ transmission function $\mathcal{T}_{RL}(\epsilon) = \text{tr}[\mathcal{S}^\dagger(\epsilon) \mathcal{S}(\epsilon)]$

◇ Fermi-Dirac for ingoing particles: $f[(\epsilon - eV_j)/k_B T_j]$

♣ obeys 2nd law thermodyn, etc. Whitney PRB (2013)

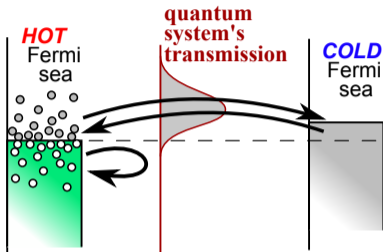
beyond linear-response : Hartree-like interactions – *self-consistent*

Christen-Büttiker (1996)

Self-consistent loop:



ORIGIN of THERMOELECTRICITY



$$I = 0$$

$$V = V_{\text{stop}}$$

$$P = IV = 0$$

Mahan,Sofo (1996). Humphrey,Linke (2005)

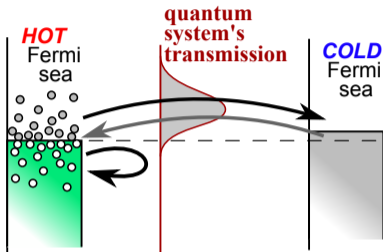
Vanishing transmission width

⇒ reversibility (no entropy generated)

⇒ Carnot efficiency $\eta = \eta_{\text{carnot}} = 1 - T_R/T_L$

... but *no power*

ORIGIN of THERMOELECTRICITY



$$I \neq 0$$

$$V \neq 0$$

$$P = IV = \text{max.}$$

Efficiency at max. power

- vanishing transmission width;

Esposito, Lindenberg, van den Broeck (2009) \Rightarrow Curzon Ahlborn efficiency

Curzon, Ahlborn (1975), Novikov (1957), Chambadal (1957)

- non-vanishing transmission width:

Nakpathomkun, Xu, Linke (2010), Leijnse, Wegewijs, Flenberg (2010)

Hershfield, Muttalib, Nartowt (2013), ...Others

... *higher* max power but *lower* efficiency at that power

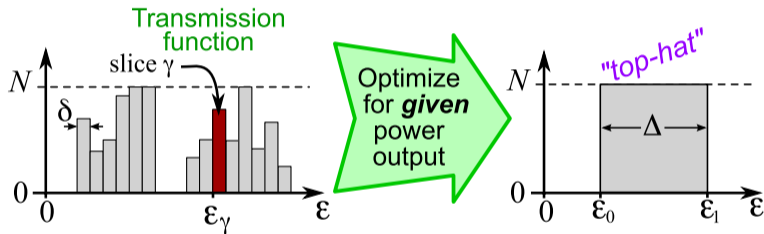
ANSWERING MY QUESTION

What is **MAXIMUM EFFICIENCY** for **GIVEN** power output?

OPTIMIZING EFFICIENCY for GIVEN POWER OUTPUT

$(n + 1)$ variables: n slices + bias, V
 one constraint : power = P

♣ *want* minimum heat-flow J for given P



Proof: changing height τ_γ of slice γ , decreases J (increases efficiency)

$$\text{if } 0 > \left. \frac{\partial J}{\partial \tau_\gamma} \right|_P = \left(\frac{\epsilon_\gamma}{eV} - \frac{J'}{P'} \right) \times \left. \frac{\partial P}{\partial \tau_\gamma} \right|_V$$

primed = d/dV

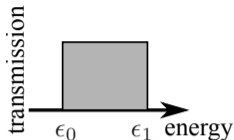
TRANSCENDENTAL EQUATION

For given temperatures T_L (hot) & T_R (cold)

$$\epsilon_0 = \frac{eV}{1 - T_R/T_L}$$

$$\epsilon_1 = eV \frac{J'}{P'}$$

primed = d/dV



Energy-integrals in J and P are Fermi-functions \times top-hat

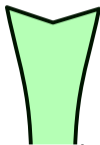
P & J are sums of *logs* and *dilog.-functions*

$$\ln [1 + e^{-(\epsilon - eV_j)/k_B T_j}] \text{ \& } \text{Li}_2 [-e^{-(\epsilon - eV_j)/k_B T_j}]$$

Get ϵ_1 from above *transcendental eq.* for given T_L (hot) & T_R (cold)

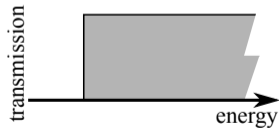
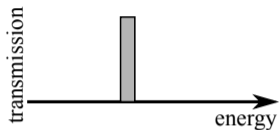
OPTIMAL TOP-HAT WIDTH

zero power output



increasing
power
output

max. power output



UPPER-BOUND on POWER OUTPUT for N transverse modes

Refrigerator cooling power: $J \leq \frac{1}{2} J_{\text{qb}} \equiv \frac{\pi^2}{12h} N (k_B T_L)^2$

Heat-engine electrical power:

$$P \leq P_{\text{qb}} \equiv \frac{A_0 \pi^2}{6h} N (k_B T_L - k_B T_R)^2 \quad \text{with } A_0 \simeq 0.192$$

- Purely quantum, i.e. irrelevant for $N \rightarrow \infty$
- $J_{\text{qb}} =$ Pendry (1983) as limit on entropy flow
 \implies “single mode fermionic” analogue of black-body
- Large N — Bjorn Sothmann’s talk Jordan et al (2013)

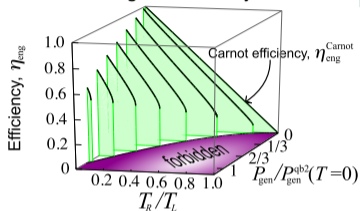
For Ioffe’s “Kerosene Radio” set-up :

$$J_{\text{qb}}, P_{\text{qb}} \sim 10\text{nW per transverse mode} \\ \implies 100\text{W needs cross-section } 1\text{cm} \times 1\text{cm}$$



MAX. EFFICIENCY for GIVEN POWER OUTPUT

Maximal heat-engine efficiency

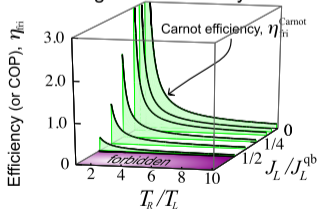


Heat-eng. : *small* power output, P .

$$\eta = \eta^{\text{Carnot}} \left(1 - \alpha_1 \sqrt{\frac{P}{P_{\text{qb}}}} + \dots \right)$$

where P_{qb} is upper-bound

Maximal refrigerator efficiency



Fridge : *small* power output, J .

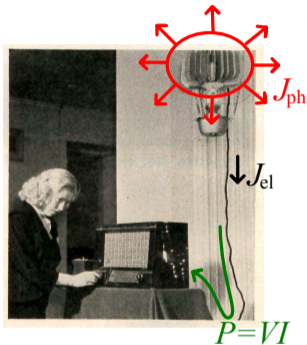
$$\eta = \eta^{\text{Carnot}} \left(1 - \alpha_2 \sqrt{\frac{J}{J_{\text{qb}}}} + \dots \right)$$

where J_{qb} is upper-bound

PARASITIC PHONON/PHOTON FLOWS

Black-body photons: $J_{\text{ph}} \propto (T_{\text{hot}}^4 - T_{\text{cold}}^4)$

phonon in nanostructures Heron et al (2009-11)



$$\text{Total efficiency } \eta_{\text{el\&ph}} = \frac{P}{J_{\text{el}} + J_{\text{ph}}}$$

Max efficiency - don't care what P
(not given P)

- *No phonons/photons:*
 $\max \eta_{\text{el\&ph}} = \text{NARROW transmission}$
 $\implies \eta_{\text{el\&ph}} \rightarrow \eta_{\text{Carnot}}$
- *Phonons/photons dominate:*
 $\max \eta_{\text{el\&ph}} \Leftrightarrow \max P$
 $= \text{WIDE transmission}$

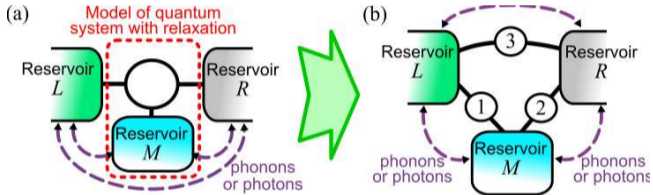
Max efficiency at given P :

$$\eta_{\text{el\&ph}}(P) = \frac{P \eta_{\text{el}}(P)}{P + \eta_{\text{el}}(P) J_{\text{ph}}}$$

RELAXATION modelled as Buttiker “voltage probe” (1988)

Sometime – inelastic scattering may *increase* efficiency

see Casati’s talk & Ora’s talk



REALLY HARD PROBLEM !!

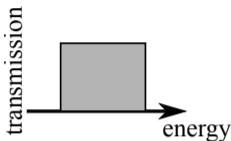
ANSWERED in 2 limits : *low* power and *max* power

Over-estimate *never* exceed results *without* relaxation.

... *open question* for intermediate powers

CONCLUSIONS

- ♣ Max. efficiency at *given* power : “top-hat”
transcendental eq. for position/width
⇒ *Width grows with power*



- ♣ Results : [1] max. possible power (*quantum*)
[2] max. possible efficiency (*quantum*)

Is this the *BEST* thermoelectric at finite power output??

- ♣ *Open question:* relaxation at intermediate power outputs?
- ♣ *Open question:* strongly correlated systems (Kondo, Luttinger, etc)?
- ◇ *How to make top-hat?*

Buttiker said “top-hat = band = chain quantum-dots”
