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

Robert S. Whitney

- + Phys. Rev. Lett. **112**, 130601 (2014),
- + Phys. Rev. B **91**, 115425 (2015) (all the details),
- + arXiv:1603.09216 (three-terminal)

OVERVIEW

♣ Question about textbook *thermodynamics*

♣ INTRODUCTION — Thermoelectrics

♣ Landauer scattering theory

⇒ *Most efficient* thermoelectric at *given* power output

QUESTIONS about basic THERMODYNAMICS

$$\eta = \frac{\text{power output}}{\text{heat input}}$$

less than Carnot: $\eta_{\text{Carnot}} \equiv 1 - T_{\text{cold}}/T_{\text{hot}}$

Carnot \Leftrightarrow *reversibility* \Rightarrow “zero” power output

♣ What does “zero” mean?

\Rightarrow system specific or universal?

♣ Stricter upper bound at finite power?



THERMOELECTRICS MACHINES

HEAT FLOW \leftrightarrow CHARGE FLOW

POWER GENERATION or REFRIGERATION

Seebeck or Peltier

EXAMPLE : NASA POWER SOURCE



Heat source: 5kg plutonium α -decay

$$T_{\text{hot}} \simeq 1000\text{K}$$

$$T_{\text{cold}} \simeq 230\text{K}$$

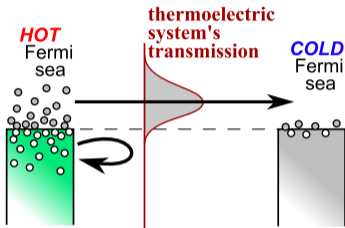
Power output = 120W

Efficiency $\eta = 6\%$

ORIGIN of THERMOELECTRICITY

Thermoelectric effects

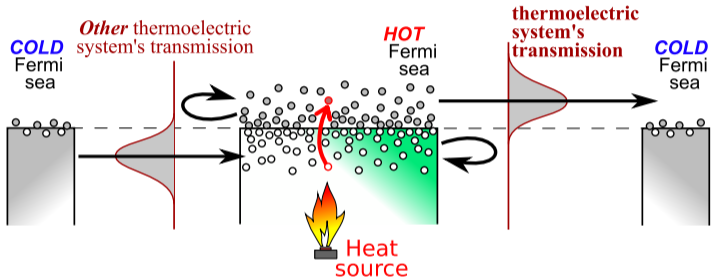
= *difference between dynamics above and below Fermi surface*



Origin of *energy filter*: MESOSCOPIC or CRYSTAL STRUCTURE

Thermoelectric effects

= *difference between dynamics above and below Fermi surface*

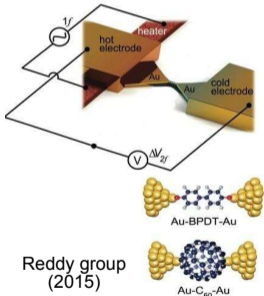


Origin of *energy filter*: MESOSCOPIC or CRYSTAL STRUCTURE

QUANTUM THERMOELECTRICS

TWO RESERVOIRS

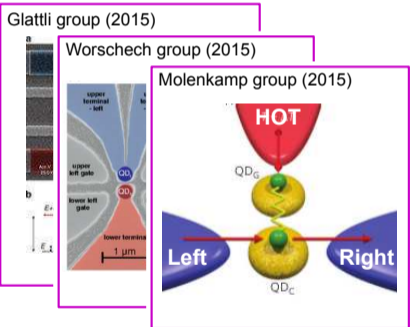
Quantum thermoelectrics
in traditional thermocouple



THREE RESERVOIRS

1 for heat & 2 for current

“Quantum Thermocouple”



2 reservoir theory (& older expts) = Molenkamp group, Mahan-Sofa, Linke group

3 reservoir theory = Entin-Wohlmann et al, Sánchez & Büttiker

PLAYGROUND

DEFINITIONS

- ◇ Heat?
- ◇ Work?
- ◇ Entropy?



QUANTUM MACHINES

- ♡ Heat engines
- ♡ Refrigerators
- ♡ Cooling by heating
- ♡ Maxwell demons

Testing quantum theories versus thermodynamics

- ♣ Markovian (Lindblad) master equation Kosloff's review
 - ♣ Scattering theory R.W. 2013
 - ♣ Keldysh non-equil. Green functions Esposito 2015
-

MAXIMUM EFFICIENCY AT GIVEN POWER OUTPUT

Inspired by engineering question:



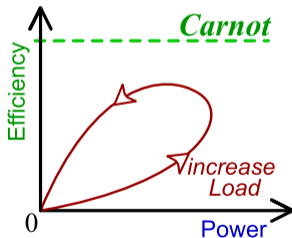
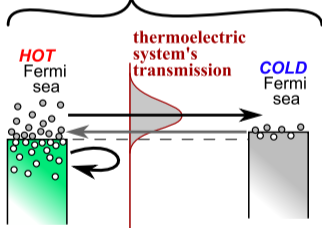
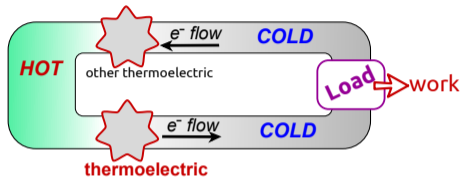
$$T_{\text{hot}} \simeq 1000\text{K} \quad T_{\text{cold}} \simeq 230\text{K}$$

Power output = 120W \Leftarrow **NECESSARY**

Efficiency $\eta = 6\%$ \Leftarrow **“nice” if bigger**

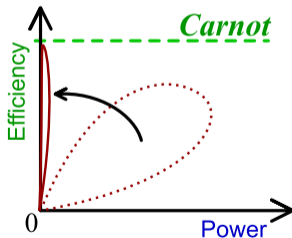
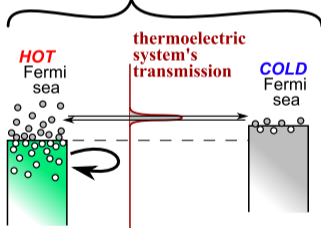
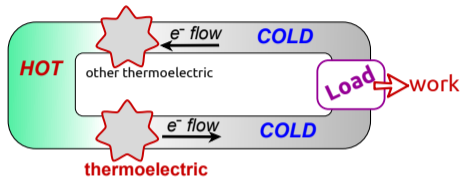
THERMOCOUPLE CIRCUIT

Mahan, Sofo (1996). Humphrey, Linke (2005)
Esposito, Lindenberg, Van den Broeck (2009)



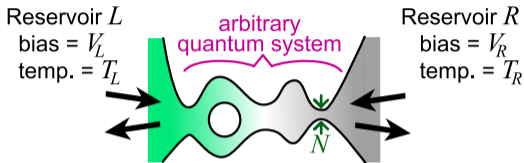
THERMOCOUPLE CIRCUIT

Mahan, Sofo (1996). Humphrey, Linke (2005)
Esposito, Lindenberg, Van den Broeck (2009)



SCATTERING THEORY \Rightarrow *thermodynamics*

Landauer scattering theory



Heat current:
$$J_L = \int_{-\infty}^{\infty} \frac{dE}{h} (E - eV_L) \mathcal{T}(E) (f_L(E) - f_R(E))$$

Transmission at energy E

Fermi-function

e-e interactions: only mean-field self-consistent Hartree-like

Christen-Büttiker (1996)

No Coulomb blockade, no Kondo Physics ...

Scattering theory \implies Thermodynamics

Bruneau Jakšić Pillet, Commun. Math. Phys. **319**, 501 (2013)

R.W., PRB **87**, 115404 (2013)

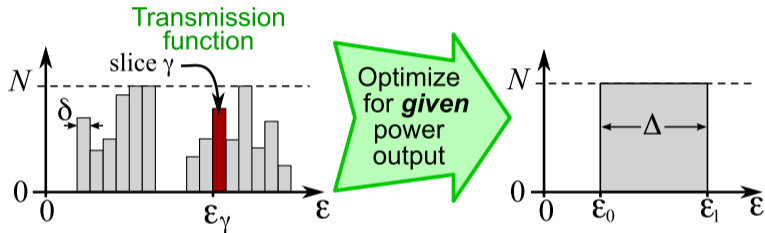
Energy Conservation }
HEAT \Leftrightarrow WORK } *1st law thermodynamics*

Proved scattering theory \Rightarrow *2nd law thermodynamics*

... using Clausius definition of entropy, $S = \frac{\text{heat}}{T}$

OPTIMIZING EFFICIENCY for GIVEN POWER OUTPUT

OPTIMIZING EFFICIENCY for GIVEN POWER OUTPUT



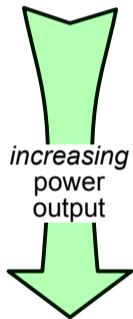
Variables: height of each slice & bias, V

Constraint : power = P

OPTIMAL TOP-HAT WIDTH

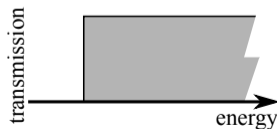
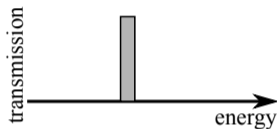
Transcendental equation for top-hat position and width

zero power output



*increasing
power
output*

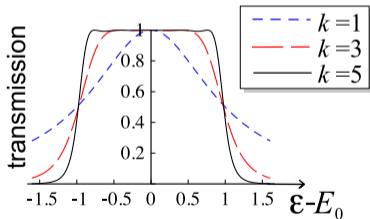
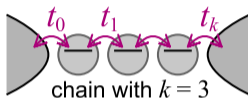
max. power output



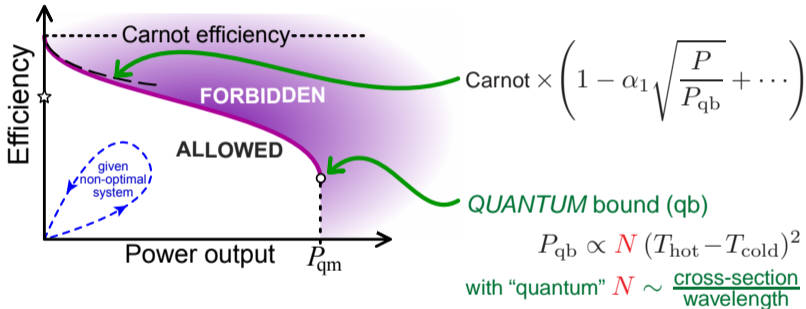
POTENTIAL REALIZATION

Make chain of sites (tight-binding model) \implies states form a *band*

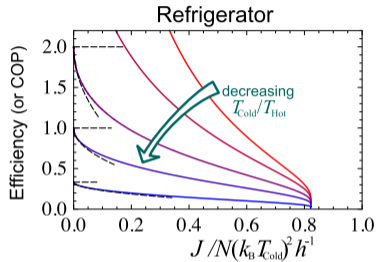
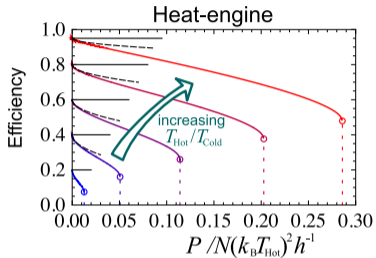
Chains of k quantum dots or molecules



Max. EFFICIENCY for GIVEN POWER

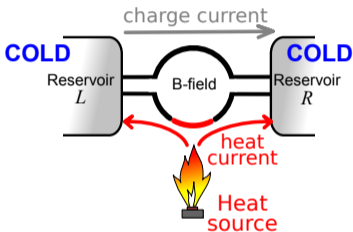


Max. EFFICIENCY for GIVEN POWER



Three-terminal thermoelectric : “quantum thermocouple”

R.W. arxiv:1603.09216



Fully-coherence inside quantum system

Four independent processes :

Hot \rightarrow L
Hot \rightarrow R
L \rightarrow R
R \rightarrow L

RESULT : max. eff. at given power
exactly the same as before

CONCLUSIONS

Max. efficiency at *zero*-power (Carnot) is **classical**

Max. efficiency at *finite*-power is **quantum**

PRL **112**, 130601 (2014), PRB **91**, 115425 (2015)

Preprint : arXiv:1603.09216

Is quantum bound relevant for REAL applications?



Cross-section for 100W of power ?

with wavelength $\lambda_F \sim 10^{-8} \text{m}$

- ◇ Minimal cross-section $\sim 4\text{mm}^2$
- ◇ 90% of Carnot requires $> 0.4\text{cm}^2$

=== EXTRAS ===

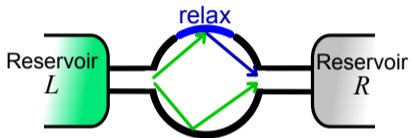
RELAXATION modelled as Buttiker “voltage probe” (1988)

Saito, Benenti, Casati & Prosen, PRB (2011). D. Sánchez & Serra, PRB (2011)

Entin-Wohlman & Aharony, PRB (2012)

VERY DIFFICULT

\implies treat only B-field = 0



PROOF of same bound
over-estimation in 2 limits

- low power
- high power

