Scattering theory of thermoelectric transport

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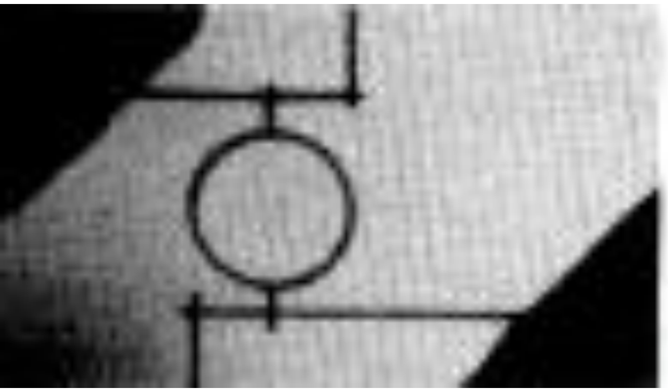
NANOPOWER

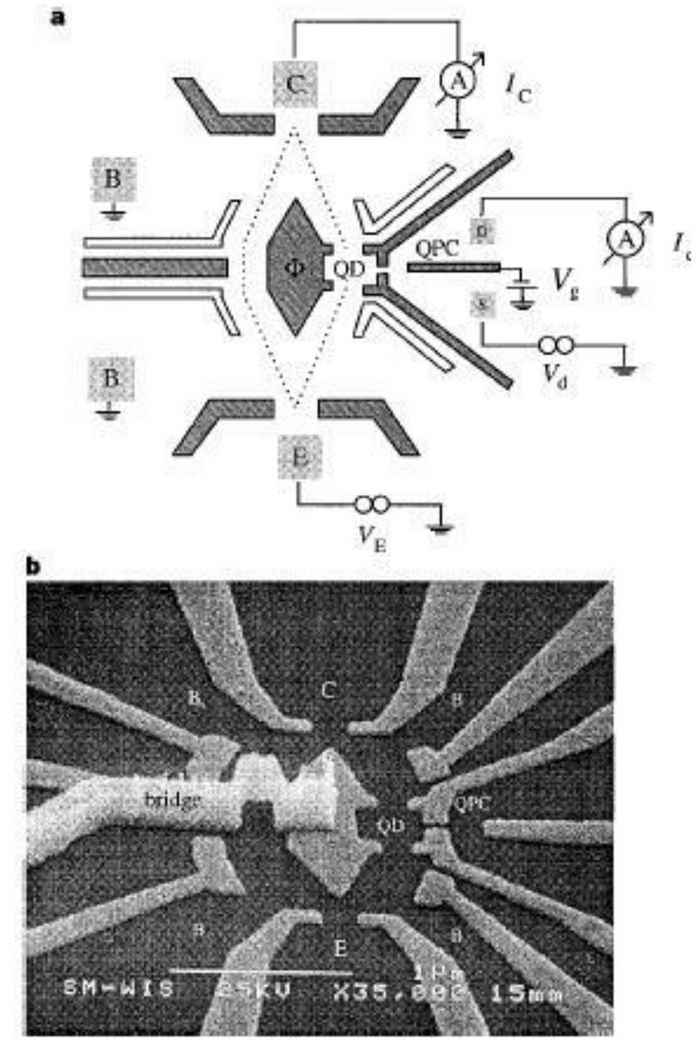
Summer School "Energy harvesting at micro and nanoscales“,
Workshop "Energy harvesting: models and applications“,
Erice, Italy, July 23-27, 2012

Mesoscopic Physics

Wave nature of electrons becomes important

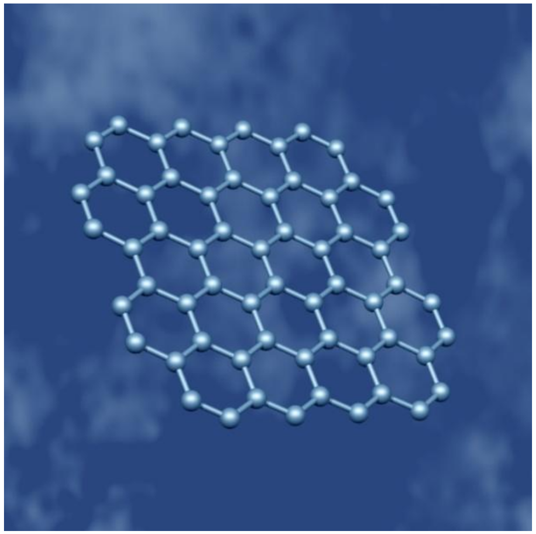


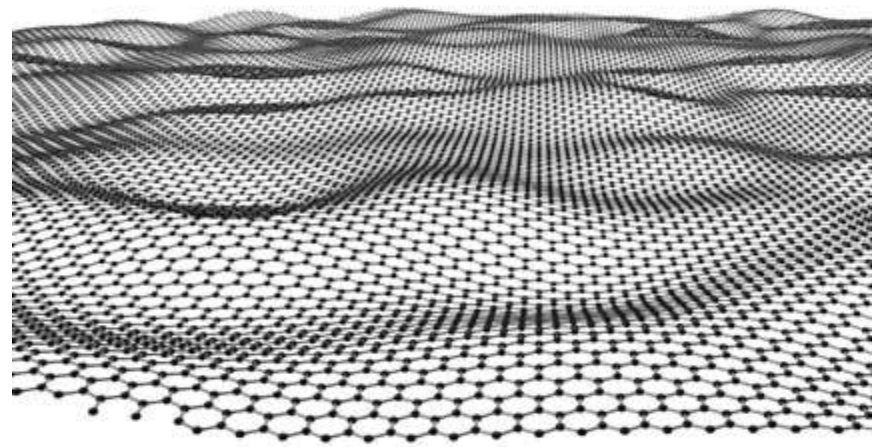
Webb et al., 1985

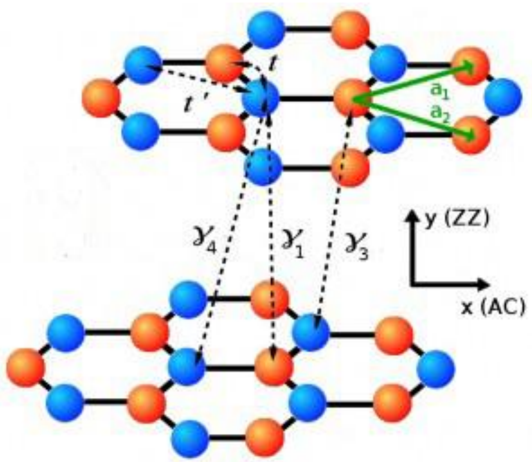


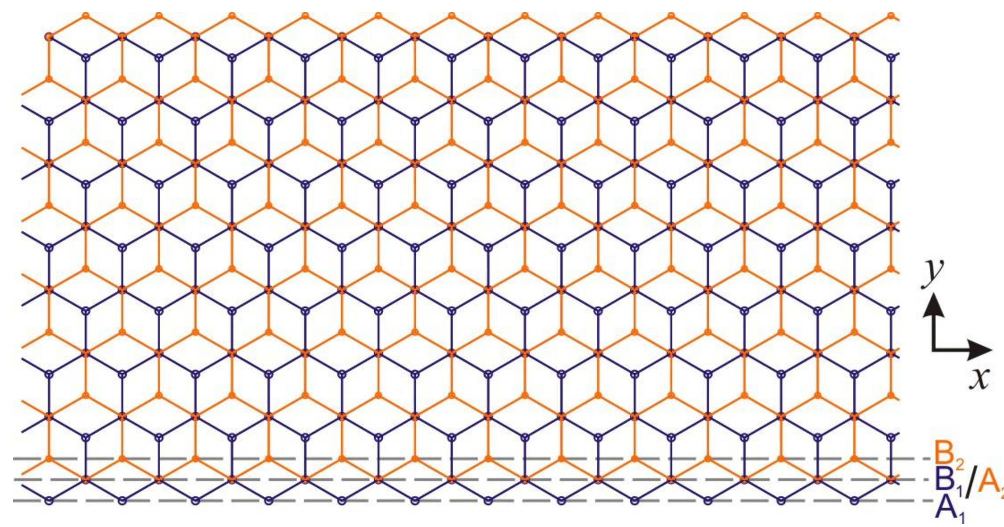
Yacoby et al. 1995

Graphene: single and bilayer



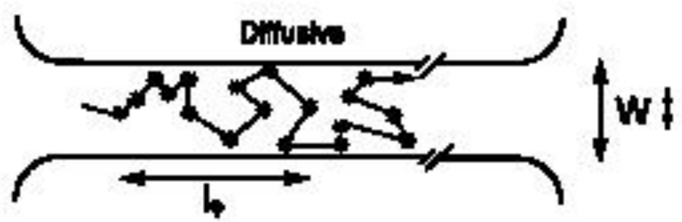






@Jian Li unige

Length scales



Beenakker and van Houten, 1991

Geometrical dimension L

(size of conductor)

Phase coherence length l_ϕ

(distance an electron travels before suffering a phase change of 2π)

Elastic scattering length l_e

(mean free path between elastic scattering events)

Inelastic scattering length l_{in}

(distance an electron travels before loosing an energy kT)

Macroscopic conductor $l_e << l_\phi \leq l_{in} << L$

Mesoscopic conductor $l_e << L << l_\phi \leq l_{in}$

Physics versus geometry

Mesoscopic physics = « Between mircoscopic and macroscopic »

Nano physics = on the geometrical length of a nanometer

Definition of mesoscopic physics is based on physical length scales. In contrast, nanophysiscs, is a definition based on a geometrical length scale.

Lecture contents

Conductance from transmission

1. Single channel conductors
2. Multichannel conductors
3. Multiprobe conductors (omitted)

Thermoelectric transport

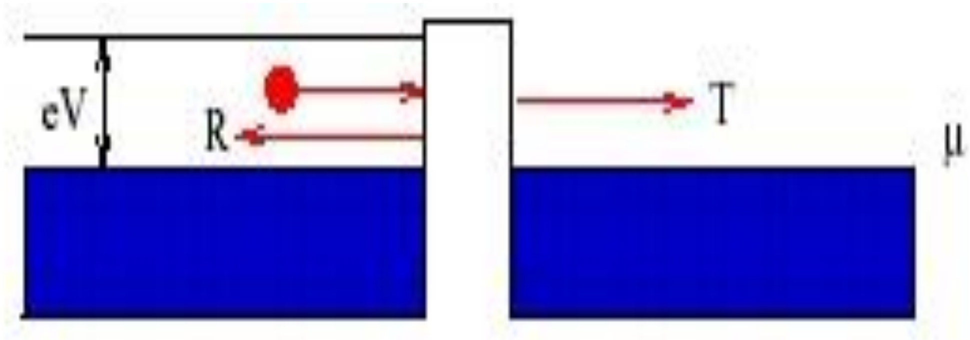
1. Two-terminal coductors
2. Thermoelectrics of a quantum dot
3. Multiprobe conductors (omitted)
4. Magnetic field symmetry (omitted)

Conductance from Transmission

1. Single channel conductors

Conductance from scattering theory

Heuristic discussion



Fermi energy left contact $\mu + eV$

Fermi energy right contact μ ,

applied voltage eV ,

transmission probability T ,

reflection probability R ,

incident current $I_{in} = e v_F \Delta\rho$

density $\Delta\rho = (d\rho/dE)\, eV$

density of states $d\rho/dE = (d\rho/dk)\,(dk/dE) = (1/2\pi)\,(1/\hbar v_F)$

$\Longrightarrow$ $I_{in} = (e/h) eV$ independent of material !!

$I = (e/h) T eV$ $\Longrightarrow$

$$G = dI/dV = \frac{e^2}{h} T$$

« Landauer formula »

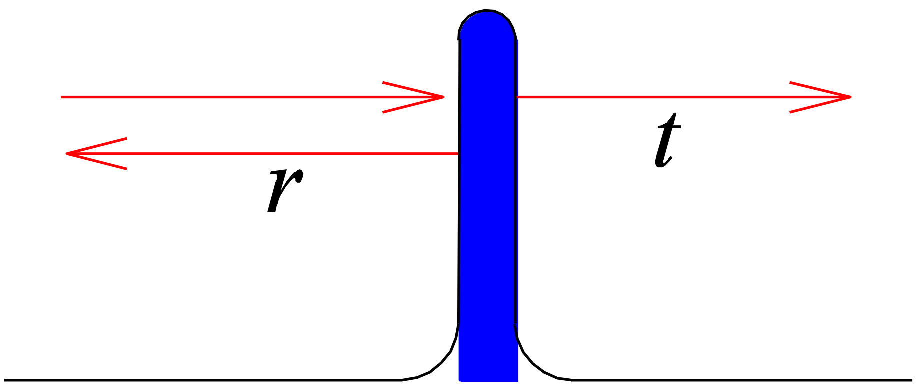
Scattering matrix

scattering state

$$|\Psi>_{inc} = \; e^{ikx}$$

$$|\Psi>_{ref} = r e^{-ikx}$$

$$|\Psi>_{tra} = t\, e^{ikx}$$



scattering matrix

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

current conservation $\Rightarrow$ S is a unitray matrix

In the absence of a magnetic field S is an orthogonal matrix

$$t' = t$$

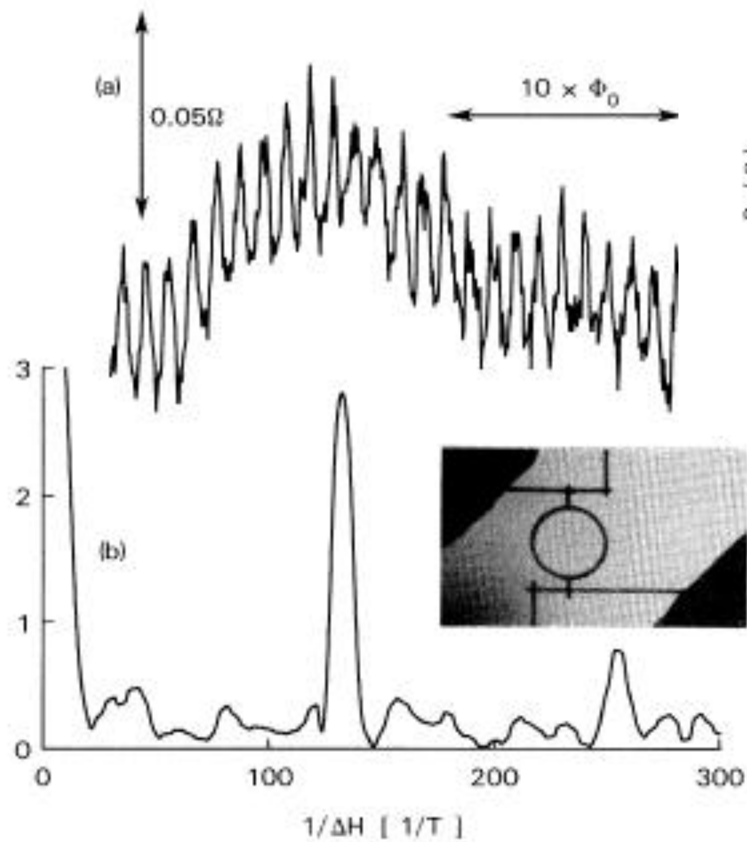
Aharonov-Bohm oscillations

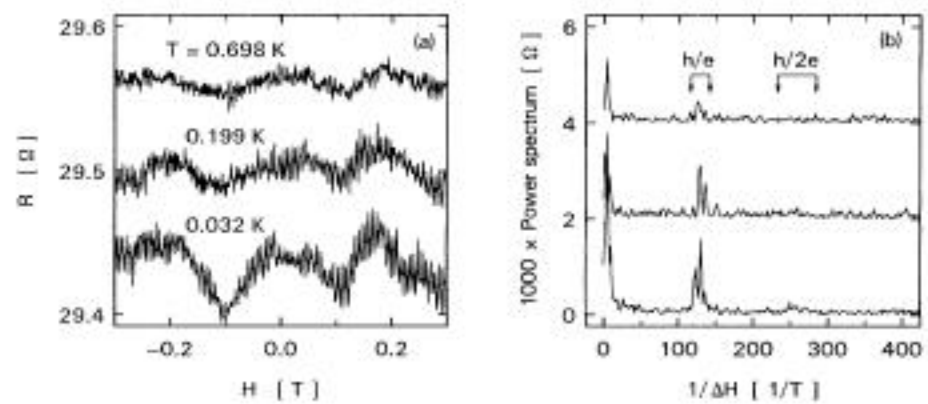
VOLUME 54, NUMBER 25 PHYSICAL REVIEW LETTERS 24 JUNE 1985

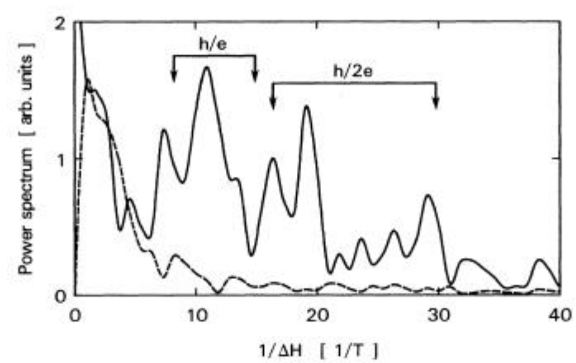
Observation of h/e Aharonov-Bohm Oscillations in Normal-Metal Rings

R. A. Webb, S. Washburn, C. P. Umbach, and R. B. Laibowitz
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598
(Received 27 March 1985)

Magnetoresistance oscillations periodic with respect to the flux h/e have been observed in submicron-diameter Au rings, along with weaker $h/2e$ oscillations. The h/e oscillations persist to very large magnetic fields. The background structure in the magnetoresistance was *not* symmetric about zero field. The temperature dependence of both the amplitude of the oscillations and the background are consistent with the recent theory by Stone.



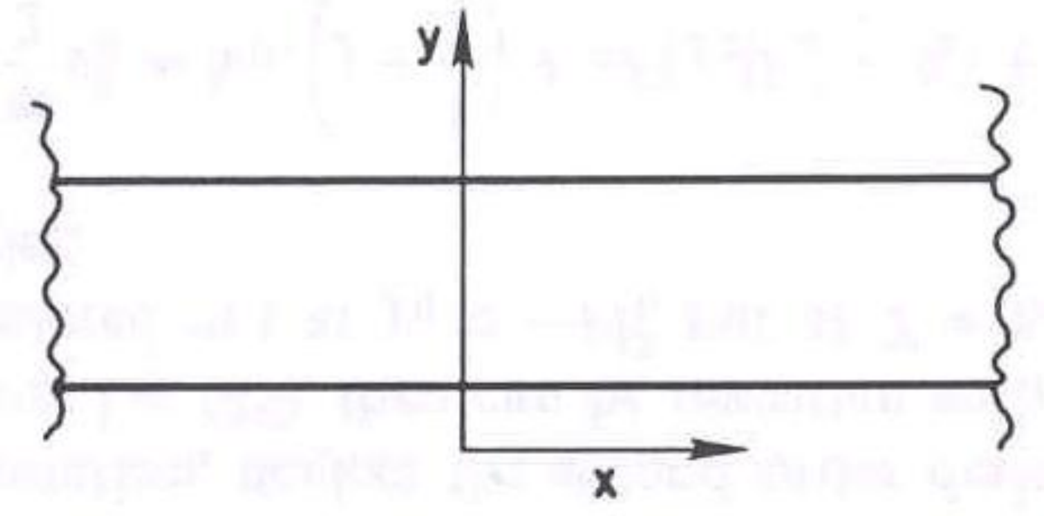


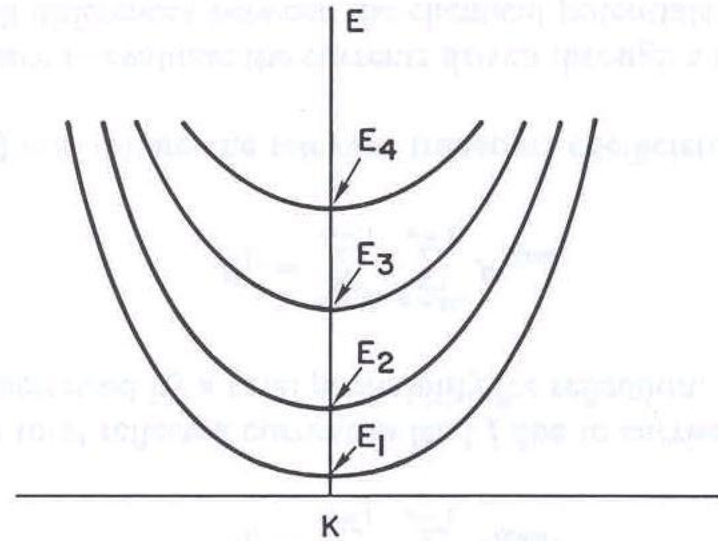


Conductance from Transmission

2. Two-probe multi-channel conductors

Multi-channel conductance: leads





asymptotic perfect translation invariant potential

$$V(x,y) = V(y) \quad \Longrightarrow$$

seprable wave function

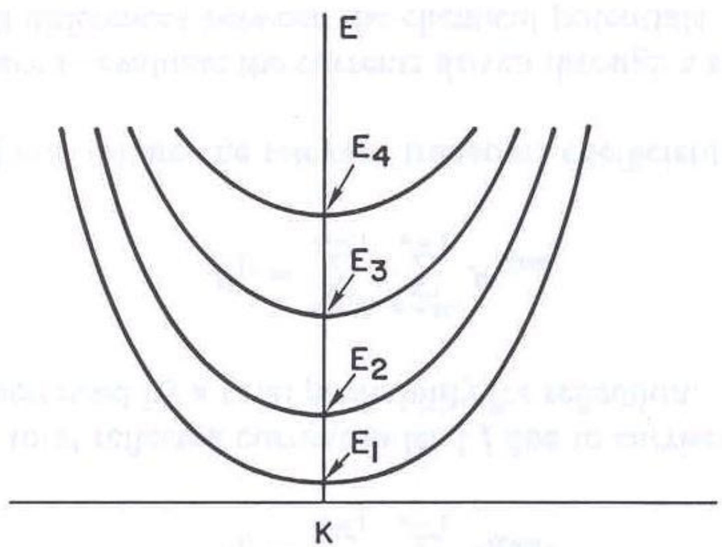
$$\phi^{\pm}_{\alpha n}(\mathbf{r}, E) = e^{\pm i k_n(E) x}\, \chi_{\alpha n}(y)$$

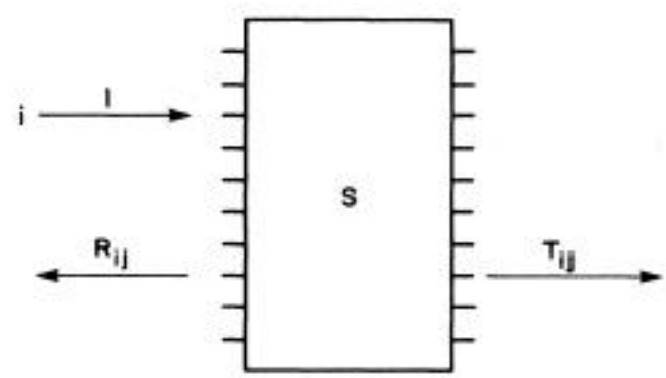
energy of transverse motion E_n channel threshold

energy for transverse and longitudnial motion

$$E = E_n + \hbar^2 k^2/2m \quad \Leftrightarrow \quad \text{scattering channel}$$

Mulit-channel conductance





incident current in channel i

$$I_{in} = e v_i \Delta\rho_i$$

density in channel i

$$\Delta\rho_i = (d\rho_i/dE)\, eV$$

density of states in channel i

$$\frac{d\rho_i}{dE} = \frac{d\rho_i}{dk}\frac{dk}{dE_i} = \frac{1}{2\pi}\frac{1}{\hbar v_i}$$

$\Longrightarrow$ independent of channel

$$I_{in} = (e/h)eV \Longrightarrow$$

$$I = (e/h)eV \sum_i \sum_j T_{ij} \Longrightarrow G = dI/dV = \frac{e^2}{h} T$$

$$T \equiv \sum_i \sum_j T_{ij}$$

« Landauer formula »

Eigen channels

$$T = \sum_{mn} T_{\beta\alpha,mn} = \sum_{mn} |s_{\beta\alpha,mn}|^2 = Tr[s^{\dagger}_{\alpha\beta} s_{\alpha\beta}] = Tr[t^{\dagger} t]$$

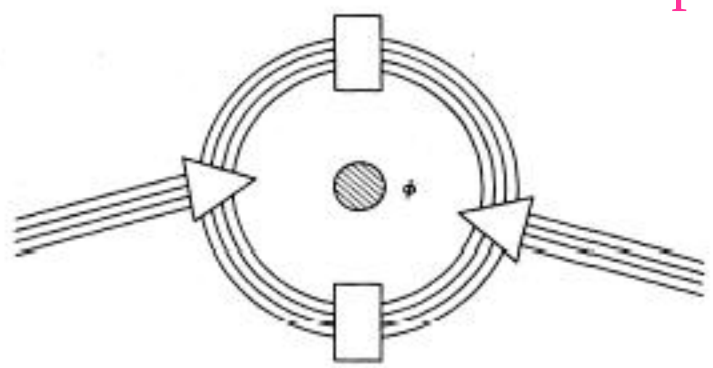
$t^{\dagger} t$ hermitian matrix; real eigenvalues T_n

$r^{\dagger} r$ hermitian matrix; real eigenvalues R_n

$$T = Tr[t^{\dagger} t] = \sum_n T_n$$

$$G = \frac{e^2}{h} \sum_n T_n$$

T_n are the genetic code of mesoscopic conductors !!



$\Longrightarrow$

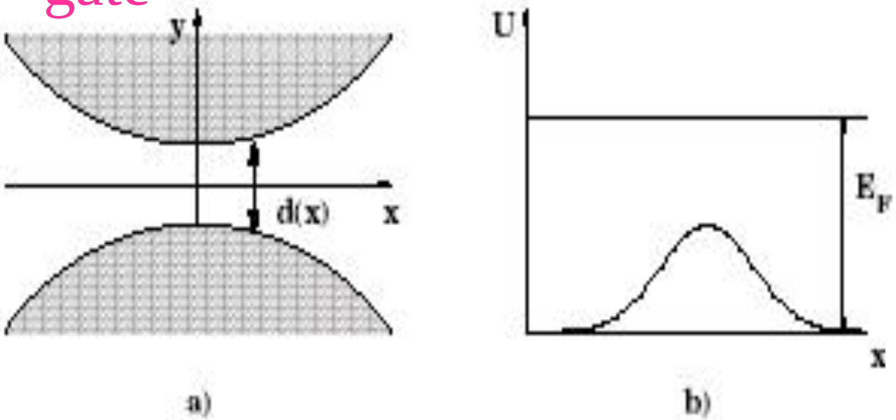
Many single channel conductors in parallel.
All the properties we discussed for single-channel two-probe conductors apply equally to many-channel multi-probe conductors: in particular

$$G(B) = G(-B)$$

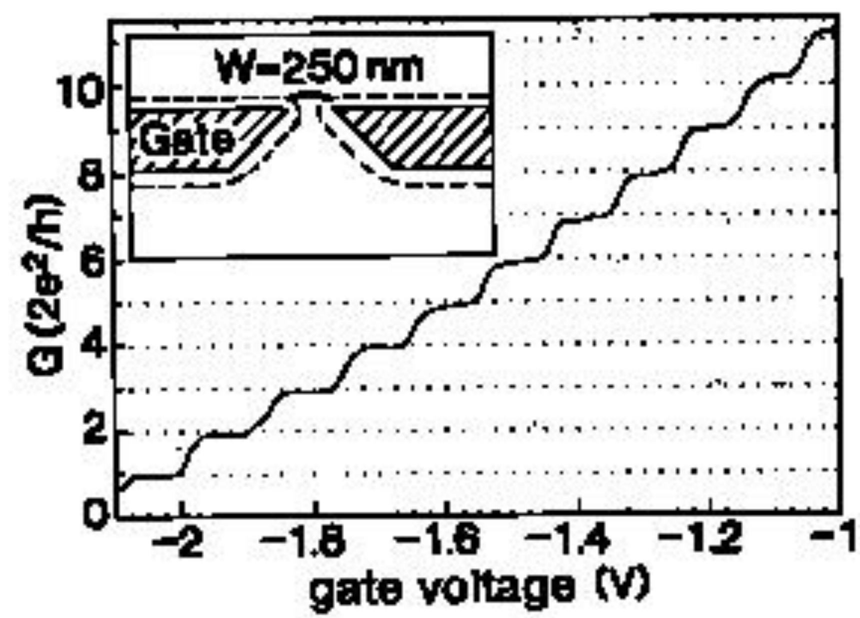
Quantum point contact

van Wees et al., PRL 60, 848 (1988)
Wharam et al, J. Phys. C 21, L209 (1988)

gate



gate



Quntum point contact

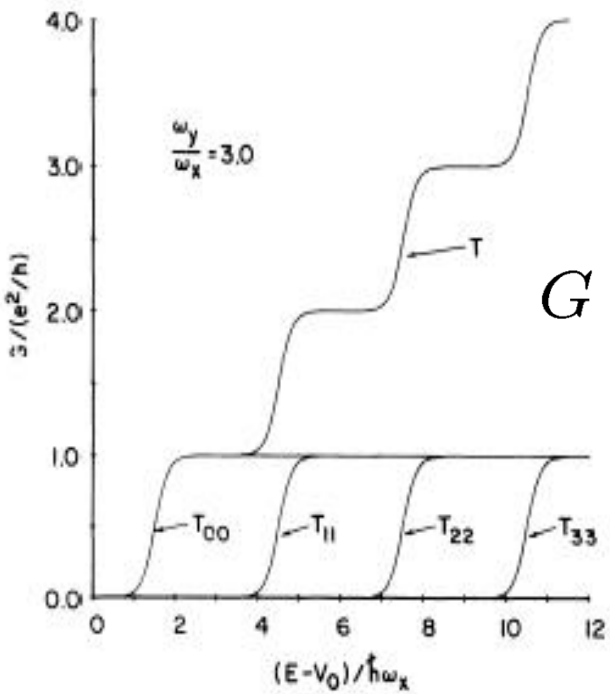
Buttiker, Phys. Rev. B41, 7906 (1990)

Saddle-point potential

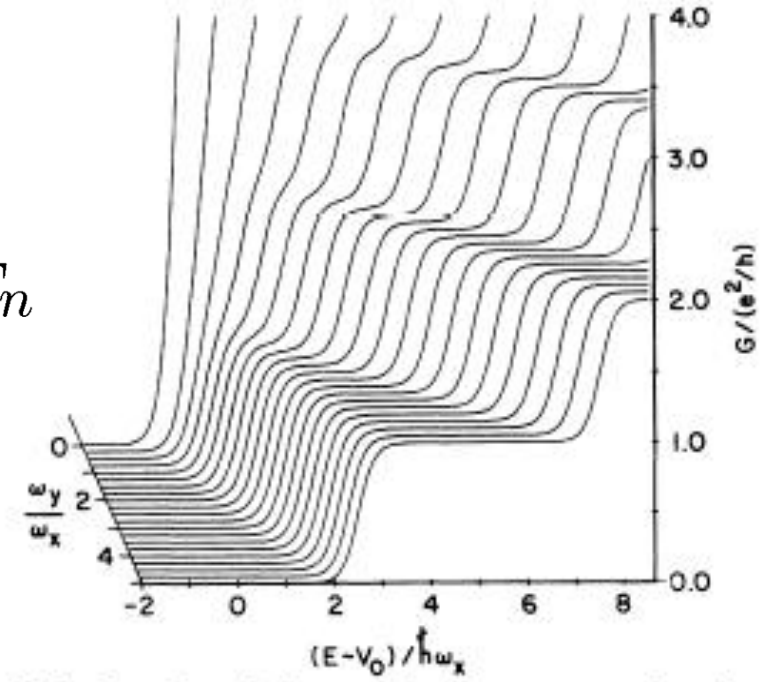
$$V(x,y) = V_0 - (1/2)m\omega_x^2 x^2 + (1/2)m\omega_y^2 y^2 + \ldots$$

Transmission probability

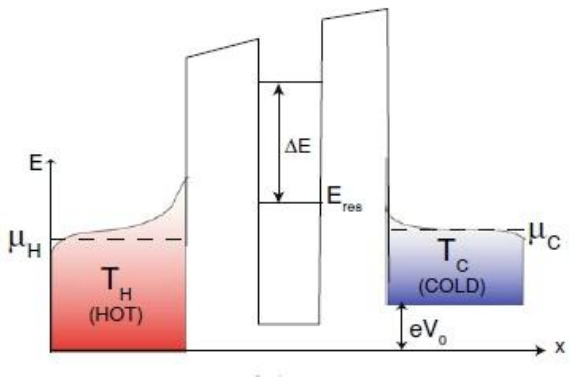
$$T_n = \frac{1}{1+e^{-\pi\epsilon_n}}\ ; \qquad \epsilon_n = 2[E - V_0 - \hbar\omega_y(n+1/2)]/\hbar\omega_x$$



$$G = \frac{e^2}{h}\sum_n T_n$$



Conductance of resonant level



Transmission probability oof single level

$$T(E) = \frac{\Gamma_L \Gamma_R}{(E - E_r)^2 + \Gamma^2/4}$$

Energy of resonant level E_r

Level width $\Gamma = \Gamma_L + \Gamma_R$

$$\Gamma_L = h\nu T_L, \ \Gamma_R = h\nu T_R$$

Conductance

$$G = \frac{e^2}{h} \int dE T(E)(-df/dE)$$

Low temperature limit $k_B T \ll \Gamma$

$$G = \frac{e^2}{h} \frac{\Gamma_L \Gamma_R}{(\mu - E_r)^2 + \Gamma^2/4}$$

High temperature limit $k_B T \gg \Gamma \Longrightarrow T(E) = 2\pi \frac{\Gamma_L \Gamma_R}{\Gamma} \delta(E - E_r)$

$$G = \frac{e^2}{h} 2\pi \frac{\Gamma_L \Gamma_R}{\Gamma} (-df/dE)|_{Er}$$

Thermoelectric Transport

1. Two terminal conductors

Energy current

Energy flux in a quantum channel: reservoirs at T1 and T2:

$$I_E = \frac{1}{h}\int dEE(f_1(E,T_1) - f_2(E,T_2))$$

Small temperature difference

$$I_E \approx \frac{\pi^2 k_B^2 T_2}{3h}(T_1 - T_2)$$

Thermal quantum (independent of electron or channel properties!!)

$$\frac{\pi^2 k_B^2 T}{3h}$$

H. L. Engquist and P. W. Anderson, Phys. Rev. B24, 1151 (1981)

$$L_S = \frac{\pi^2 k_B^2}{3e^2}$$

Lorentz factor (Sommerfeld theory)

Heat current

Heat current in perfect quantum channel, (linear response)

$$U = \frac{1}{h}\int dE\,(E-\mu)\,(f_1(E,T_1) - f_2(E,T_2))$$

Heat current (elastic backscattering , linear response)

$$U = \frac{1}{h}\int dE\,(E-\mu)\,(\sum_n T_n)\,(f_1(E,T_1) - f_2(E,T_2))$$

Connection with energy and electrical current

$$U = I_E - \mu(I/e)$$

Thermoelectric transport (linear response)

$$\begin{pmatrix} I \\ U \end{pmatrix} = \begin{pmatrix} L_0 & L_1 \\ L_1 & L_2 \end{pmatrix} \begin{pmatrix} (\mu_1 - \mu_2) \\ (T_1 - T_2)/T \end{pmatrix}$$

$$L_\nu = \frac{1}{h}\int dE\,(E-\mu)^\nu\,(\sum_n T_n)\,(-\frac{df}{dE})\,, \qquad \nu = 0, 1, 2$$

Thermoelectric transport

Fluxes in response to potentials

$$\begin{pmatrix} I \\ U \end{pmatrix} = \begin{pmatrix} L_0 & L_1 \\ L_1 & L_2 \end{pmatrix} \begin{pmatrix} (\mu_1 - \mu_2) \\ (T_1 - T_2)/T \end{pmatrix}$$

Current and temperature differences as driving forces

$$\begin{pmatrix} V \\ U \end{pmatrix} = \begin{pmatrix} R & S \\ \pi & \kappa \end{pmatrix} \begin{pmatrix} I \\ (T_1 - T_2) \end{pmatrix}$$

R resistance

S thermopower

π Peltier

κ thermal conductance

Multi-terminal expressions:

P. N. Butcher , J. Phys.: Condensed Matter 2, 4869 (1990).

Thermopower

$$S = \frac{\Delta V}{\Delta T} = \frac{(\mu_1 - \mu_2)}{e(T_1 - T_2)} = -\frac{1}{eT}\frac{L_1}{L_0}$$

Cutler-Mott formula

$$S = -\frac{1}{eT}\frac{\int dE\,(E-\mu)\,(\sum_n T_n)\,(df/dE)}{\int dE\,(\sum_n T_n)\,(df/dE)}$$

Sommerfeld integral

$$M_3 = -\frac{1}{2}\int dE\,(E-\mu)^2\,(df/dE) = \frac{\pi^2}{6}(k_B T)^2$$

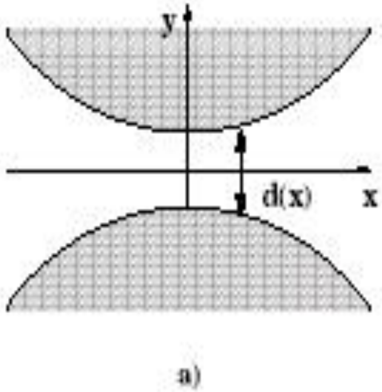
zero temperature limit

$$S = \frac{\pi^2 k_B^2 T}{3e}\frac{d}{dE}\ \ln T(E)|_{E=E_F}$$

Thermopower of a QPC

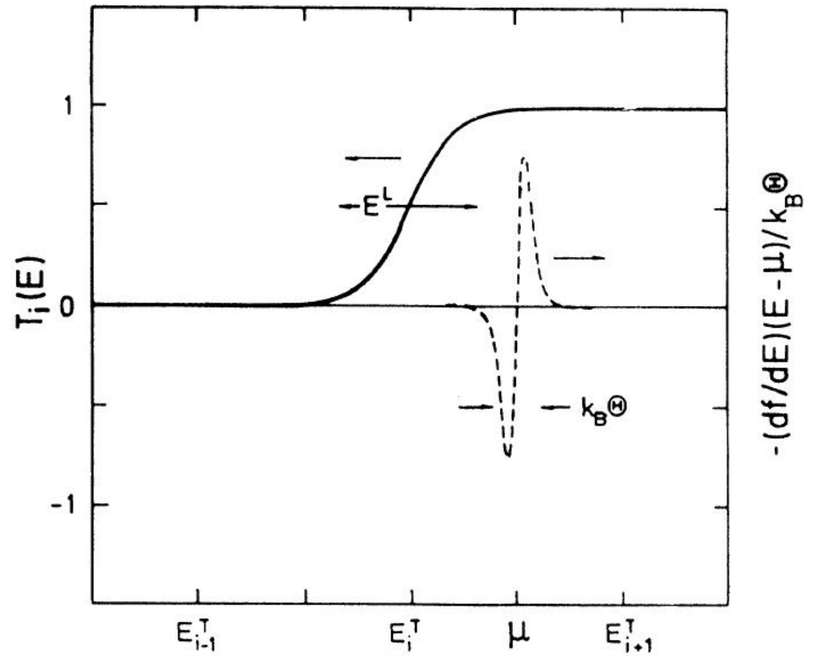
Proetto, PRB 44, 9096 (1991)

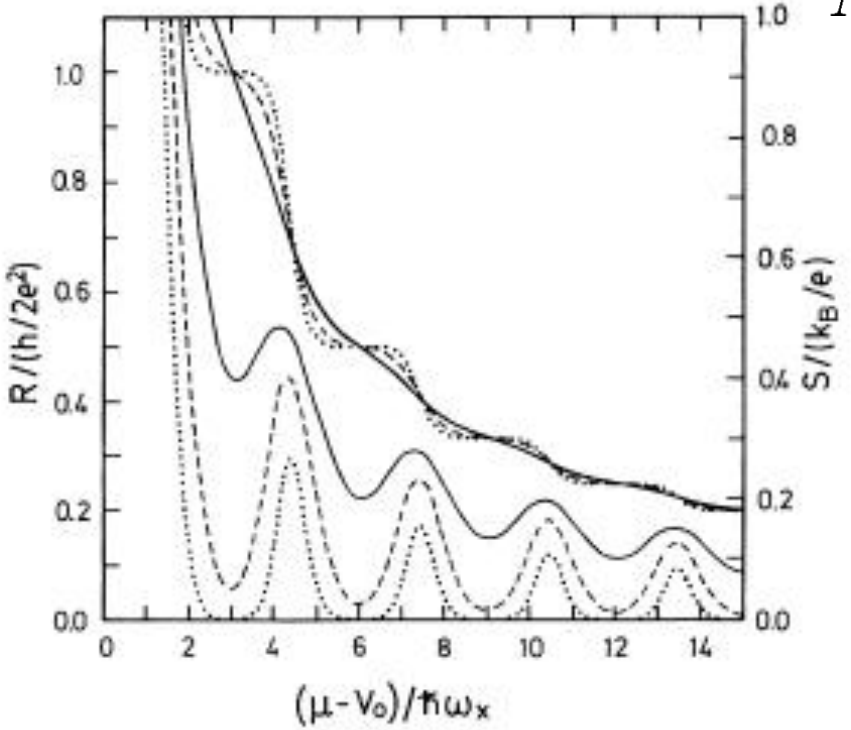
$$S = -\frac{1}{eT}\frac{\int dE\,(\sum_n T_n)\,(E-\mu)\,(df/dE)}{\int dE\,(\sum_n T_n)\,(df/dE)}$$



$$T_n = \frac{1}{1+e^{-\pi\epsilon_n}}\;;$$

Channel dependence $\frac{1}{N}$



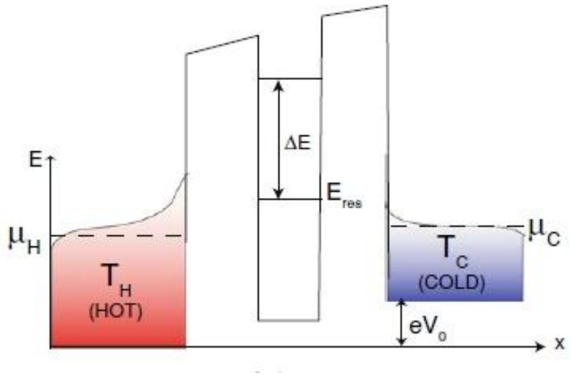


Thermoelectric transport

2. Thermoelectric transport of a quantum dot

Thermopower for resonant transmission

P. Mani, N. Nakpathomkun, H. Linke, Journal of Electronic Materials 38, 1163 (2009).



$$S = -\frac{k_B}{ek_BT}\frac{\int dE\,(E-\mu)\left(\sum_n T_n\right)(df/dE)}{\int dE\left(\sum_n T_n\right)(df/dE)}$$

Resonant transmission probability

$$T(E) = \frac{\Gamma_L\Gamma_R}{(E-E_r)^2+\Gamma^2/4}$$

Level width $\Gamma = \Gamma_L + \Gamma_R$

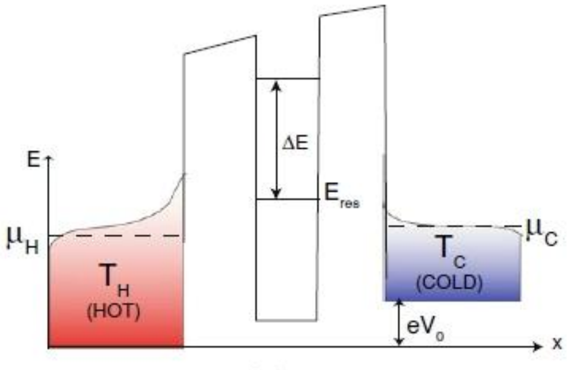
High temperature limit $k_BT \gg \Gamma \implies T(E) = 2\pi\frac{\Gamma_L\Gamma_R}{\Gamma}\delta(E-E_r)$

$$S = -\frac{k_B}{ek_BT}(\mu - E_r)$$

Universal ! But only as long as thermal energy is small compared to the level separation.

Thermopower for resonant transmission

P. Mani, N. Nakpathomkun, H. Linke,
Journal of Electronic Materials 38, 1163 (2009).



Cutler-Mott

$$S = -\frac{k_B}{ek_BT}\frac{\int dE\,(E-\mu)\,(\sum_n T_n)\,(df/dE)}{\int dE\,(\sum_n T_n)\,(df/dE)}$$

Low temperature limit of CM-formula

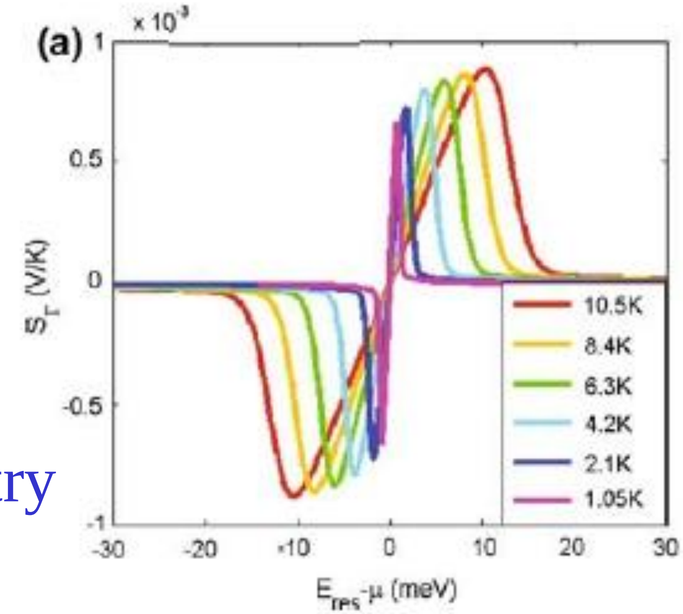
$$S = \frac{\pi^2 k_B^2 T}{3e}\frac{d}{dE}\ln T(E)|_{E=E_F}$$

Resonant transmission probability

$$T(E) = \frac{\Gamma_L \Gamma_R}{(E-E_r)^2 + \Gamma^2/4}$$

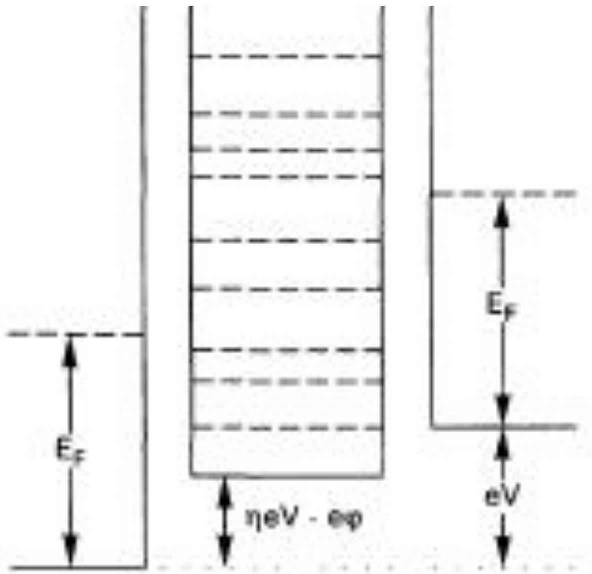
$$S = \frac{\pi^2 k_B^2 T}{3e}\frac{2(\mu - E_r)}{(\mu - E_r)^2 + \Gamma^2/4}$$

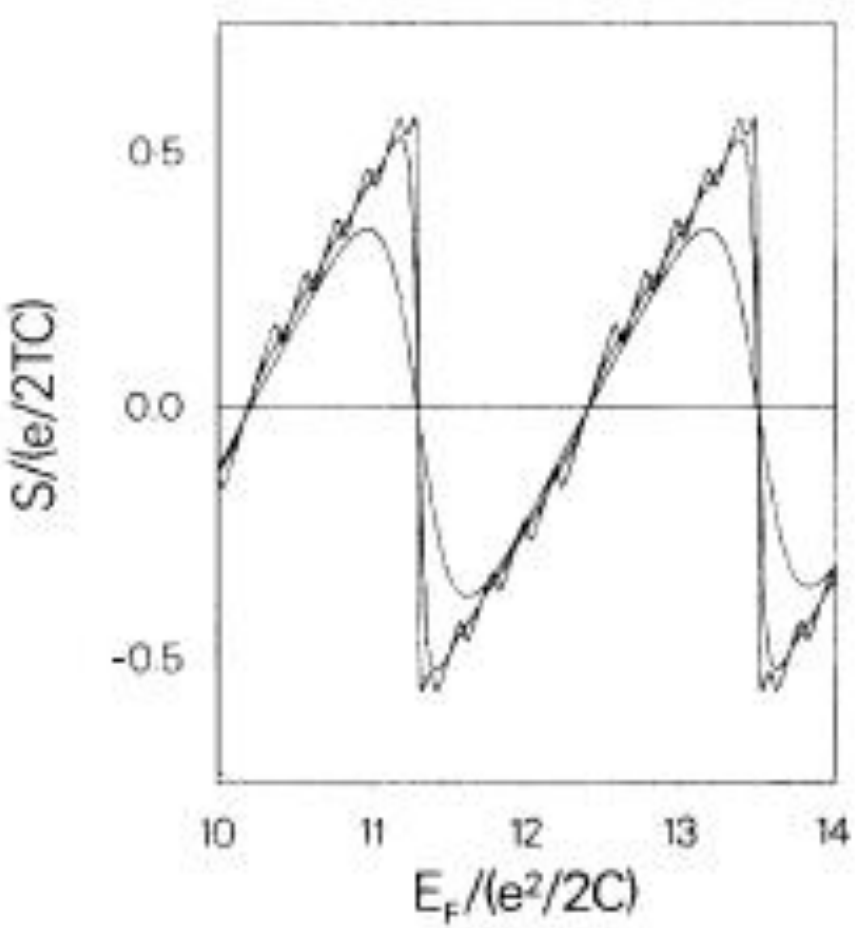
Note that this is independent of symmetry



Thermopower of a multilevel dot

C. W. J. Beenakker and A. A. M. Staring Phys. Rev. B 46, 9667 (1992)





Thermopower of a chaotic cavity

S. F. Godijn, S. Möller, H. Buhmann, L. W. Molenkamp, S. A. van Langen **PRL 82, 2927–2930 (1999)**

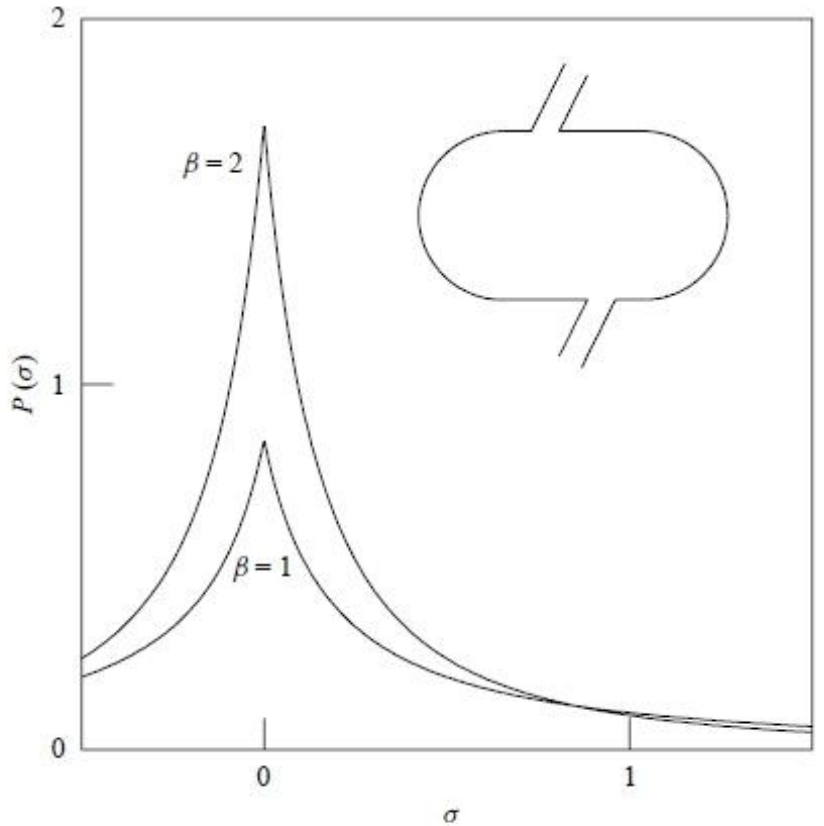
Cutler-Mott-formula

$$S = -\frac{1}{eT}\frac{\int dE\,(E-\mu)\,(\sum_n T_n)\,(df/dE)}{\int dE\,(\sum_n T_n)\,(df/dE)}$$

zero temperature limit

$$S = \frac{\pi^2 k_B^2 T}{3e}\frac{d}{dE}\ln T(E)|_{E=E_F}$$

Probability distribution of the thermopower of a chaotic cavity one channel leads



S. A. van Langen, P. G. Silvestrov, C. W. J. Beenakker, Supperlattice and Microstructures, 23, 691 (1999).

Efficiency of a single level dot

Efficiency $\eta = P/U$

Power $P = IV$

Current $I = \frac{e}{h}\int dE\, T(E)\,(f_C(E,T_C) - f_H(E,T_H))$

Heat current $U_\alpha = \frac{1}{h}\int dE\,(E-\mu_\alpha)\,T(E)\,(f_H(E,T_H)-f_C(E,T_C))$

High temperature limit $k_B T \gg \Gamma \implies T(E) = 2\pi \frac{\Gamma_L \Gamma_R}{\Gamma}\delta(E - E_r)$

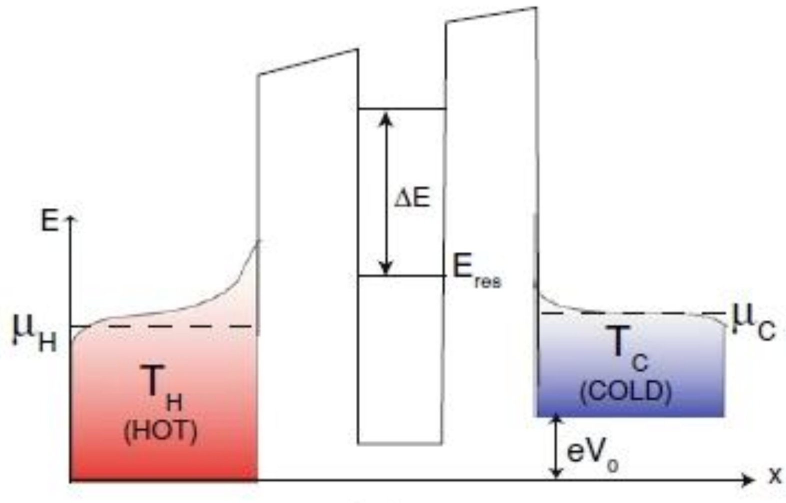
Efficency

$$\frac{\eta}{\eta_C} = \frac{\mu_C - \mu_H}{(E_r - \mu_H)} = \frac{eV}{(E_r - \mu_H)}$$

Carnot efficiency is reached when $E_r = \mu_C$

Stall voltage $I = 0$

$$\frac{(E_r - \mu_H)}{k_B T_H} = \frac{(E_r - \mu_C)}{k_B T_C}$$

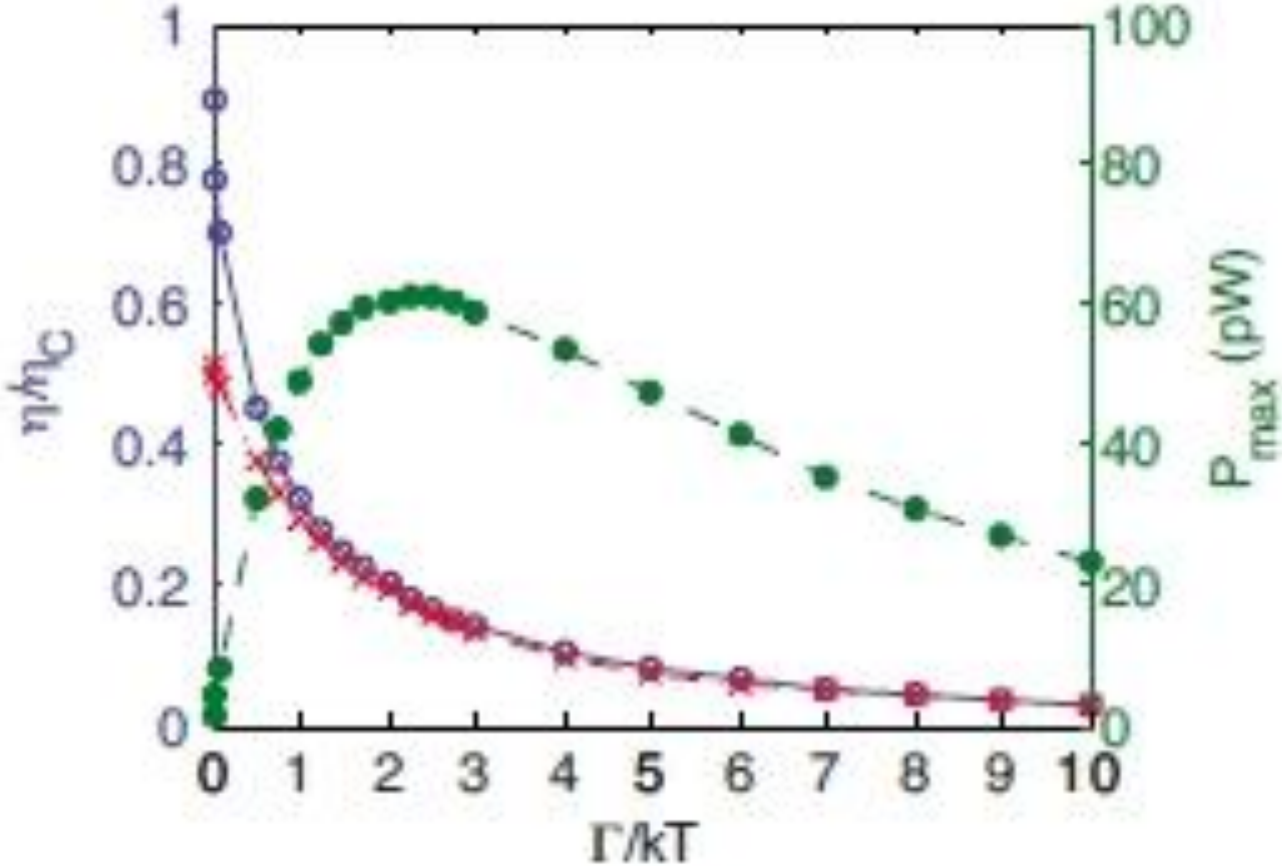


Efficiency at maximum power

Nakpathomkun, Xu, Linke, PRB 82, 235428 (2012)

------- efficiency at maximum power
------- maximum efficiency
------- maximum power

Maximization is with regards to the position of the resonant level position



Summary

Brief review of scattering approach to elctrical conductance

Magnetic field symmetry of conductance

Brief review of scattering approach to thermoelectric transport

Thermoelectric transport through a single level dot

Power, efficiency and efficiency at maximum power