Thermoelectric conversion at the spectrum edges of disordered nanowires

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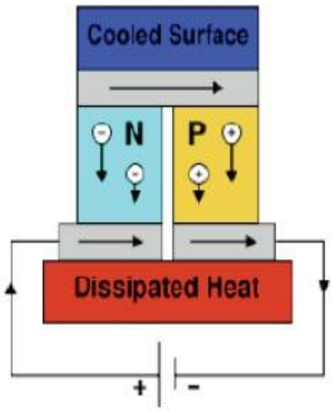
OUTLINE

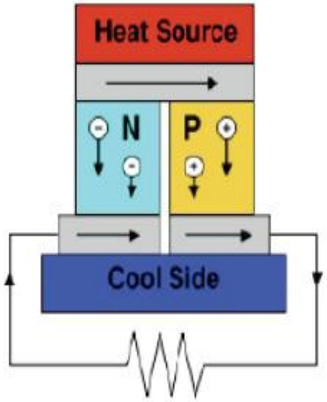
- Effects of gate voltage on thermoelectric conversion in 1D disordered nanowires
- Results in the Low-Temperature regime
- Results in the Variable-Range Hopping Regime

THERMOELECTRIC EFFECT

Peltier-Seebeck effect: describes the possibility of generating an electrical potential difference from a temperature gradient, and vice-versa.

Peltier (Π)





Seebeck (S)

Thermopower (Seebeck coefficient):

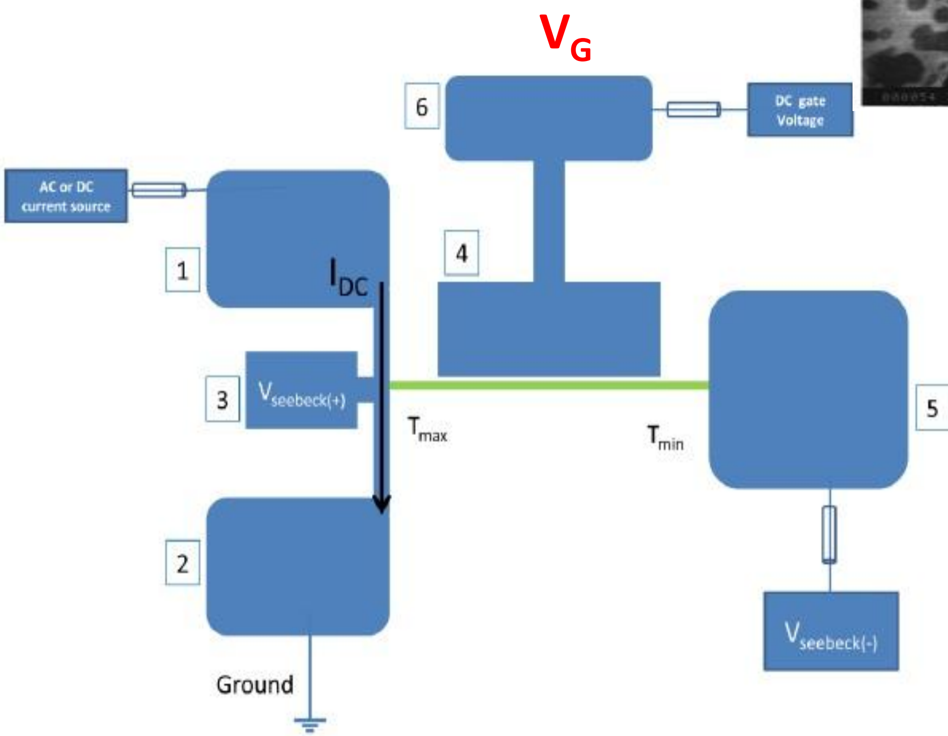
$$S = -\frac{\Delta V}{\Delta T} \quad \left(\frac{\mu V}{K}\right)$$

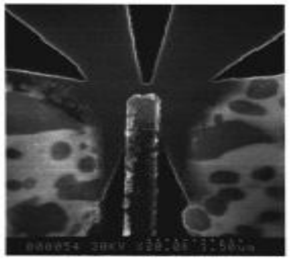
It measures the magnitude of the induced voltage in response to a temperature difference across a material.

Time-Reversal Symmetry: **Π = TS** (second Thomson relation)

GOAL : UNDERSTANDING HOW THERMOELECTRIC TRANSPORT DEPENDS ON CARRIER DENSITY IN THE WIRE

Gate-modulated thermoelectric conversion of one-dimensional disordered nanowires: sketch of a possible experimental setup



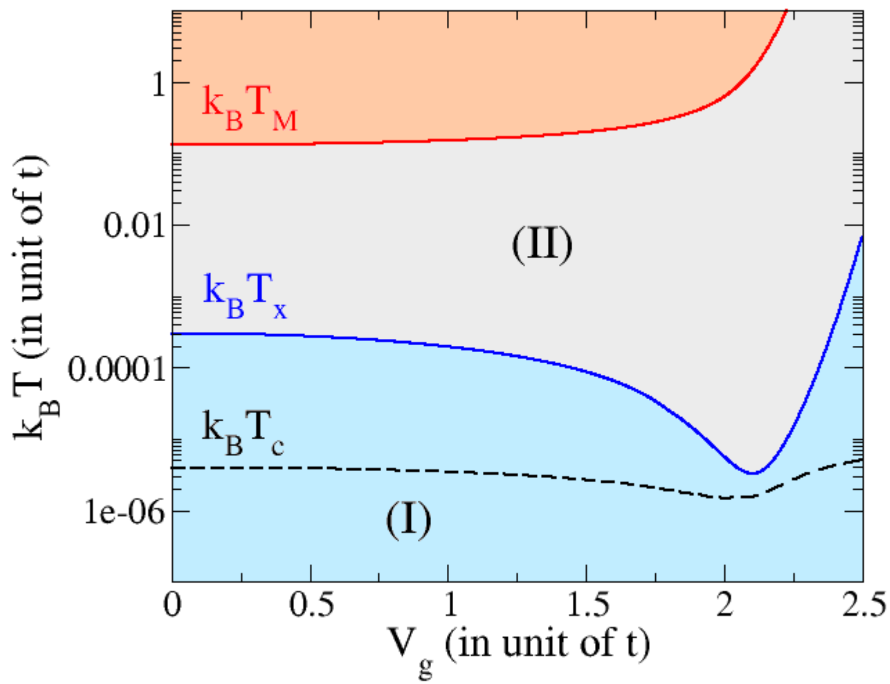


From [1]

[1] W. Poirier, D. Mailly & M. Sanquer, PRB **59**, 10856 (1999)

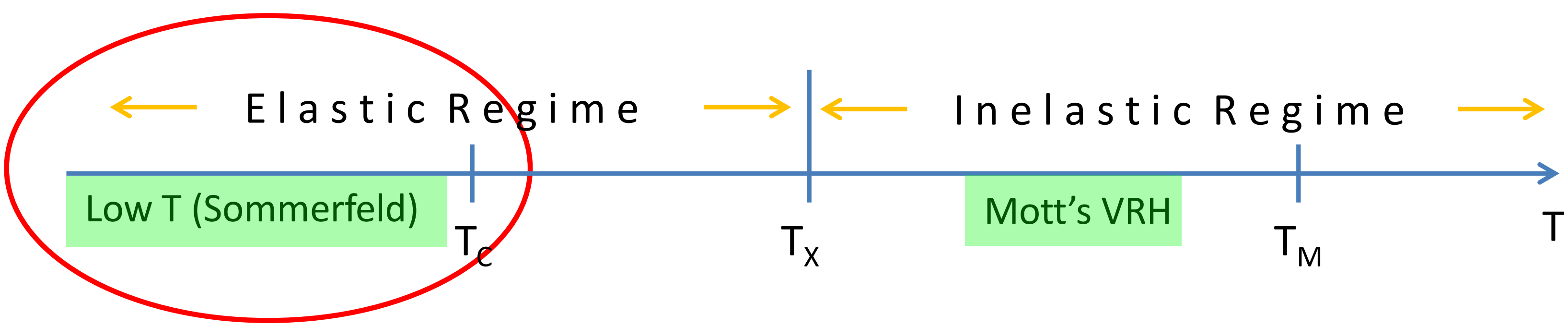
TEMPERATURE SCALES AND TRANSPORT MECHANISMS

1D Disordered Nanowire of size L and W=1 → spectrum edge at V_g = 2.5 t



- **T_C** - "Sommerfeld" temperature (Sommerfeld expansion - Elastic Transport)
- **T_X** - Activation temperature (Onset of inelastic transport - VRH)
- **T_M** - Mott temperature (Onset of simple activated regime - NNH)

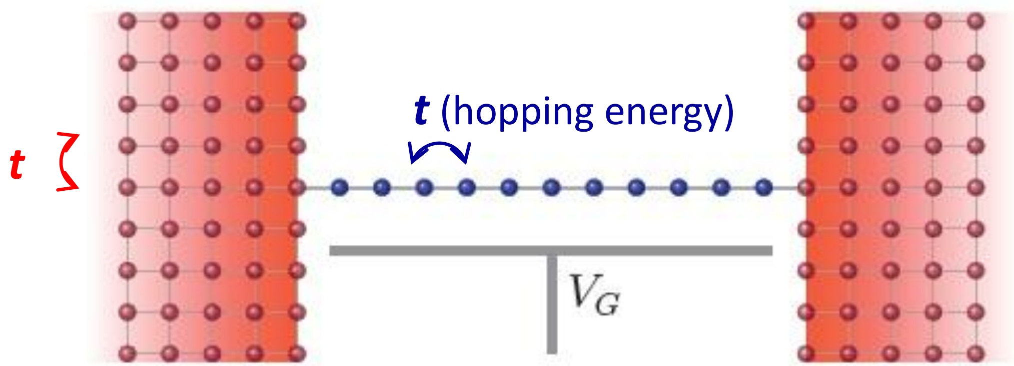
(I) Low-T Regime
(II) VRH Regime



THERMOPOWER IN LOW T REGIME: THEORY

1D system with disorder W → Anderson Localization with Localization length ξ(E)

Left lead (described by self-energy Σ_L)



Right lead (described by self-energy Σ_R)

Nanowire: lattice of length L (***N*** sites)
with on-site disorder (uniform distribution **W**)

Assumptions: Low Temperatures + Linear Response = **Mott's Formula**

$$S = t \left.\frac{\mathrm{d}\ln \mathcal{T}}{\mathrm{d}E}\right|_{E_F}$$

In physical units: $$S = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)\left(\frac{k_B T}{t}\right) s$$

Typical transmission in the localized regime: $$[\ln \mathcal{T}]_0(E) = -\frac{2N}{\xi(E)}$$

By knowing ξ(E) we can predict the behaviour of the typical thermopower

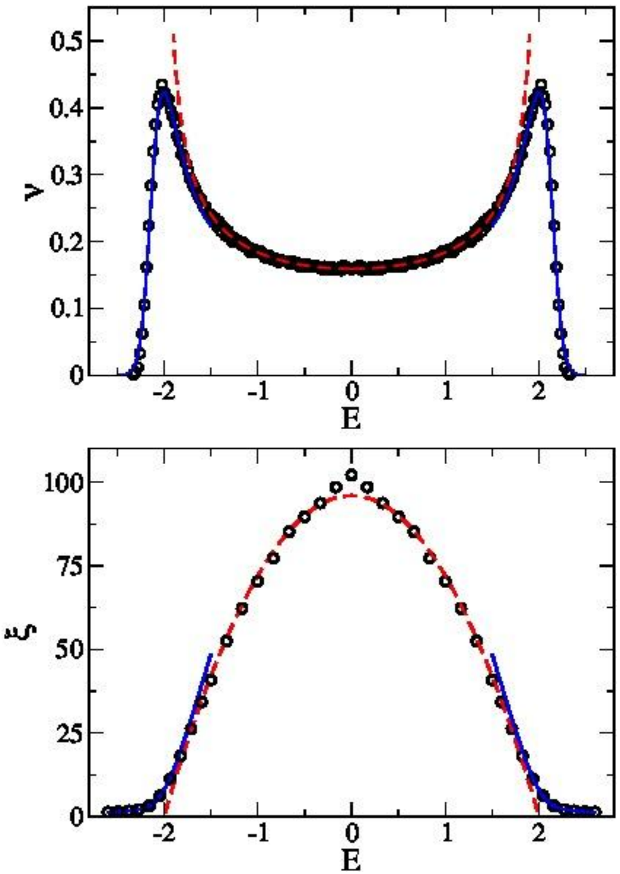
Numerics: tight binding Hamiltonian, RGF calculation

1D DENSITY OF STATES ν=ρ/N AND LOCALIZATION LENGTH ξ

1D nanowire of **N** sites with hopping **t** and disorder **W**

Analytical expressions derived in weak disorder limit

W=1 : spectrum edge at ~ 2t+W/2 ~ 2.5t



"Bulk" formulas:

$$\rho_b(E)/N = \frac{1}{2\pi t\sqrt{1-(E/2t)^2}}$$

$$\xi_b(E) = \frac{24}{W^2}\left(4t^2 - E^2\right)$$

"Edge" formulas (from [1]):

$$\rho_e(E)/N = \sqrt{\frac{2}{\pi}}\left(\frac{12}{tW^2}\right)^{1/3} \frac{\mathcal{I}_1(X)}{[\mathcal{I}_{-1}(X)]^2}$$

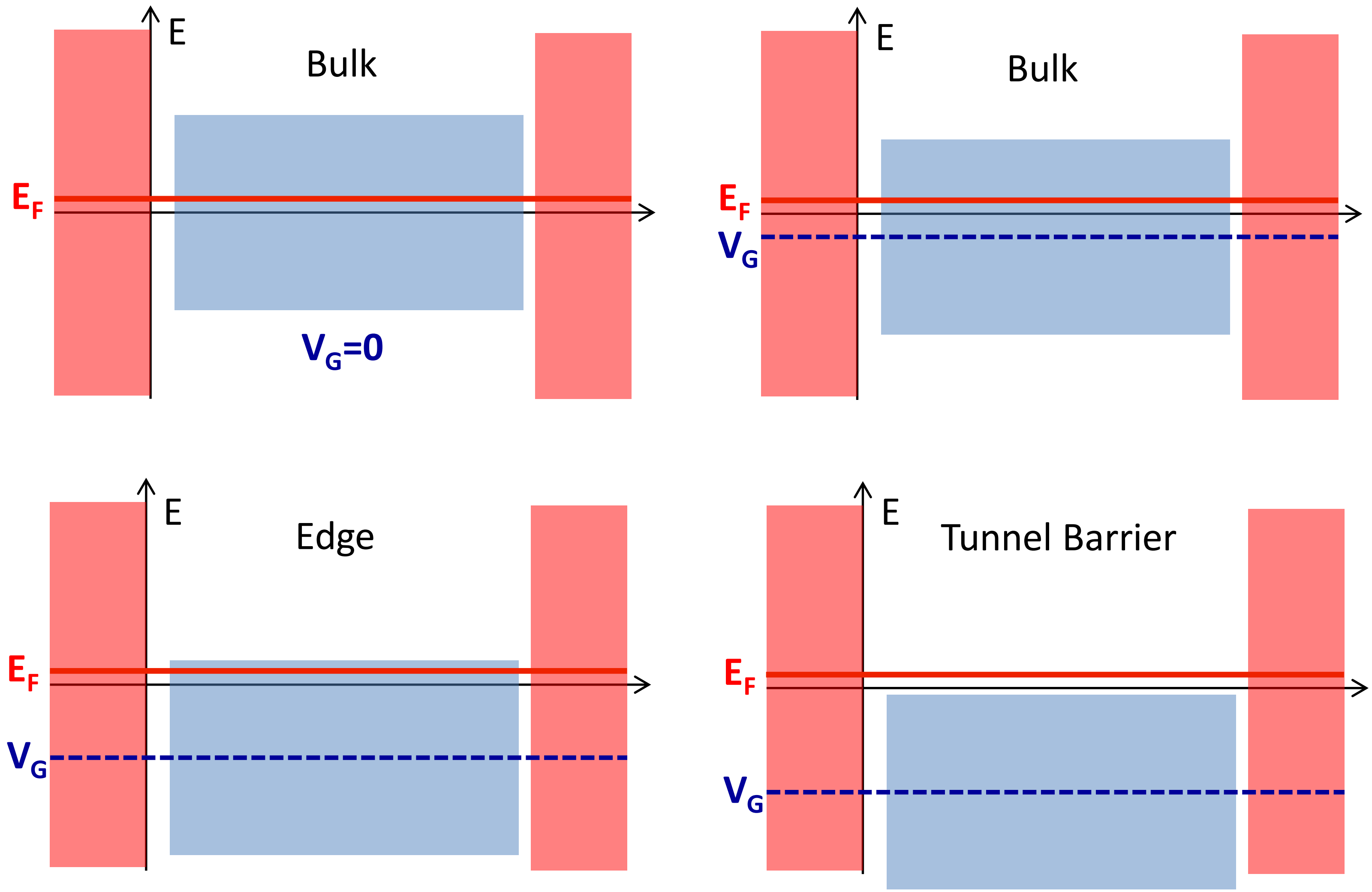
$$\xi_e(E) = 2\left(\frac{12t^2}{W^2}\right)^{1/3} \frac{\mathcal{I}_{-1}(X)}{\mathcal{I}_1(X)}$$

$$\mathcal{I}_n(X) = \int_0^\infty y^{n/2}\, e^{-\frac{1}{6}y^3+2Xy}\, dy$$

$$X = (|E| - 2t)t^{1/3}(12/W^2)^{2/3}$$

[1] B. Derrida & E. Gardner, J. Physique 45, 1283 (1984)

EFFECT OF GATE VOLTAGE ON THE ENERGY SPECTRUM



What matters is the <u>relative</u> position of E_F inside the energy spectrum

TYPICAL THERMOPOWER AT LOW T: WEAK DISORDER THEORY & NUMERICAL CHECK WITH W=1

From Mott's formula:

Bulk:

$$S_0^b = -N \frac{(E_F - V_g)\, W^2}{96t^3[1-((E_F-V_g)/2t)^2]^2}$$

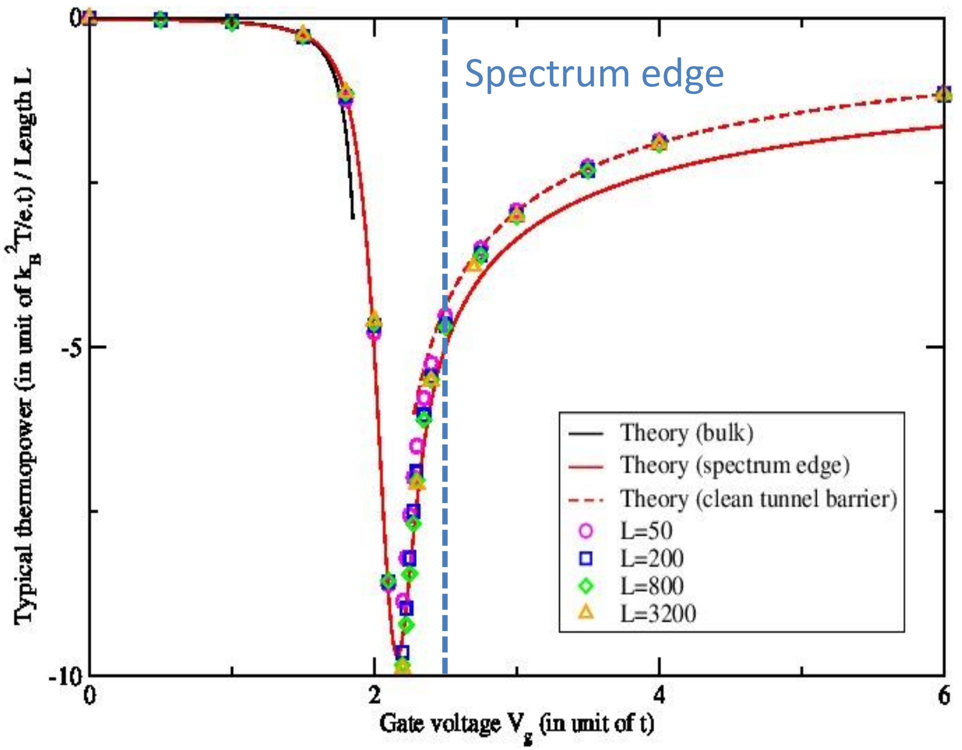
Edge:

$$S_0^e = -2N\left(\frac{12t^2}{W^2}\right)^{1/3}\left\{\frac{\mathcal{I}_3(X)}{\mathcal{I}_{-1}(X)} - \left[\frac{\mathcal{I}_1(X)}{\mathcal{I}_{-1}(X)}\right]^2\right\}$$

$$X = (|E_F - V_g| - 2t)t^{1/3}(12/W^2)^{2/3}$$

Tunnel Barrier:

$$\frac{S_0^{TB}}{N} \underset{N\to\infty}{\approx} \frac{1}{N}\frac{2t}{\Gamma(E_F)}\left.\frac{d\Gamma}{dE}\right|_{E_F} \pm \frac{1}{\sqrt{\left(\frac{E_F-V_g}{2t}\right)^2 - 1}}$$



Large Enhancement of the Thermopower near the spectrum edge of the nanowire

R. Bosisio, G. Fleury and J-L. Pichard, (2013)

MESOSCOPIC FLUCTUATIONS: THERMOPOWER DISTRIBUTIONS

In the Bulk → Cauchy distribution (demonstrated in [1] for the case S_0=0)

$$P(S) = \frac{1}{\pi}\frac{\Lambda}{\Lambda^2 + (S - S_0)^2}$$

$$\Lambda = \frac{2\pi t}{\Delta_F}$$

S_0 = typical thermopower
Δ_F = mean level spacing near E_F

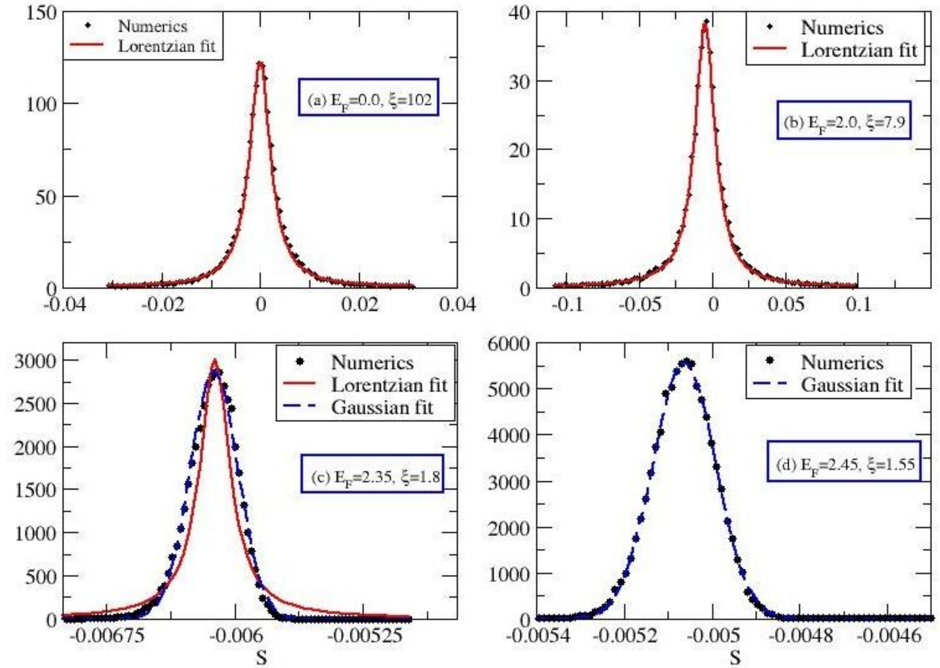
Near the Edge → Gauss distribution (characterized numerically)

$$P(S) = \frac{1}{\sqrt{2\pi}\lambda}\exp\left[-\frac{(S - S_0)^2}{2\lambda^2}\right]$$

$$\lambda \approx 0.6\frac{Wt\sqrt{N}}{(E_F - V_g)^2 - (2t + W/4)^2}$$

1D nanowire with disorder W=1 → Spectrum edge at E=2.5t

V_g = 0.0 V_g = 2.0



V_g = 2.35 V_g = 2.45

[1] S. A. van Langen, P. G. Silvestrov, and C.W. J. Beenakker, Supperlattices Microstruct. 23, 691 (1998).
[2] R.Bosisio, G. Fleury and J-L. Pichard, (2013)

MESOSCOPIC FLUCTUATIONS: CHARACTERIZING THE TRANSITION

$$\eta = \frac{\int dS |P(S) - P_G(S)|}{\int dS |P_L(S) - P_G(S)|}$$

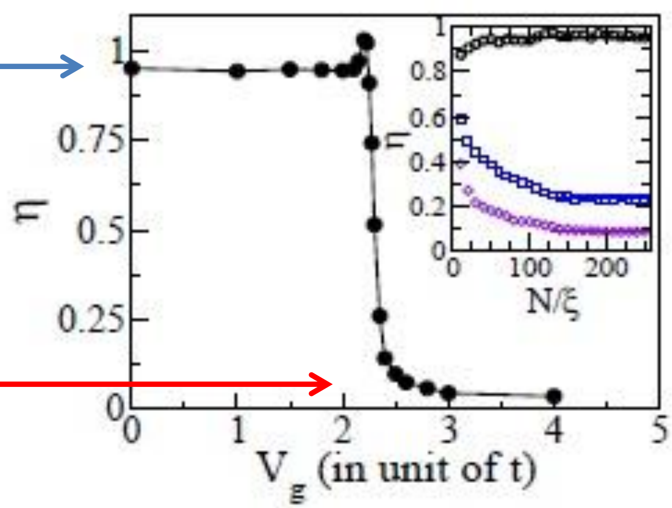
Parameter which measures the "distance" between the observed numerical distribution and the best Lorentzian (P_L) and Gaussian (P_G) fits

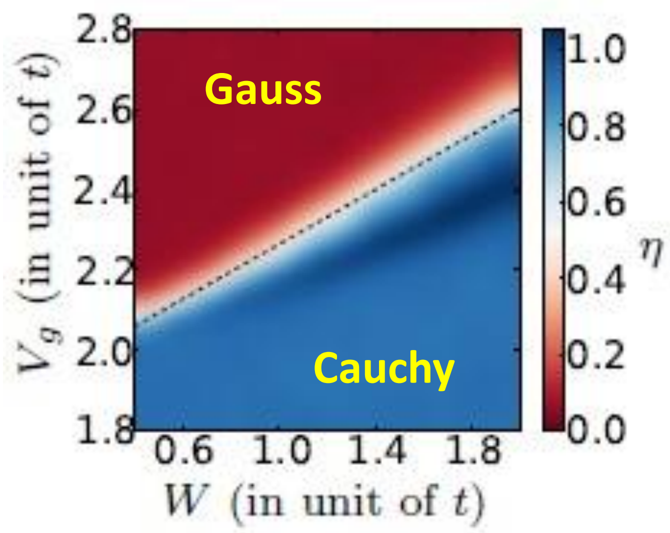
- $\eta = 1$ if Cauchy distribution
- $\eta = 0$ if Gauss distribution

W=1

Cauchy

Gauss





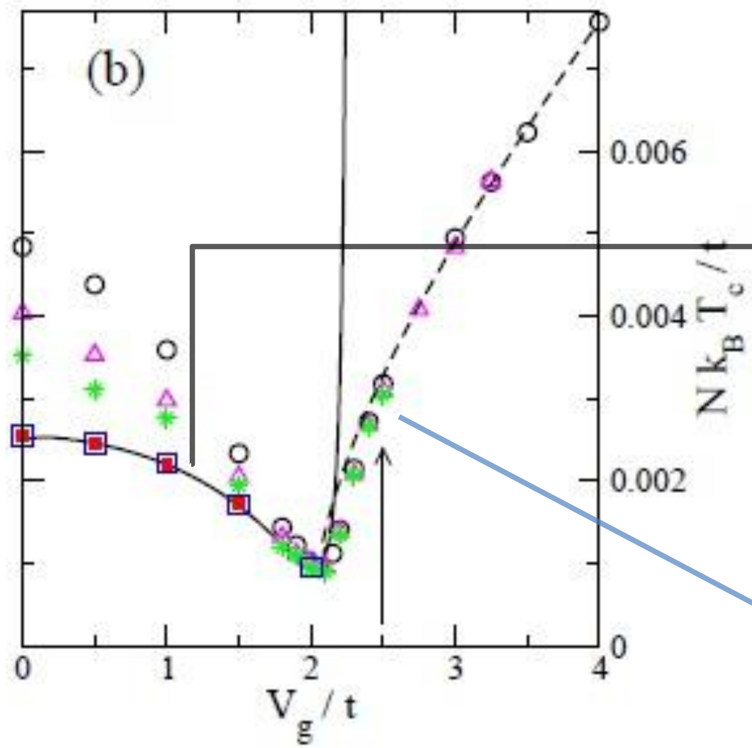
[1] R.Bosisio, G. Fleury and J-L. Pichard, (2013)

"SOMMERFELD" TEMPERATURE

Q: Validity of the Mott's formula for S

Validity of Sommerfeld Expansion → Wiedemann-Franz (WF) law, Mott's formula

Looking at the range of validity of W-F law



Sommerfeld temperature is proportional to the mean energy level spacing in the system:

$$k_B T_c \propto \Delta_F$$

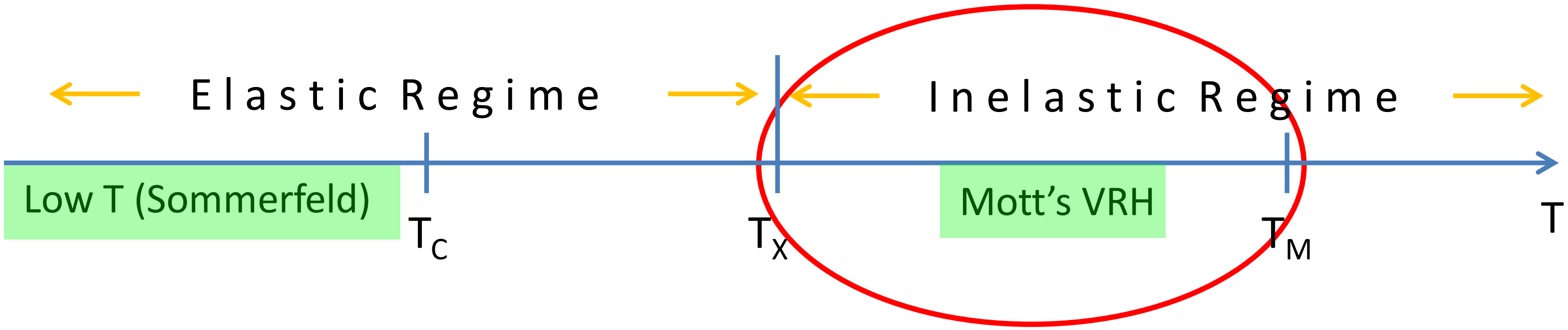
Proportionality constant depends on required precision

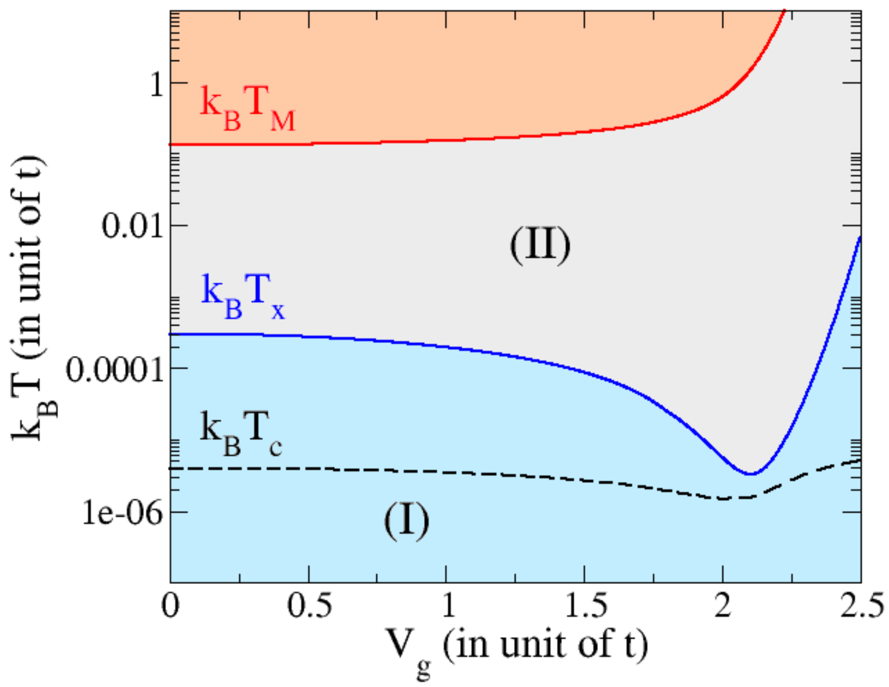
Result for the tunnel barrier:

$$N k_B T_c \propto t\sqrt{[(E_F - V_g)/(2t)]^2 - 1}$$

Estimation for Si nanowire: ~ 100 mK

PART 2: VRH TRANSPORT (II)



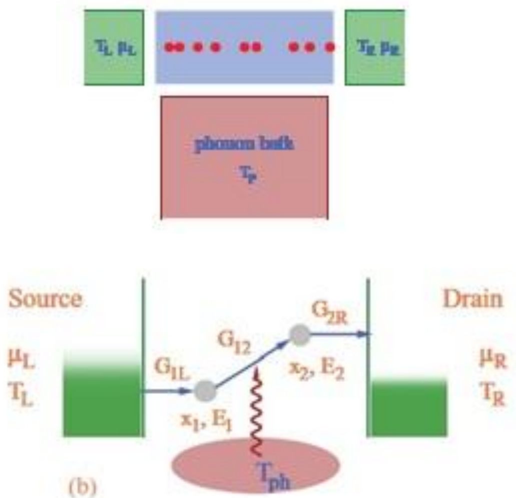


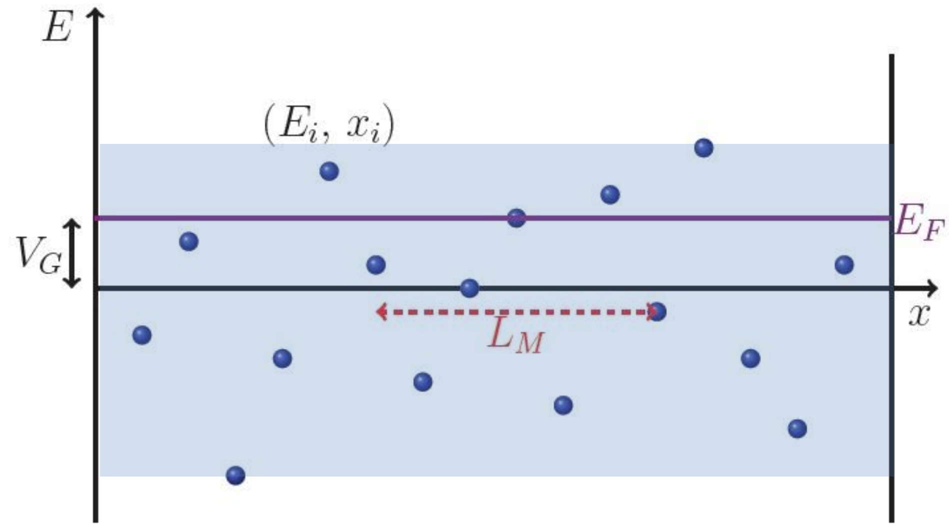
VRH: MODEL

Hopping between pairs of localized states mediated by phonons

Conductance: competition between **tunneling** and activated processes

$$G_{ij} \sim e^{-2|x_i - x_j|/\xi} \, e^{-(|E_i-\mu|+|E_j-\mu|+|E_i-E_j|)/2k_BT}$$





Maximization of the conductance yields the scale of typical hop:

$$L_M \simeq \left(\frac{\xi}{2\nu T}\right)^{1/2}$$

Mott's Hopping length

ξ = localization length

ν = density of states / volume

[1] J-H. Jiang, O. Entin-Wohlman and Y. Imry, Phys. Rev. B 87, 205420 (2013).

[2] R.Bosisio, G. Fleury and J-L. Pichard, (2013)

TEMPERATURE SCALES

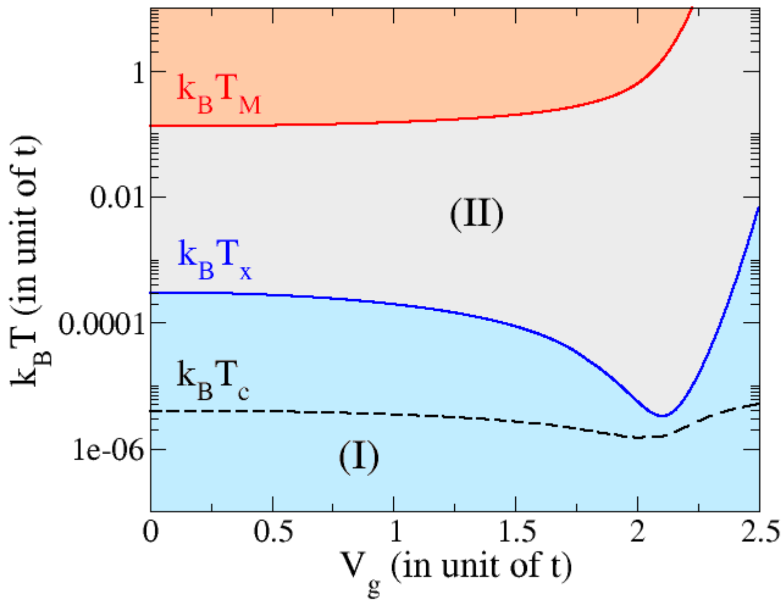
$L_M \simeq \left(\frac{\xi}{2\nu T}\right)^{1/2}$

T ↓

Low T: $L_M >> L$ → elastic transport

Increasing T: $L_M \sim L$ → onset of inelastic processes → $T_x \sim \frac{\xi}{2\nu L^2}$

Increasing T: $L_M \sim \xi$ → simple activated transport → $T_M \simeq (\xi^d \nu)^{-1}$



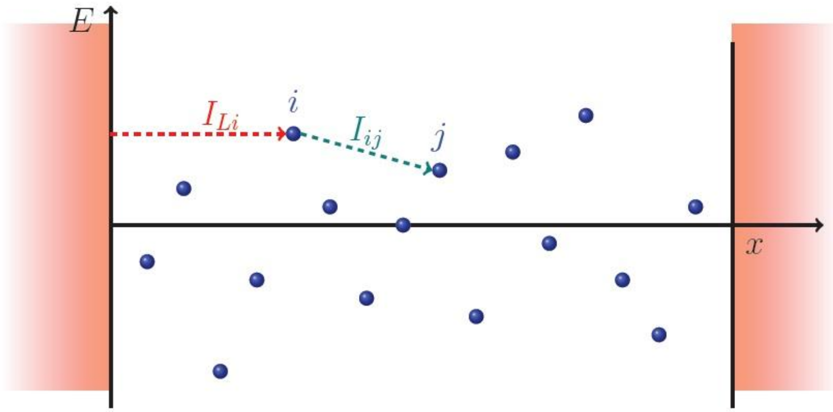
VRH Typical Conductance : (Mott's picture) $G(T) \sim exp\left\{-\left(\frac{T_M}{T}\right)^{1/(d+1)}\right\}$ d=1 (dimensionality)

What about the thermopower?

Conductance: Kurkijärvi (1973), Lee (1984), Fogler (2005)
Thermopower: Zvyagin (~80's)

RANDOM RESISTOR NETWORK [1,2]

E_i: set of energy levels localized at (random) positions $\mathbf{x}_i$



I_{ij}: hopping current between sites i and j

$I_{iL(R)}$: tunneling current between site i and leads

$f_i = f_i^0 + \delta f_i$ "local" FD distribution

Current conservation at node i :
$$\left(\sum_{j \neq i} I_{ij} \right) + I_{iL} + I_{iR} = 0$$

Electric current:
$$I_L^e = \sum_i I_{iL} = -\sum_i I_{iR}$$

Heat current:
$$I_{L(R)}^Q = \sum_i \left(\frac{E_i - \mu_{L(R)}}{e} \right) I_{iL(R)}$$

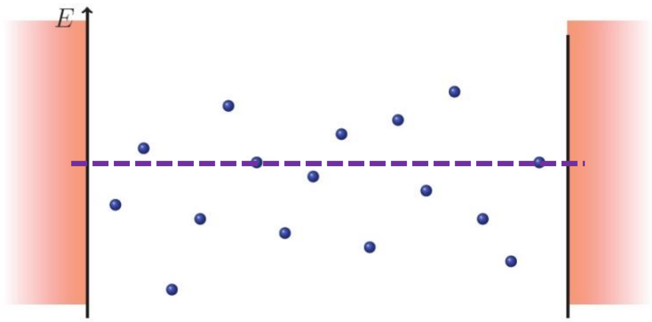
Peltier: $\Pi = \frac{I_L^Q}{I_L^e}$

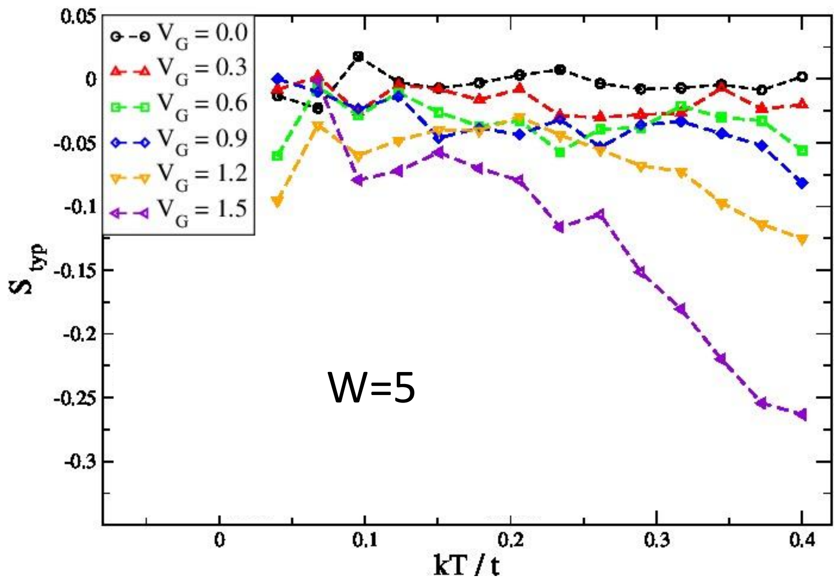
Thermopower: (from Onsager relations) $S = \frac{\Pi}{T}$

[1] A. Miller and E. Abrahams, Phys. Rev. 120, 745 (1960)
[2] J-H. Jiang, O. Entin-Wohlman and Y. Imry, Phys. Rev. B 87, 205420 (2013).

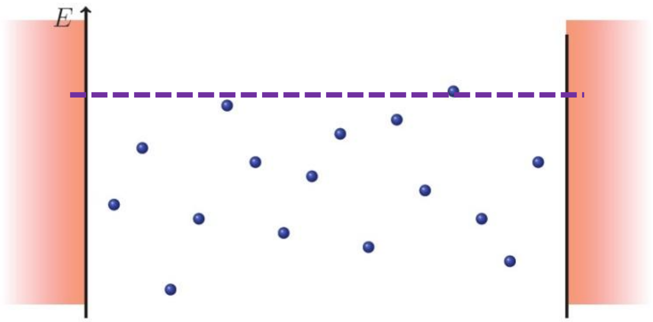
EFFECT OF V_g ON TYPICAL THERMOPOWER IN VRH

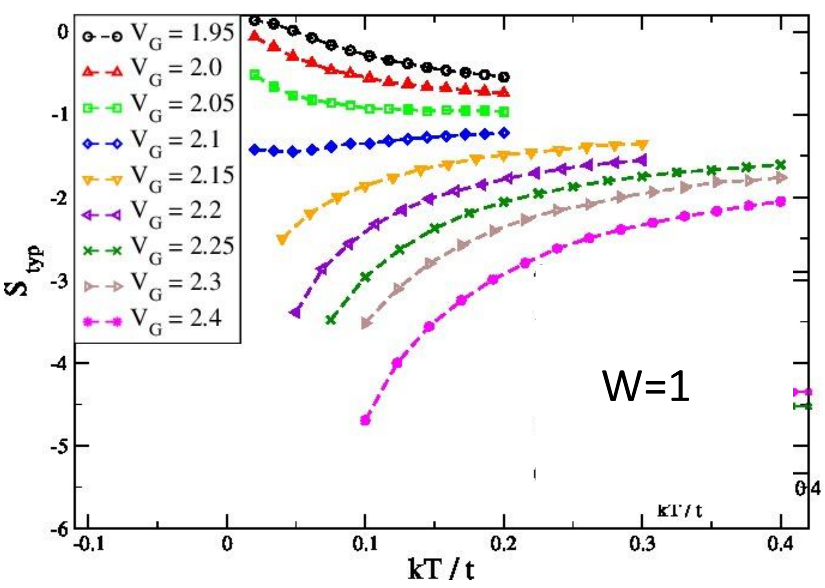
Bulk





Edge

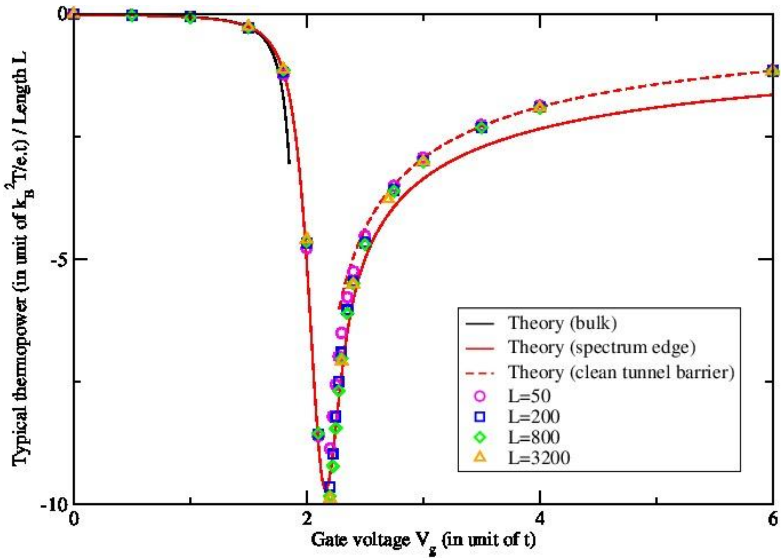




[1] R.Bosisio, G. Fleury and J-L. Pichard, (2013)

CONCLUSIONS

Enhanced thermoelectric conversion at the spectrum edge of disordered nanowires



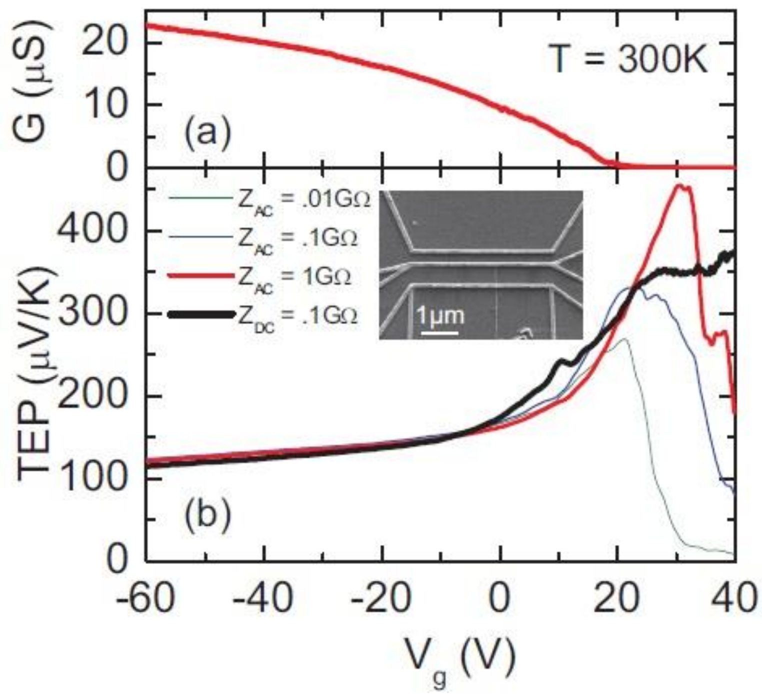
→**Low T**: Analytical description of the typical thermopower as a function of V_G.

→**VRH**: Preliminary results indicate similar behaviour.

Recent experimental work by the group of P.Kim:

Electric Field Effect Thermoelectric Transport in Individual Silicon and Germanium/Silicon Nanowires

Yuri M. Brovman[1], Joshua P. Small[1], Yongjie Hu[2], Ying Fang[2], Charles M. Lieber[2], and Philip Kim[1]
[1] *Department of Applied Physics and Applied Mathematics and Department of Physics, Columbia University, New York, New York, 10027, USA and*
[2] *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02139, USA*



[1] P. Kim et al., arXiv:1307.0249 (2013)