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# Thermoelectric Conversion at the band edges of disordered nanowires :

## Coherent elastic regime and Activated inelastic regime

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# OUTLINE

## ☐ I . Elastic Coherent Regime (Low temperatures)

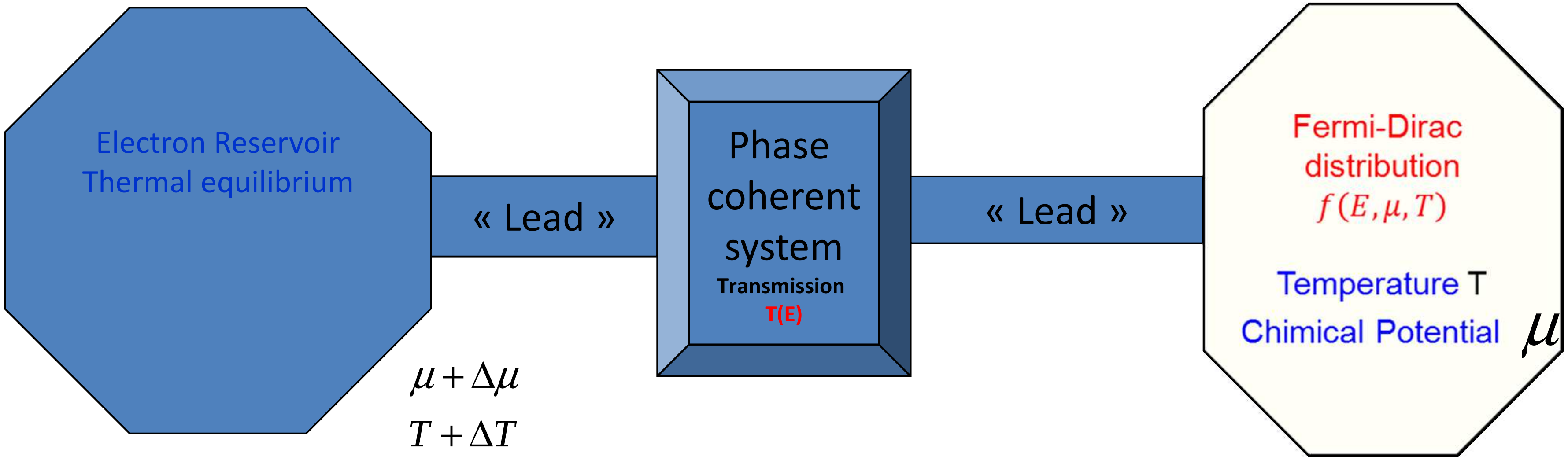
- **Measure of the conductance** of disordered nanowires in the field effect transistor device configuration **(Sanquer et al)** and the Mott formula for the thermopower.
- **Theory using an Anderson model for a 1d disordered chain** Thermoelectric transport (i) the bulk; (ii) the edge and (iii) eventually the outside of the impurity band - Typical behavior and fluctuations of the thermopower

## ☐ II. Inelastic Activated Regime (Intermediate temperatures) in 1d.

Mott variable range hopping and Miller-Abrahams resistor network,
Seebeck and Peltier coefficients near the edges of the impurity band.

## ☐ III. Thermoelectric transport at room temperature (Kim et al).

# Linear Response (mesoscopic regime) Imry and Sivan
# Charge and heat currents induced by generalized forces



Electron Reservoir
Thermal equilibrium

« Lead »

Phase coherent system
Transmission
$T(E)$

« Lead »

Fermi-Dirac distribution
$f(E,\mu,T)$

Temperature T
Chemical Potential $\mu$

$\mu+\Delta\mu$
$T+\Delta T$

$$\begin{pmatrix} J_e \\ J_Q \end{pmatrix} = \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix} \begin{pmatrix} \Delta\mu/eT \\ \Delta T/T^2 \end{pmatrix}$$

$$L_{ij} = \frac{e^2 T}{h} \int dE \begin{bmatrix} 1 & E-\mu/e \\ E-\mu/e & \left(E-\mu/e\right)^2 \end{bmatrix} T(E)\left(\partial f/\partial E\right)$$

**Conductances**
**(electrical and thermal)**

$$G_e = \frac{L_{11}}{T}$$

$$G_Q = \frac{\det L}{T^2 L_{11}}$$

**Thermo-electric coefficients**
**Seebeck and Peltier**

$$S = \frac{L_{12}}{T L_{11}}$$

P=ST

(Onsager)

**Importance to break particle-hole symmetry**

# LOW TEMPERATURE COHERENT ELASTIC TRANSPORT
# VALIDITY OF MOTT FORMULA FOR THE THERMOPOWER

VOLUME 81, NUMBER 16 PHYSICAL REVIEW LETTERS 19 OCTOBER 1998

**Thermometer for the 2D Electron Gas using 1D Thermopower**

N. J. Appleyard, J. T. Nicholls, M. Y. Simmons, W. R. Tribe, and M. Pepper
*Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, United Kingdom*

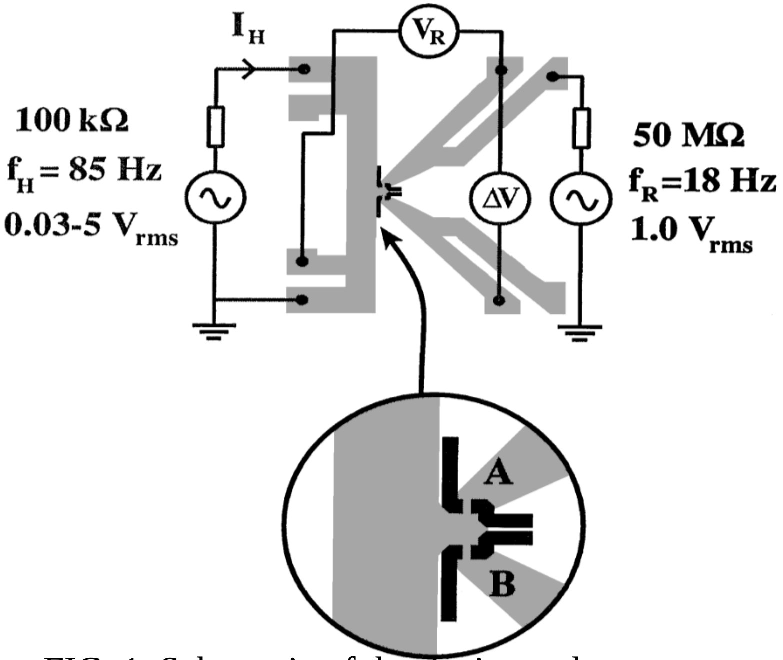


FIG. 1. Schematic of the device and measurement circuit. The etched mesa, shown in grey, consists of a heating channel and two voltage probes, where the two 1D constrictions are defined. The four-terminal resistance *R* is measured simultaneously with the thermopower *S*, but at a different frequency. Magnified view: The two pairs of split gatesdefining the constrictions *A* and *B* are shown in solid black.

## Sommerfeld Expansion
## Mott Formula

$$S = \frac{\Delta V}{T_e - T_l}\Big]_{I=0} = \frac{(\pi k_B)^2}{3e}(T_e + T_l)\frac{\partial(\ln G)}{\partial \mu}$$

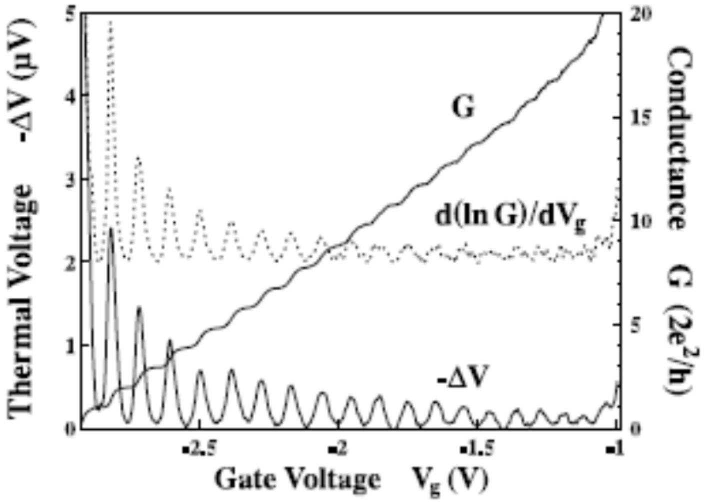


FIG. 2. Experimental traces of the conductance *G* and the thermopower voltage from constriction *A*, using a heating current of **1.5 mA** at a lattice temperature of **305 mK,** so that ***Te*** **~ 600 mK**. The dashed line shows the predicted thermopower signal from the Mott relation [Eq. (1)].

# TUNNELING AND INTERFERENCES IN VERY SMALL GA AS METAL-SEMICONDUCTOR FIELD-EFFECT TRANSISTORS

PHYSICAL REVIEW B VOLUME 59, NUMBER 16 15 APRIL 1999-II

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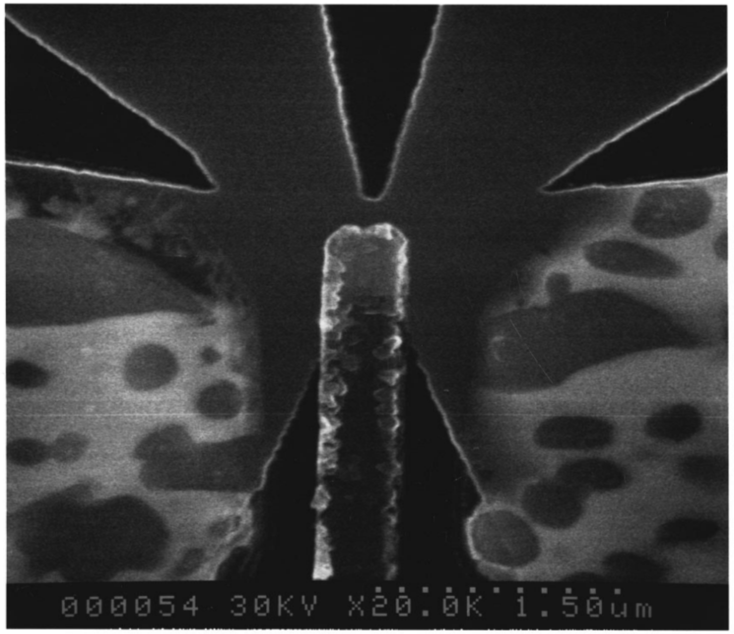


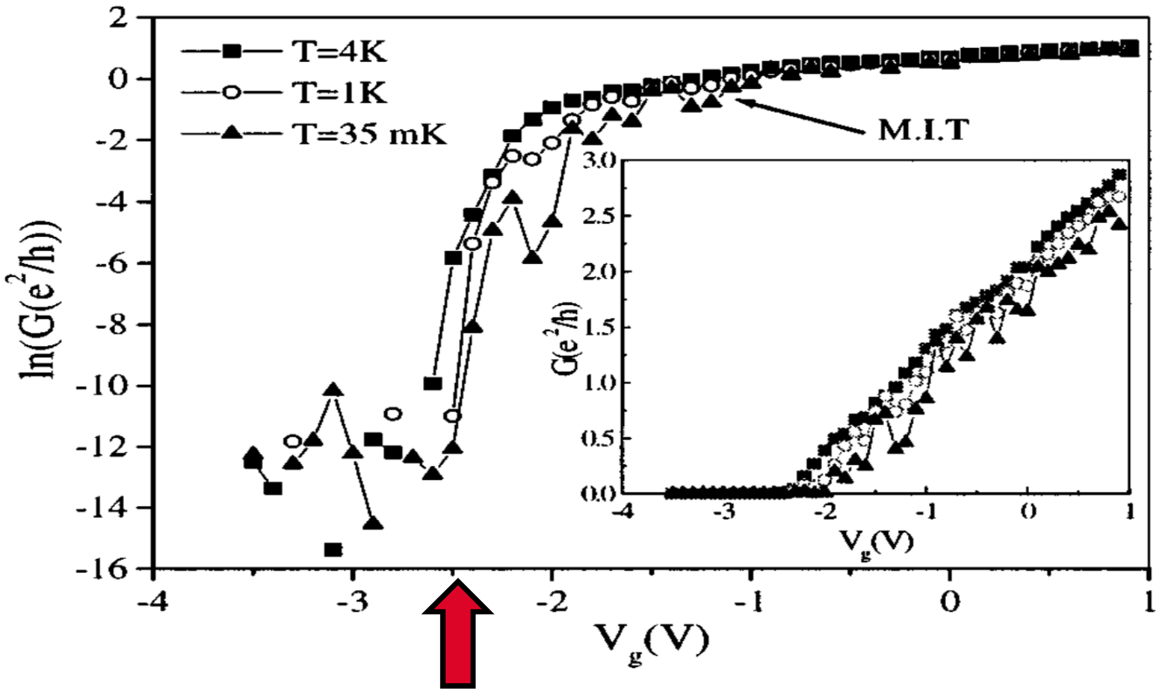
**Quantum coherent elastic transport in the field effect transistor device configuration at very low temperature**

**We study the transport through gated GaAs:Si wires of 0.5 $\mu$m length in the insulating regime and observe transport via tunneling at very low temperature. We describe the mean positive magnetoconductance and the mesoscopic fluctuations of the conductance ~versus energy or magnetic field! purely within one-electron interference model.**

FIG. 1. SEM picture of the GaAs:Si **submicronic** MESFET. The 0.5-mm-thick aluminum Schottky gate is visible on the bottom. **The gate** does not cover the whole constriction width, but **covers entirely the conducting channel if one considers the depletion width**. The GaAs is doped at $\mathbf{10^{23}}$ **Si** $\boldsymbol{m^{-3}}$) 300-nm-thick layer is etched toform four large contact pads to the active region under the gate.Au$x$Ge12$x$Ni Ohmic contacts are visible on the right and the left. The volume of the active region is estimated to be **0.2 x 0.2 x 0.5** $\boldsymbol{\mu m^{3}}$ (taking into account depletion layers for $V_{gate}$= 0 V, about 120 nm).

# GATE MODULATED CARRIER DENSITY

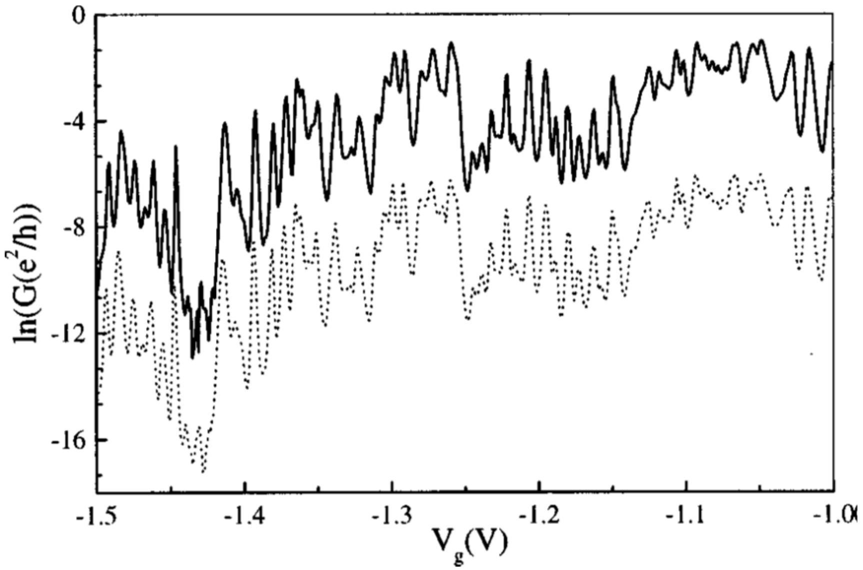
**Anderson Insulator** → ← **Conductor**



**ln *G*(*V* gate)** at three temperatures in a large gate voltage range
(details of the conductance pattern are not seen for this gate voltage sampling)
Inset: the same curve in a linear scale. Note the linearity at voltages above the transition.

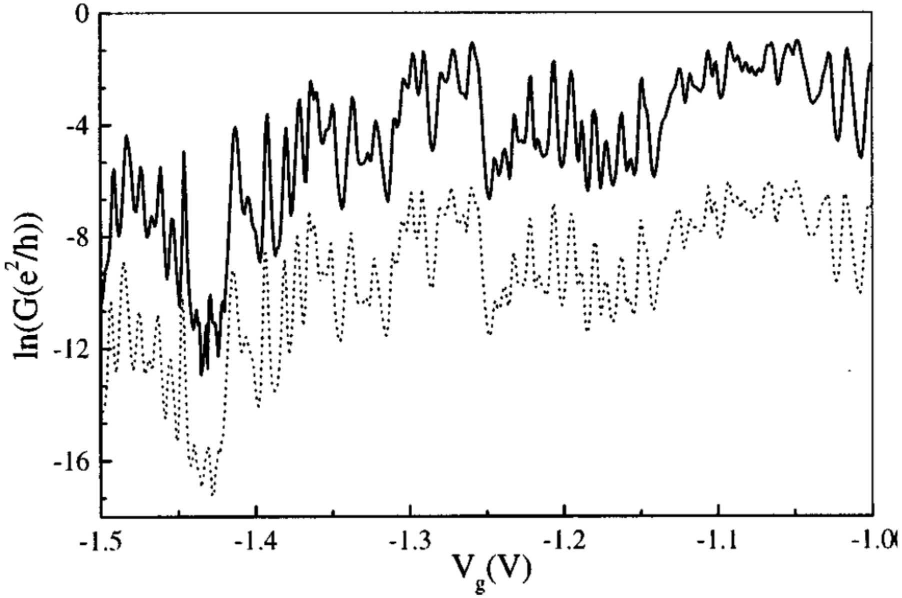
**Edge of the impurity band = -2,5 V**
**(Complete depletion of the disordered nanowire)**

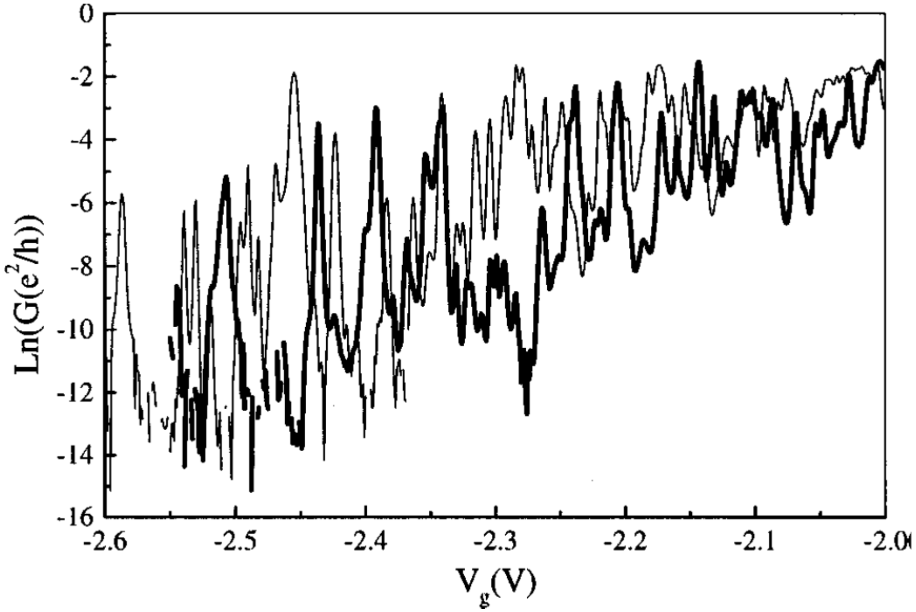
# REPRODUCIBLE CONDUCTANCE FLUCTUATIONS INDUCED BY A VARIATION OF THE GATE VOLTAGE IN THE INSULATING REGIME



**ln $G$($V$ gate)** at **$T$ =100 $m$K** in the **0.5-$\mu$m-long** sample for two successive experiments without thermal cycling, showing the excellent reproducibility of the conductance pattern (curves are shifted for clarity).

# CONDUCTANCE FLUCTUATION S INDUCED BY VARYING THE GATE VOLTAGE


**Bulk** of the impurity band


**Edge** of the impurity band

**Mott Formula :**

$$S \approx \frac{\partial \ln(G)}{\partial V_g}$$

**Larger thermopower at the band edges**

# Disordered nanowire in the field effect transistor device configuration:

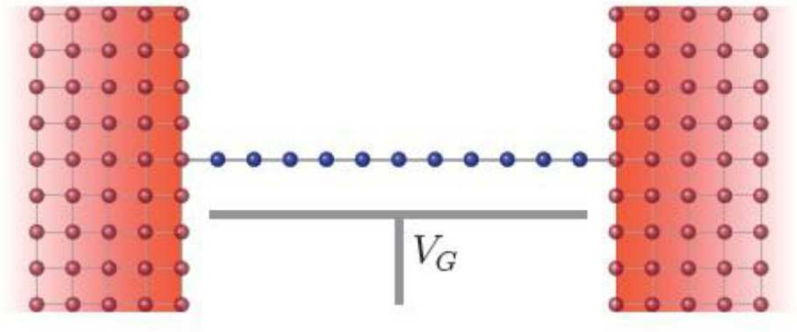
R. Bosisio, G. Fleury and JLP

arXiv:1310.4923v2 [cond-mat.mes-hall]

1d lattice of length L (***N*** sites) with nearest hopping terms t, random on-site potentials and gate potential $V_G$

Anderson Localization with **localization length ξ(E)**

Left lead
(self-energy $\Sigma_L$)



Right lead
(self-energy $\Sigma_R$)

$$H_{1d} = -\boldsymbol{t}.\Sigma_{ij}\left(c_j{}^{+}c_i + H.C\right) + \Sigma_i\, \boldsymbol{\varepsilon}_i n_i$$

$$H_{gate} = \Sigma_i \boldsymbol{V_G}\, n_i$$

$\boldsymbol{\varepsilon_i}$ Box distribution of **width W** and **center 0**

# Study of the localized limit $N > \xi$

*Elastic coherent transport, Linear Response, Sommerfeld expansions*

→ **“Mott Formula “**

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

*Typical thermopower*

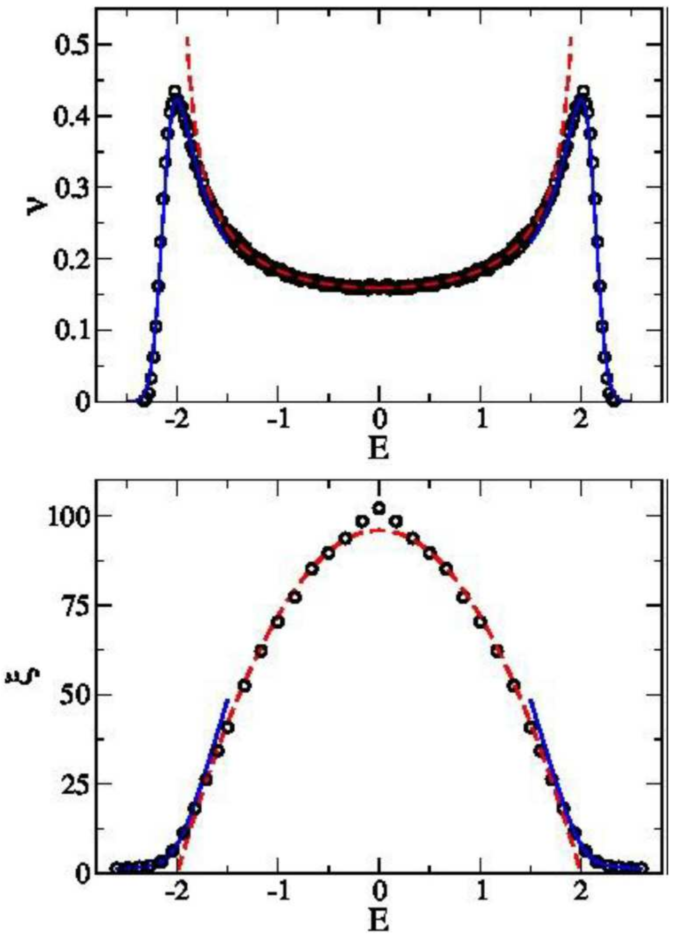
$$[\ln \mathcal{T}]_0(E) = -\frac{2N}{\xi(E)}$$

$$S = \frac{\pi^2}{3} \left(\frac{k_B}{e}\right) \left(\frac{k_B T}{t}\right) S$$

← In physical units

To predict the typical behavior of S, one just need to know how the localization length $\xi$ depends on the energy E.

# Weak Disorder expansions of the 1d density of states ν=ρ/N and of the localization length ξ (assuming $V_G = 0$)



Numerical check with $\boldsymbol{W = 1}$

**BULK**

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

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

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

**EDGE**

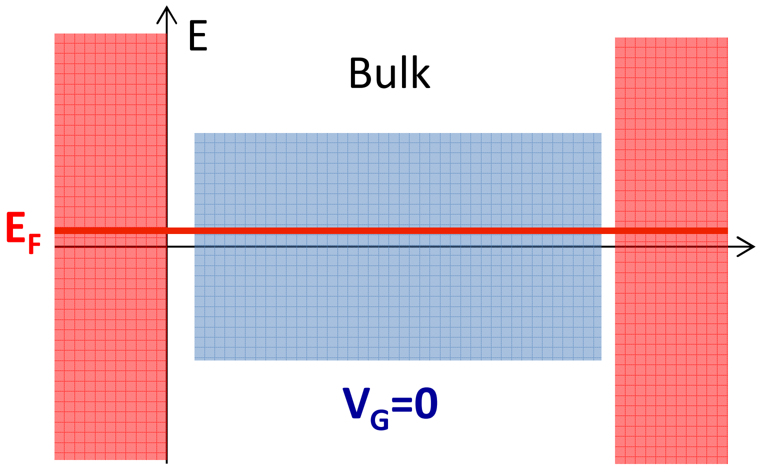
$$\rho_e(E)/N = \sqrt{\frac{2}{\pi}}\left(\frac{12}{tW^2}\right)^{1/3}\frac{\mathcal{I}_1(X)}{[\mathcal{I}_{-1}(X)]^2}$$

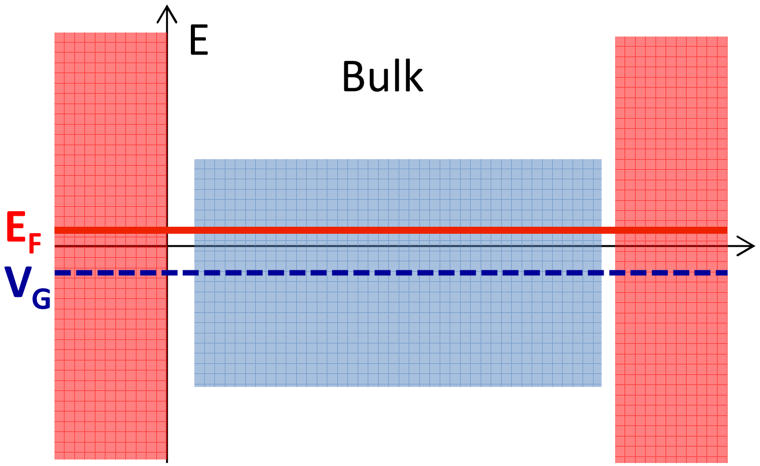
$$\xi_e(E) = 2\left(\frac{12t^2}{W^2}\right)^{1/3}\frac{\mathcal{I}_{-1}(X)}{\mathcal{I}_1(X)}$$

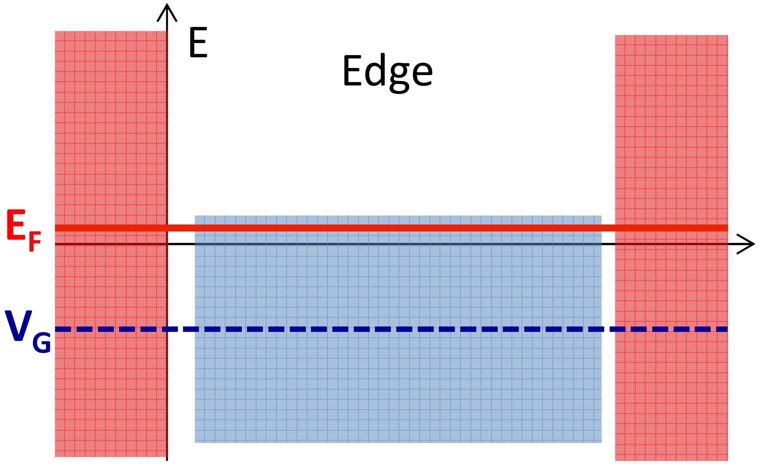
$$X = (|E| - 2t)t^{1/3}(12/W^2)^{2/3}$$

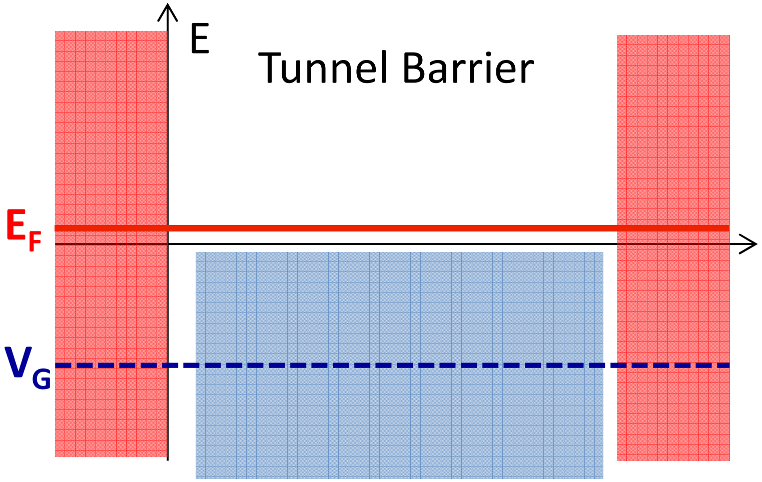
$$\mathcal{I}_n(X) = \int_0^\infty y^{n/2}\, e^{-\frac{1}{6}y^3 + 2Xy}\, dy$$

# EFFECT OF GATE VOLTAGE ON THE IMPURITY BAND









What matters is the relative position of $E_F$ inside the impurity band

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

Using Sommerfeld expansions for having Mott formula

Bulk:

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

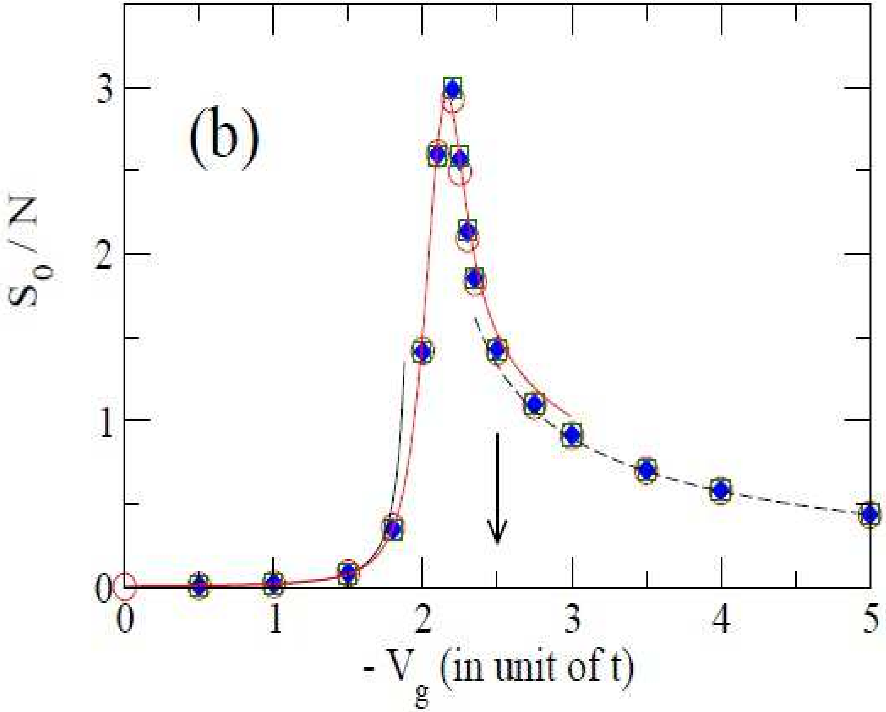
Edge:

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

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

Tunnel Barrier:

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



(N = 200 (circle), 800 (square) and 1600 (diamond)). W/t = 1. The arrow indicates the position of the edge of the impurity band of the nanowire.

**Large Enhancement of the Thermopower near the band 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)

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

$S_0$ = typical thermopower
$\Delta_F$ = mean level spacing near $E_F$

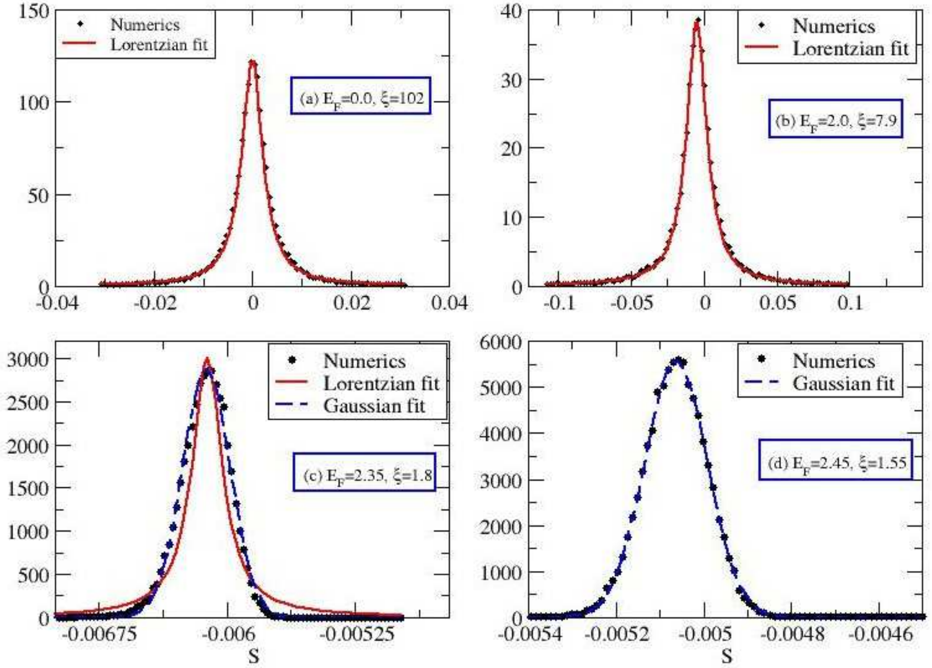
Near the Edge → Gauss distribution (characterized numerically)

$$P(S) = \frac{1}{\sqrt{2\pi}\lambda}\exp\left[-\frac{(S-S_0)^2}{2\lambda^2}\right] \qquad \lambda \approx 0.6\frac{Wt\sqrt{N}}{(E_F - V_g)^2 - (2t + W/4)^2}$$

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**

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[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

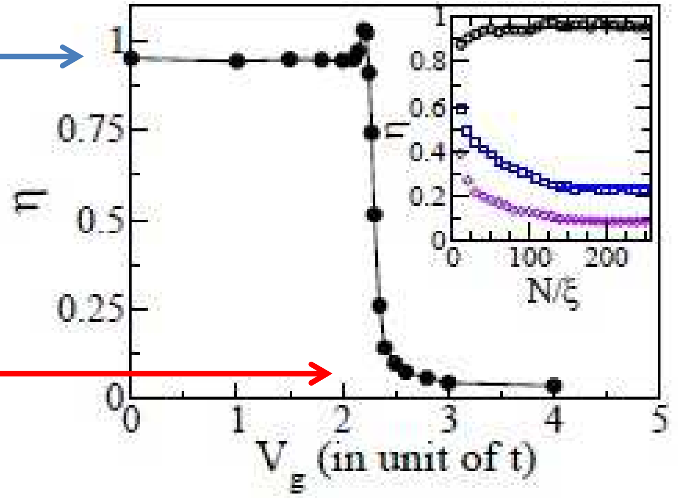
- $\eta = 1$ if Cauchy distribution
- $\eta = 0$ if Gauss distribution

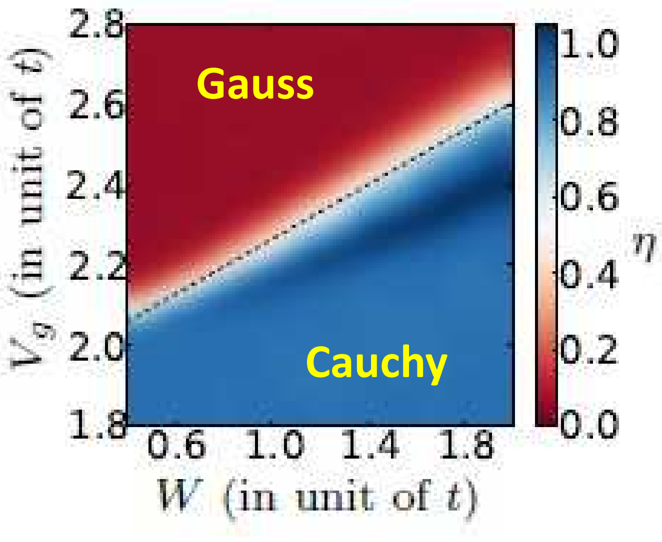
Edge: $V_G = 2{,}5$

W=1

Cauchy

Gauss





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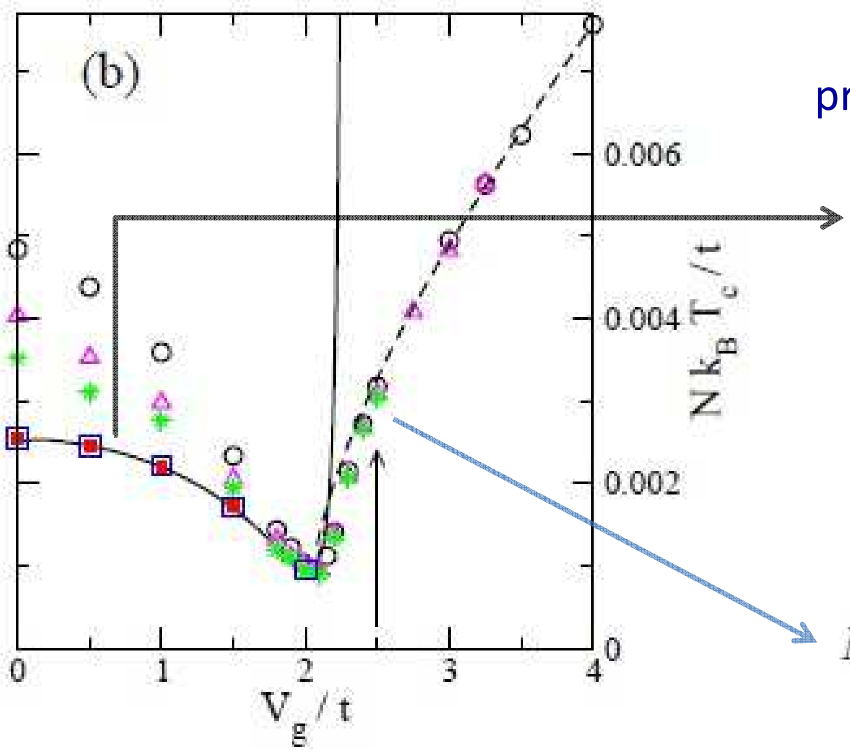
[1] R.Bosisio, G. Fleury and J-L. Pichard, arXiv:1310.4923v2 [cond-mat.mes-hall]

# “SOMMERFELD" TEMPERATURE

**Validity of the Sommerfeld expansion leading to Mott formula for S**

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

**Range of validity of W-F law for $W = 1$ and $E_F = 0$ as a function of $V_G$**



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

$$k_BT_c \propto \Delta_F$$

Proportionality constant depends on required precision

Result for the tunnel barrier:

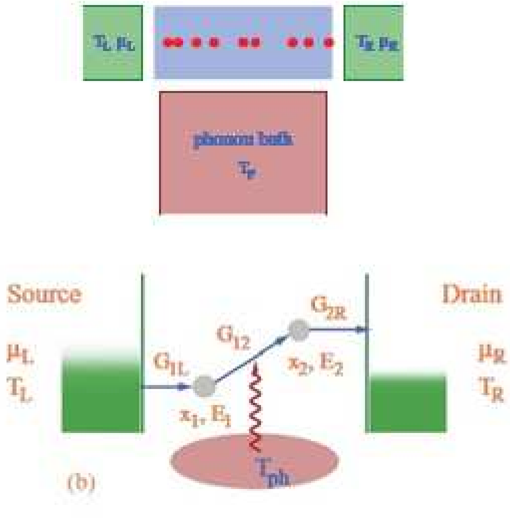
$$Nk_BT_c \propto t\sqrt{[(E_F - V_g)/(2t)]^2 - 1}$$

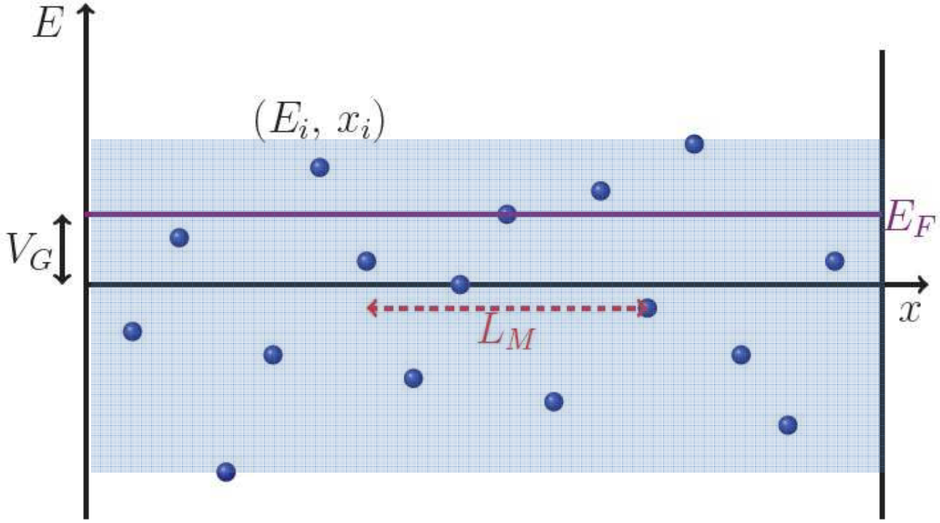
Estimation for Si nanowire: ~ 100 mK

# Variable Range Hopping (VRH) Transport in gated disordered NWS

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

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[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

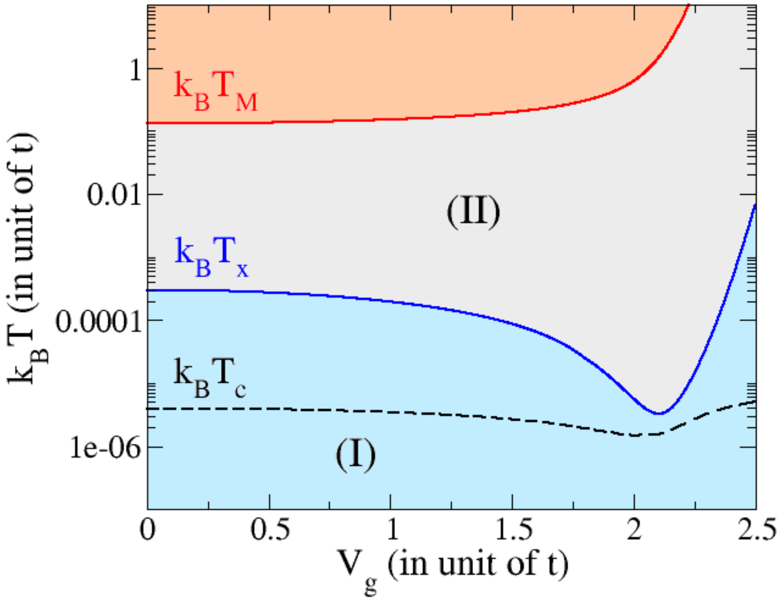
$L_M \simeq \left(\frac{\xi}{2\nu T}\right)^{1/2}$

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

What about the thermopower?

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

# MILLER-ABRAHAMS RESISTOR NETWORK (SEE ALSO AMBEGAOKAR-HALPERIN-LANGER)

1. **Transition rates**

Between localized states

**[Inelastic transition rates (Fermi Golden Rule)]**

$$\Gamma_{ij} = \gamma_{ij}\, f_i\left(1 - f_j\right)\left[N_{BE}\left(\varepsilon_i - \varepsilon_j\right) + \theta\left(\epsilon_i - \epsilon_j\right)\right]$$

$$\gamma_{ij} = \alpha_{e-ph}.\, e^{-|x_i - x_j|/\xi}$$

Between lead and localized states

[Elastic tunneling rates]

$$\Gamma_{Li} = \gamma_{Li}\, f_i\left(1 - f_j\right) \qquad \gamma_{ij} = e^{-|x_i - x_j|/\xi}$$

2. **Conductances**

$$\boldsymbol{G_{ij} = \frac{e^2}{k_B T}\Gamma_{ij}}$$

3. **Local chemical potential (out of equilibrium transport)**

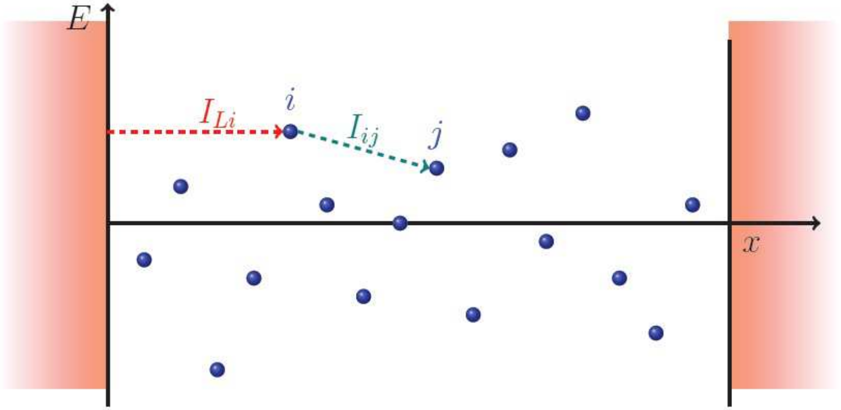
$$\boldsymbol{f_i(\mu) \rightarrow f_i(\mu + \delta\mu_i)}$$

4. **Current**

$$I_{ij} = G_{ij}\,\frac{\delta\mu_i - \delta\mu_j}{e}$$

# RANDOM RESISTOR NETWORK [1,2]

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: $\Pi = \dfrac{I_L^Q}{I_L^e}$

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

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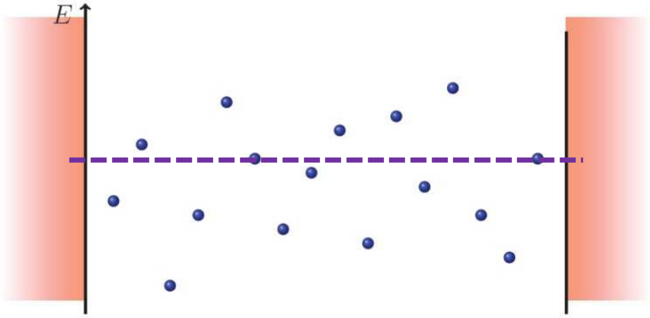
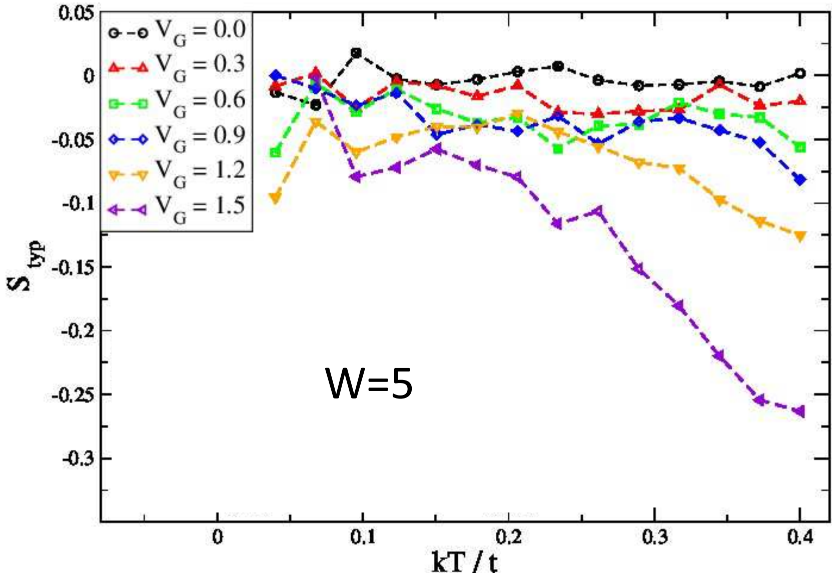
[1] A. Miller and E. Abrahams, Phys. Rev. 120, 745 (1960)
[2] J-H. Jiang, O. Entin-Wohlman and Y. Imry, Phys. Rev. B 87, 205420 (2013).

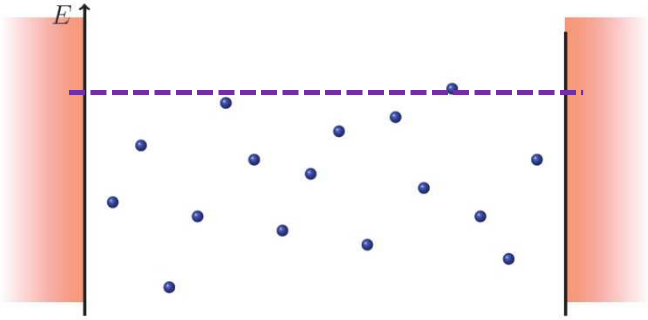
# EFFECT OF $V_g$ ON TYPICAL THERMOPOWER IN VRH

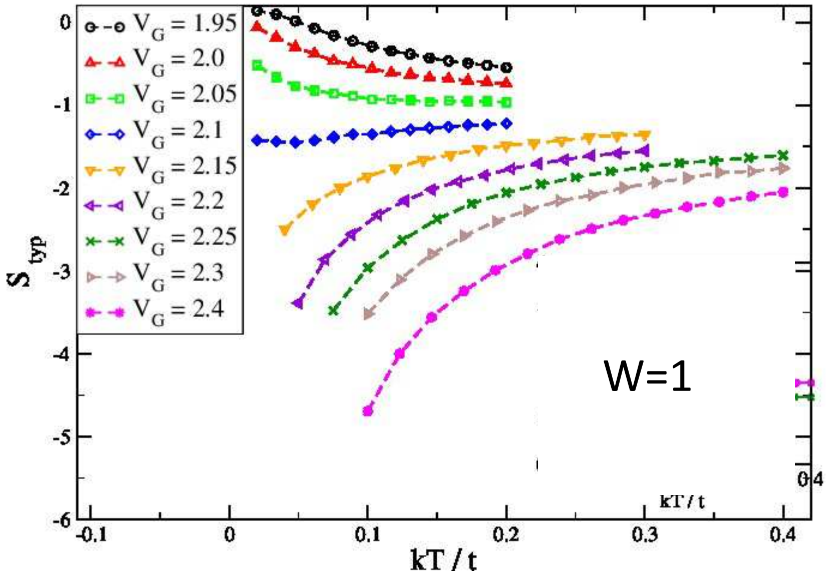
## Bulk





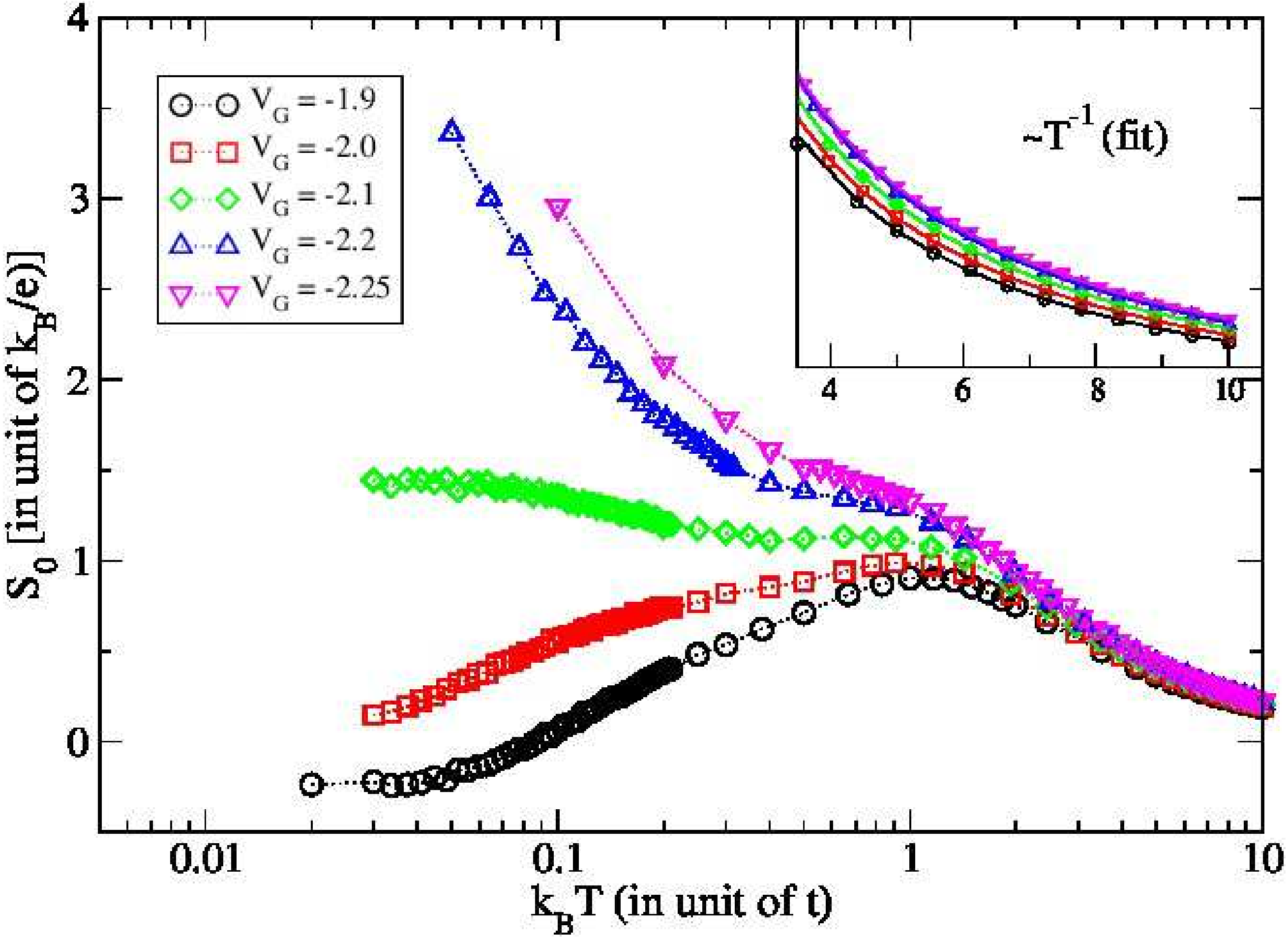
## Edge





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

# Thermopower as a function of temperature and of the gate voltage



Insert: 1/T behavior (consistent with Zviagyn) valid at high temperatures

# ENHANCED TEP NEAR THE BAND EDGE OF SEMICONDUCTING NWS AT ROOM TEMPERATURE

http://arxiv.org/pdf/1307.0249v1.pdf

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

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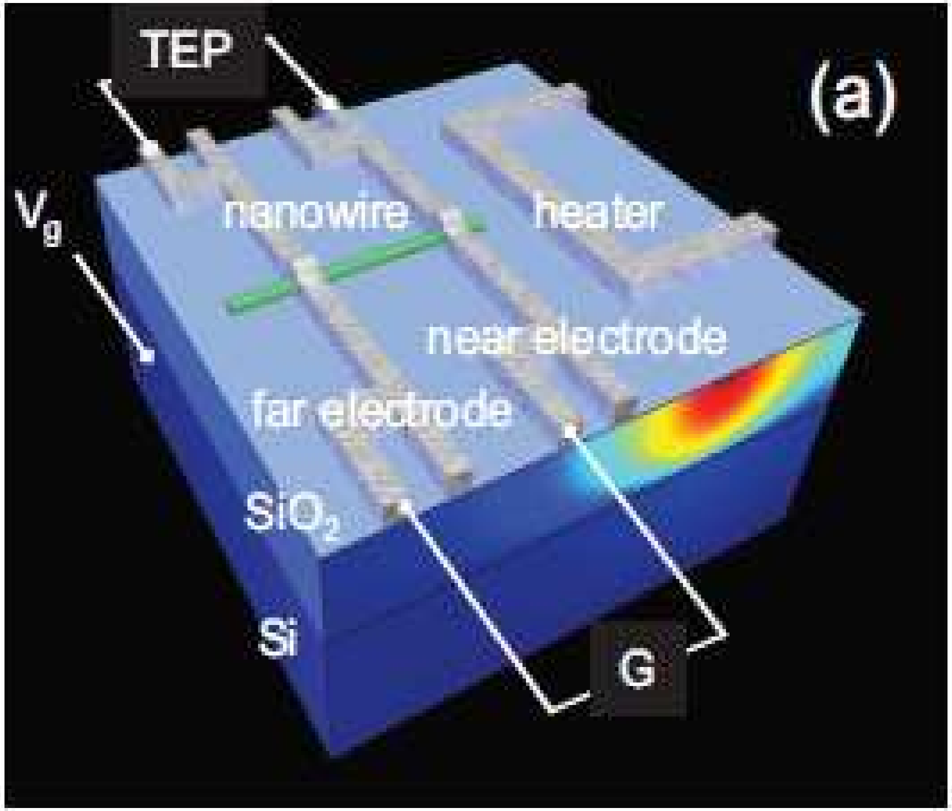
We have simultaneously measured conductance and thermoelectric power (TEP) of individual silicon and germanium/silicon core/shell nanowires in the field effect transistor device configuration. As the applied gate voltage changes, the TEP shows distinctly different behaviors while the electrical conductance exhibits the turn-off, subthreshold, and saturation regimes respectively. At room temperature, peak TEP value of ∼300μ V/K is observed in the subthreshold regime of the Si devices.

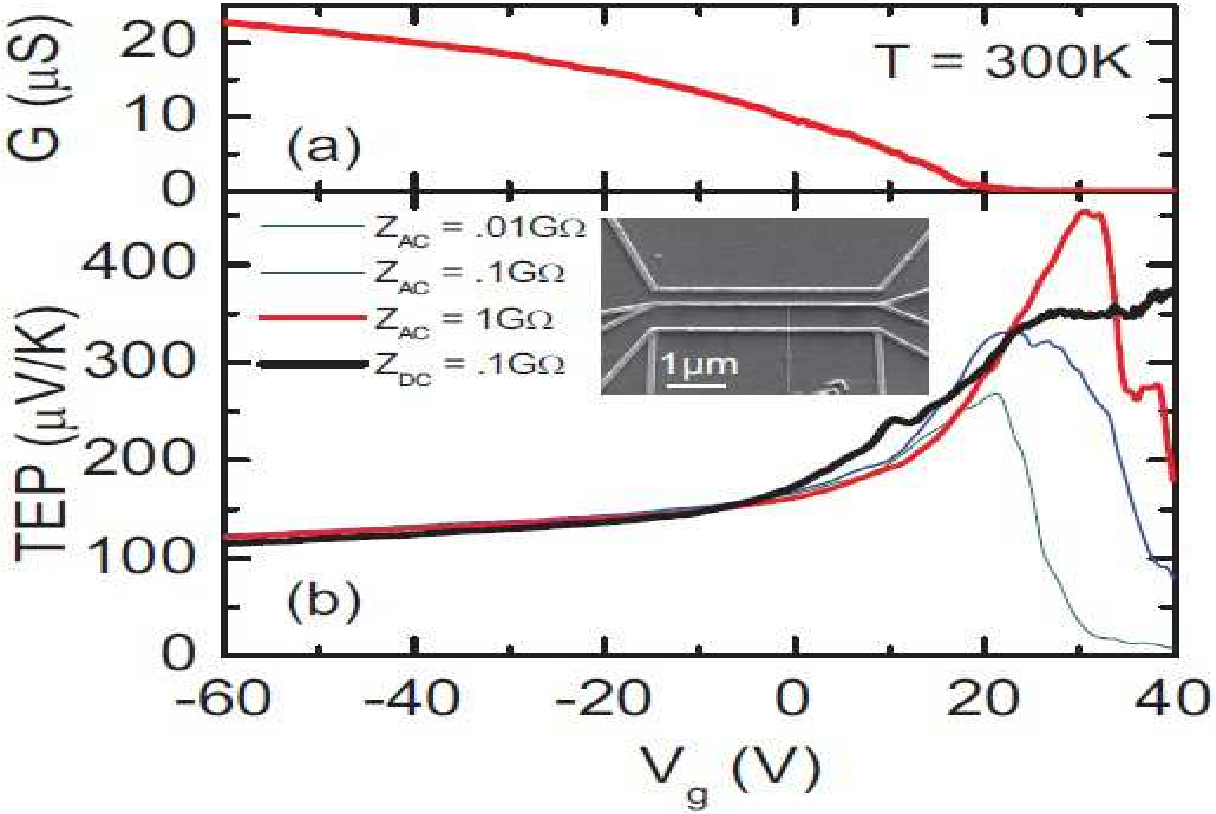
Substantially large peak TEP values are observed in the subthreshold regime of the Si and Ge/Si devices**, indicating largely enhanced TEP near the band edge of semiconducting NWs.**

# FIELD EFFECT TRANSISTOR DEVICE CONFIGURATION



Schematic diagram of the simultaneous measurement technique of conductance and thermopower on individual nanowires. The finite element simulation shows a temperature profile, with red being the hottest and blue being the bath temperature, of the cross section of the substrate.

# GE/SI NANOWIRE AT ROOM TEMPERATURE



Conductance (a) and thermopower (b) of a Ge/Si nanowire as a function of gate voltage taken at T = 300 K. The inset in (b) shows a typical SEM image of a 12 nm Ge/Si device. Large input impedance becomes important when measuring TEP near the band edge of a semiconductor, as the FET device turns off.

# THANK YOU