``Enseigner la recherche en train de se faire''

COLLÈGE DE FRANCE
1530

Chaire de
Physique de la Matière Condensée

PETITS SYSTEMES THERMOELECTRIQUES: *CONDUCTEURS MESOSCOPIQUES ET GAZ D'ATOMES FROIDS*

Cycle « Thermoélectricité »
2012 - 2014

Antoine Georges

Séance du 12 novembre 2013

- Coefficients thermoélectriques dans l'approche de Landauer -Büttiker
- Application aux contact quantiques ponctuels

Séminaires : Laurens Molenkamp
(Universität Würzburg)

10h45 : Thermoelectric Properties of Semiconductor Nanostructures

11h45 – *Topological Insulators : Recent Results and New Directions*

Matrix of Onsager Coefficients in the linear response regime

Reminders from spring 2013 lectures
- more on website -

Particle and entropy currents. Linear response :

$$I_N = L_{11}\Delta\mu + L_{12}\Delta T$$
$$I_S = L_{21}\Delta\mu + L_{22}\Delta T$$

Slight change of definition as compared to spring 2013 lectures:

$$j_n = -L_{11}\nabla\mu - L_{12}\nabla T$$
$$j_s = -L_{21}\nabla\mu - L_{22}\nabla T$$

N,S particle number and entropy (n,s: *densities per unit volume*)
I_N,I_S: currents (j_n,j_s: *current densities*)

$\Delta\mu \equiv \mu_L - \mu_R$

$\Delta T \equiv T_L - T_R$

Instead of gradients (note sign change !) $\nabla\mu \sim -\Delta\mu/L$

Conjugate thermodynamic variables:

Grand-canonical potential :

$$\Omega(T,\mu) = -k_B T \ln Z_G$$

Particle-number and Entropy:

$$N = -\frac{\partial\Omega}{\partial\mu}|_T \;\;,\;\; S = -\frac{\partial\Omega}{\partial T}|_\mu$$

In agreement with thermodynamic definition of `generalized forces', etc… cf. spring 2013 notes

Irreversible entropy production rate :

$$\frac{\partial Q}{\partial t}\Big|_{irr} = T\frac{\partial S}{\partial t}\Big|_{irr} = I_N \Delta\mu + I_S \Delta T$$

$$= I\Delta V + I_Q \frac{\Delta T}{T}$$

IΔV: Usual form of electrical power

[Uses conservation of energy and particle number,
cf. notes spring 2013]

$$T\frac{\partial S}{\partial t}\Big|_{irr} = (\Delta\mu, \Delta T)\begin{pmatrix} L_{11} & L_{21} \\ L_{21} & L_{22} \end{pmatrix}\begin{pmatrix} \Delta\mu \\ \Delta T \end{pmatrix}$$

→ Key property of the Onsager matrix (1)

- Second principle: entropy production rate is positive (or zero for an irreversible process)
- → L is a positive semi-definite matrix

$$L_{11} \geq 0 \quad , \quad L_{22} \geq 0 \quad , \quad \det L \geq 0$$

- Dimensionless coupling constant characterizing energy conversion :

$$g^2 \equiv \frac{L_{12}^2}{L_{11} L_{22}} \in [0, 1]$$

Key property of the Onsager matrix (2): Onsager-Casimir reciprocity relations

When time-reversal symmetry applies (B=0):

$$\boxed{L_{12} = L_{21}}$$

In the presence of a magnetic field:

$$\boxed{\begin{array}{l} L_{11}(-B) = L_{11}(B) \ , \ L_{22}(-B) = L_{22}(B) \\ L_{12}(-B) = L_{21}(B) \end{array}}$$

Identification of the transport coefficients from the Onsager matrix L:

Using:

$$I = -eI_N \quad , \quad \Delta\mu = -e\Delta V \quad , \quad I_Q = TI_S$$

$$I = e^2 L_{11} \Delta V - e L_{12} \Delta T$$
$$I_Q = -eTL_{21} \Delta V + TL_{22} \Delta T$$

Conductance (ΔT=0): $G = e^2 L_{11}$

Seebeck coefficient (Thermopower) α :

Open circuit I=0 → `Stopping force' $\Delta V = -\alpha \Delta T$

$$\alpha = -\frac{L_{12}}{eL_{11}}$$

Peltier coefficient (heat per unit charge):

$$I_Q \equiv \Pi \, I \big|_{\Delta T=0}$$

$$\boxed{\Pi = -T\frac{L_{21}}{eL_{11}}} \qquad L_{21} = L_{12} \Rightarrow \Pi = T\alpha$$

Onsager symmetry → Kelvin's relation

Thermal conductance:

Again, open circuit condition (I=0):

$$I_Q = G_{th} \, \Delta T \big|_{I=0} \qquad \boxed{\frac{G_{th}}{T} = \left[L_{22} - \frac{L_{12}L_{21}}{L_{11}} \right]}$$

Lorenz number
(cf. Wiedemann-Franz law, later): $\mathcal{L} \equiv \dfrac{G_{th}/T}{G}$

Considering a setup in which the current I and thermal gradient are imposed, one can rewrite the above linear-response equations as:

$$\begin{pmatrix} \Delta V \\ I_Q \end{pmatrix} = \begin{pmatrix} R & -\alpha \\ \Pi & G_{th} \end{pmatrix} \begin{pmatrix} I \\ \Delta T \end{pmatrix}$$

R = 1/G: Resistance, Π: Peltier coefficient

Rate of irreversible heat production:

$$\frac{\partial Q}{\partial t}|_{irr} = (I, \Delta T/T) \cdot \begin{pmatrix} R & -\alpha \\ \Pi & G_{th} \end{pmatrix} \begin{pmatrix} I \\ \Delta T \end{pmatrix}$$
$$= RI^2 + \frac{G_{th}}{T}\Delta T^2 + I\Delta T\left[\frac{\Pi}{T} - \alpha\right]$$

$$\frac{\partial Q}{\partial t}|_{irr} = RI^2 + \frac{G_{th}}{T}\Delta T^2 = \text{Joule} + \text{Fourier}$$

The Seebeck/Peltier terms correspond to reversible processes and do not contribute !

Generalization of the Landauer formula to thermoelectric transport

Thermal: HL Engquist and PW Anderson Phys Rev B 24, 1151 (1981)

Thermoelectric effects:

U.Sivan and Y.Imry Phys Rev B 33, 551 (1986)

P.N. Butcher J. Phys Cond Matt 2, 4869 (1990)

The Landauer formula

Conductance as Transmission

Reminder from lecture 1

$$\mu_L - \mu_R = -e(V_L - V_R)$$

$$T = 0: \quad G = \frac{2e^2}{h}\mathcal{T}(\varepsilon_F)$$

$$T \neq 0: \quad G = \frac{2e^2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$I = -\frac{2e}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[f(\varepsilon-\mu_L) - f(\varepsilon-\mu_R)\right]$$

$\mathcal{T}(\varepsilon)$: Energy-dependent transmission coefficient

Particle, Energy and Entropy Currents

For a detailed discussion,
see notes at the end of these slides

Linear Response Regime:

$$\frac{\partial}{\partial\mu} f\left(\frac{\varepsilon-\mu}{k_B T}\right) = \left(-\frac{\partial f}{\partial\varepsilon}\right) \quad , \quad \frac{\partial}{\partial T} f\left(\frac{\varepsilon-\mu}{k_B T}\right) = \frac{\varepsilon-\mu}{T}\left(-\frac{\partial f}{\partial\varepsilon}\right)$$

$$\frac{\partial}{\partial\alpha} s = \frac{\partial s}{\partial f}\frac{\partial}{\partial\alpha} f = [-k_B \ln\frac{f}{1-f}]\frac{\partial}{\partial\alpha} f = \frac{\varepsilon-\mu}{T}\frac{\partial}{\partial\alpha} f$$

$$\begin{aligned} I_N &= \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[\Delta\mu + \frac{\varepsilon-\mu}{T}\Delta T\right]\left(-\frac{\partial f}{\partial\varepsilon}\right) \\ I_S &= \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[\frac{\varepsilon-\mu}{T}\Delta\mu + \left(\frac{\varepsilon-\mu}{T}\right)^2\Delta T\right]\left(-\frac{\partial f}{\partial\varepsilon}\right) \end{aligned}$$

From which we immediately identify the Onsager coefficients defined as (cf 2012-2013 lectures):

$$\begin{pmatrix} I_N \\ I_S \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}\begin{pmatrix} \Delta\mu \\ \Delta T \end{pmatrix}$$

$$L_{11} = \frac{2}{h} I_0 \;,\; L_{12} = L_{21} = \frac{2}{h} k_B I_1 \;,\; L_{22} = \frac{2}{h} k_B^2 I_2$$

in which the *dimensionless* integrals read:

$$I_n \equiv \int d\varepsilon\, \mathcal{T}(\varepsilon)\left(\frac{\varepsilon-\mu}{kT}\right)^n\left(-\frac{\partial f}{\partial\varepsilon}\right)$$

Conductance, Thermopower and Thermal Conductance:

$$G = \frac{2e^2}{h} I_0 \;, \quad \left(\frac{h}{e^2} = 25.81 k\Omega \right)$$

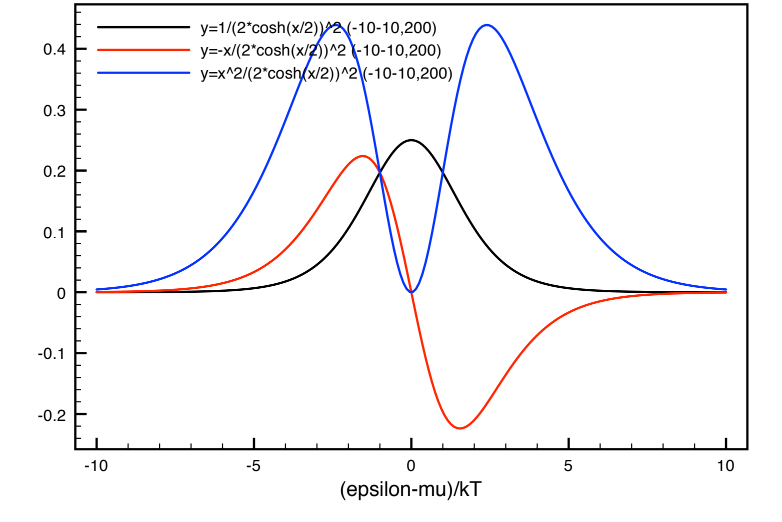
$$\alpha = -\frac{k_B}{e} \frac{I_1}{I_0} \;, \quad \left(\frac{k_B}{e} = 86.3\, \mu V K^{-1} \right)$$

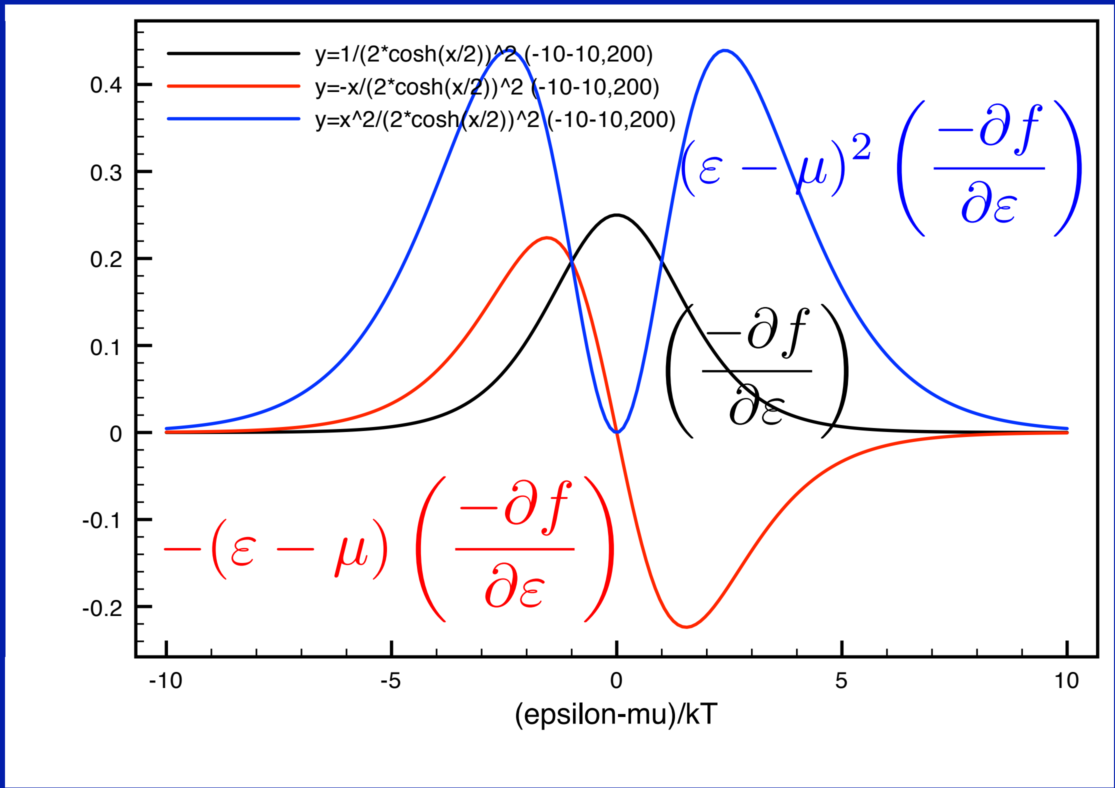
$$\frac{G_{th}}{T} = \frac{2}{h} k_B^2 \left[I_2 - \frac{I_1^2}{I_0} \right]$$

$$\mathcal{L} \equiv \frac{G_{th}}{TG} = \left(\frac{k_B}{e} \right)^2 \left[\frac{I_2}{I_0} - \left(\frac{I_1}{I_0} \right)^2 \right]$$

Dimensionless integrals:

$$I_n \equiv \int d\varepsilon\, \mathcal{T}(\varepsilon) \left(\frac{\varepsilon - \mu}{k_B T} \right)^n \left(-\frac{\partial f}{\partial \varepsilon} \right)$$





Different coefficients probe different range of energy:

- Conductance probes the immediate vicinity of E_F, in a symmetric way for particles and holes
- Thermopower probes a difference between contributions from holes (>0) and particles (<0). *It vanishes if particles and hole have the same transmission.*
- Thermal conductance probes a few kT from E_F

Note complete FORMAL similarity with expressions from Boltzmann equation for a bulk system, see spring 2013

$$\mathcal{T}(\varepsilon) \equiv \frac{2}{\hbar} \int \frac{d^d k}{(2\pi)^d} \tau(\varepsilon_{\mathbf{k}}) \left[\frac{1}{d}\sum_a (\nabla^a_{\boldsymbol{k}} \varepsilon_{\mathbf{k}})^2\right] \delta(\varepsilon - \varepsilon_{\mathbf{k}})$$

(Dimensionality: L^{2-d})

Key difference: SQUARE of velocity enters here
scattering – not ballistic
Current-current correlator

$$\begin{aligned} L_{11} &= \frac{1}{\hbar} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) \mathcal{T}(\varepsilon) \\ L_{12} &= \frac{1}{\hbar} \frac{1}{T} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) (\varepsilon - \mu) \mathcal{T}(\varepsilon) \\ L_{22} &= \frac{1}{\hbar} \frac{1}{T^2} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) (\varepsilon - \mu)^2 \mathcal{T}(\varepsilon) \end{aligned}$$

$$\sigma = e^2 L_{11} \ , \ \ \alpha = -\frac{L_{12}}{e L_{11}} \ , \ \ \kappa = T\left(L_{22} - \frac{L_{12}^2}{L_{22}}\right)$$

Low Temperature expressions

(from Sommerfeld's expansion – see notes

Warning: assumes no or weak intrinsic T-dependence of transmission
– OK for elastic scattering

$$G = \frac{2e^2}{h}\mathcal{T}(\mu = \varepsilon_F)$$ Landauer

$$\alpha = -\frac{k_B}{e}\frac{\pi^2}{3}k_B T\,\frac{\mathcal{T}'(\varepsilon_F)}{\mathcal{T}(\varepsilon_F)}$$

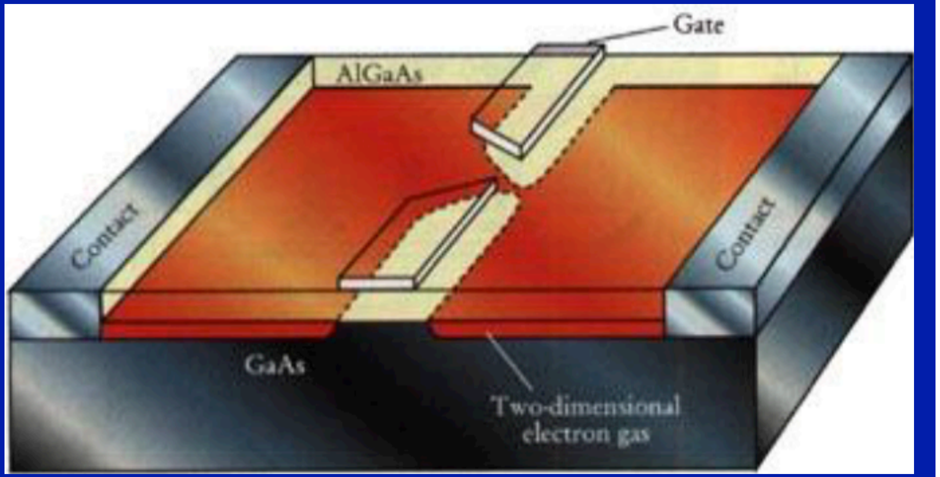
$$= -\frac{k_B}{e}\frac{\pi^2}{3}k_B T\,\frac{\partial}{\partial\mu}\ln\mathcal{T}(\mu)\big|_{\mu=\varepsilon_F}$$ Mott-Cutler

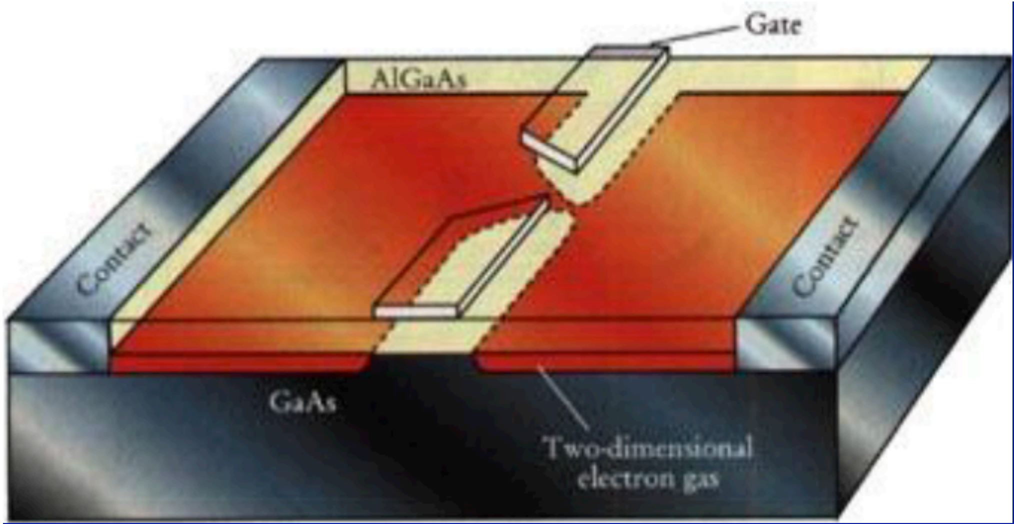
$$\frac{G_{th}/T}{G} \equiv \mathcal{L} \to \left(\frac{k_B}{e}\right)^2\frac{\pi^2}{3} \quad (T \to 0)$$

Wiedemann-Franz law

Quantum Point Contacts (QPC) The first evidence of conductance quantization

Van Wees et al. PRL 60, 848 (1988)
Quantized Conductance of Point Contacts in a Two-Dimensional Electron Gas
cf. also:
Wharam et al.
One-dimensional transport and the quantization of the ballistic resistance
J.Phys C 21 L209 (1988)





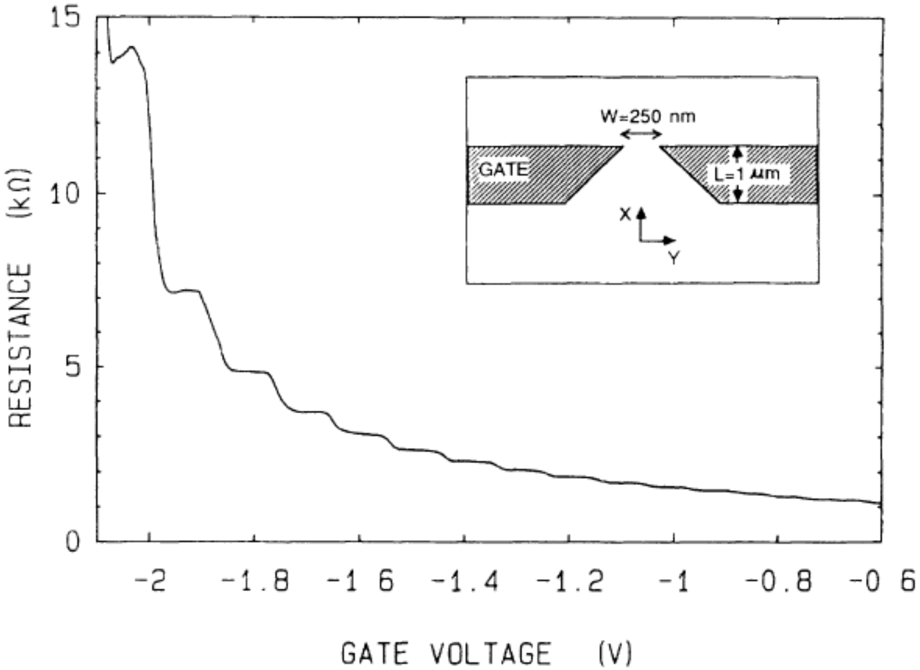


FIG. 1. Point-contact resistance as a function of gate voltage at 0.6 K. Inset: Point-contact layout.

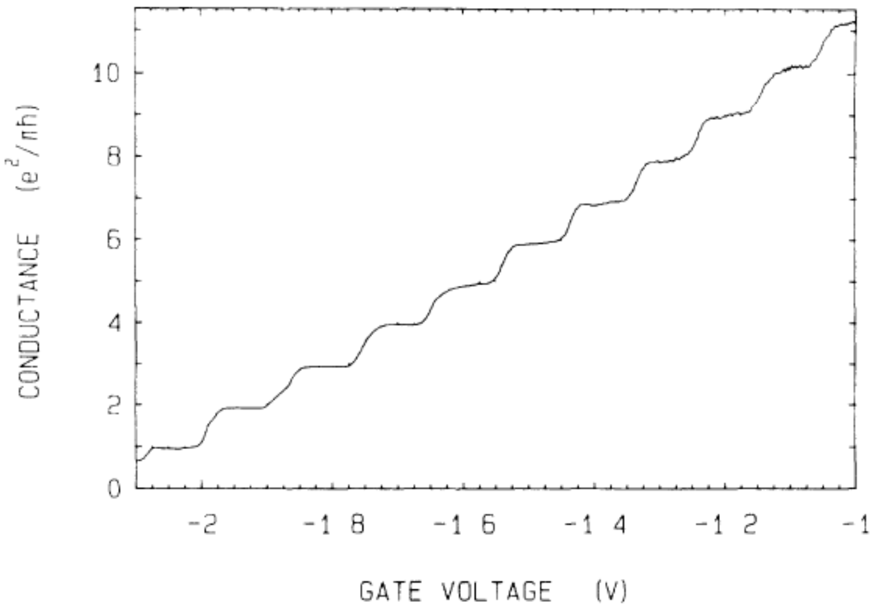


FIG. 2. Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

Transmission coefficient for an electron injected in channel m to go into channel n:

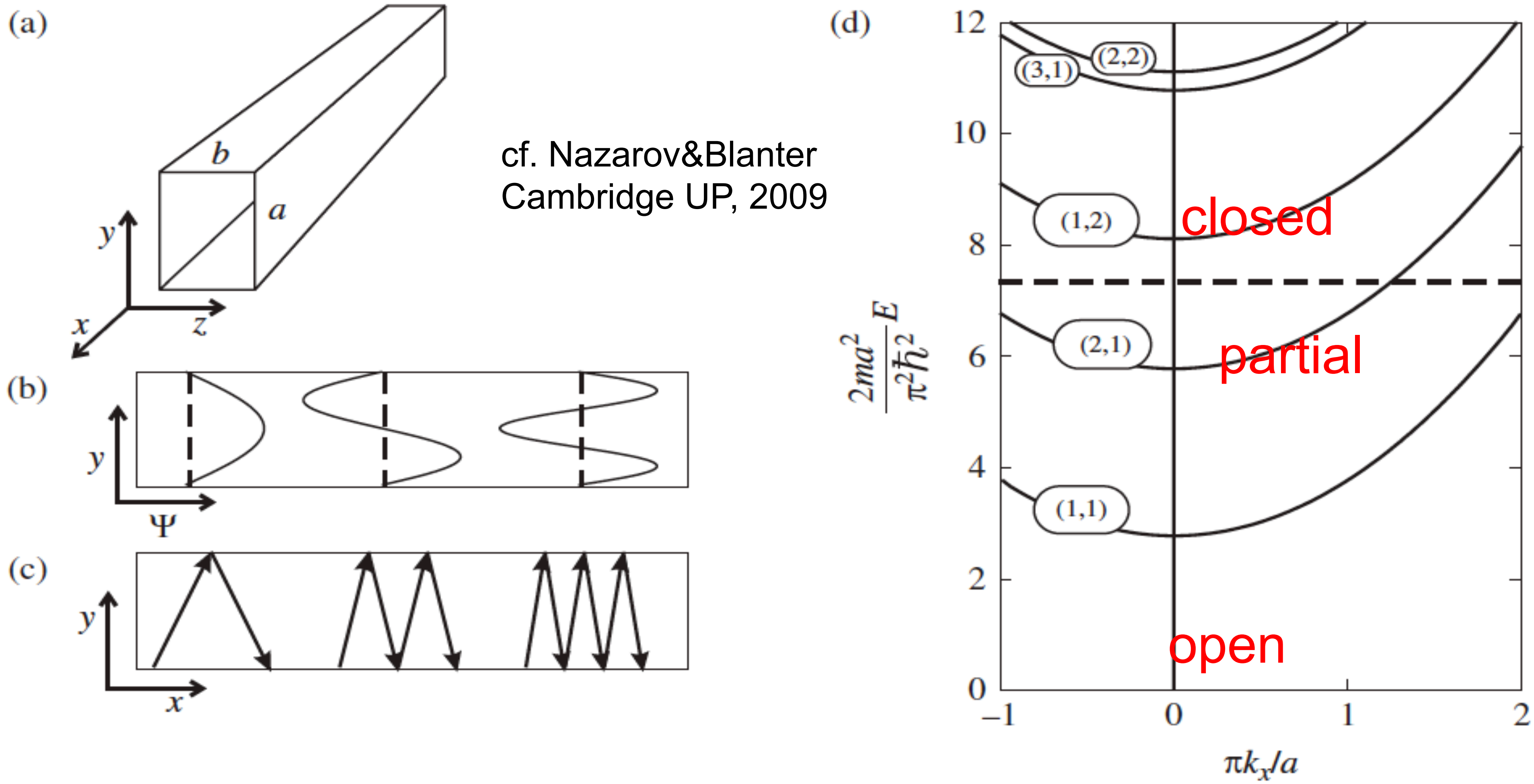
$$\mathcal{T}_{nm} = |t_{nm}|^2$$

Each mode n contributes a current proportional to $\sum_m \mathcal{T}_{nm}$

Total current finally involves transmission coefficient:

$$\mathcal{T}(\varepsilon) = \sum_{nm} \mathcal{T}_{nm} = \sum_{nm} t_{nm} t^*_{nm} = \mathrm{Tr}\, tt^\dagger$$

$$= \sum_\lambda \mathcal{T}_\lambda$$ sum of eigenvalues of tt^+ matrix



cf. Nazarov&Blanter
Cambridge UP, 2009

$$2D: \quad \varepsilon_n(k_x) = \frac{\hbar^2}{2m}\left[k_x^2 + n^2\left(\frac{\pi}{a}\right)^2\right] \quad (n > 0)$$

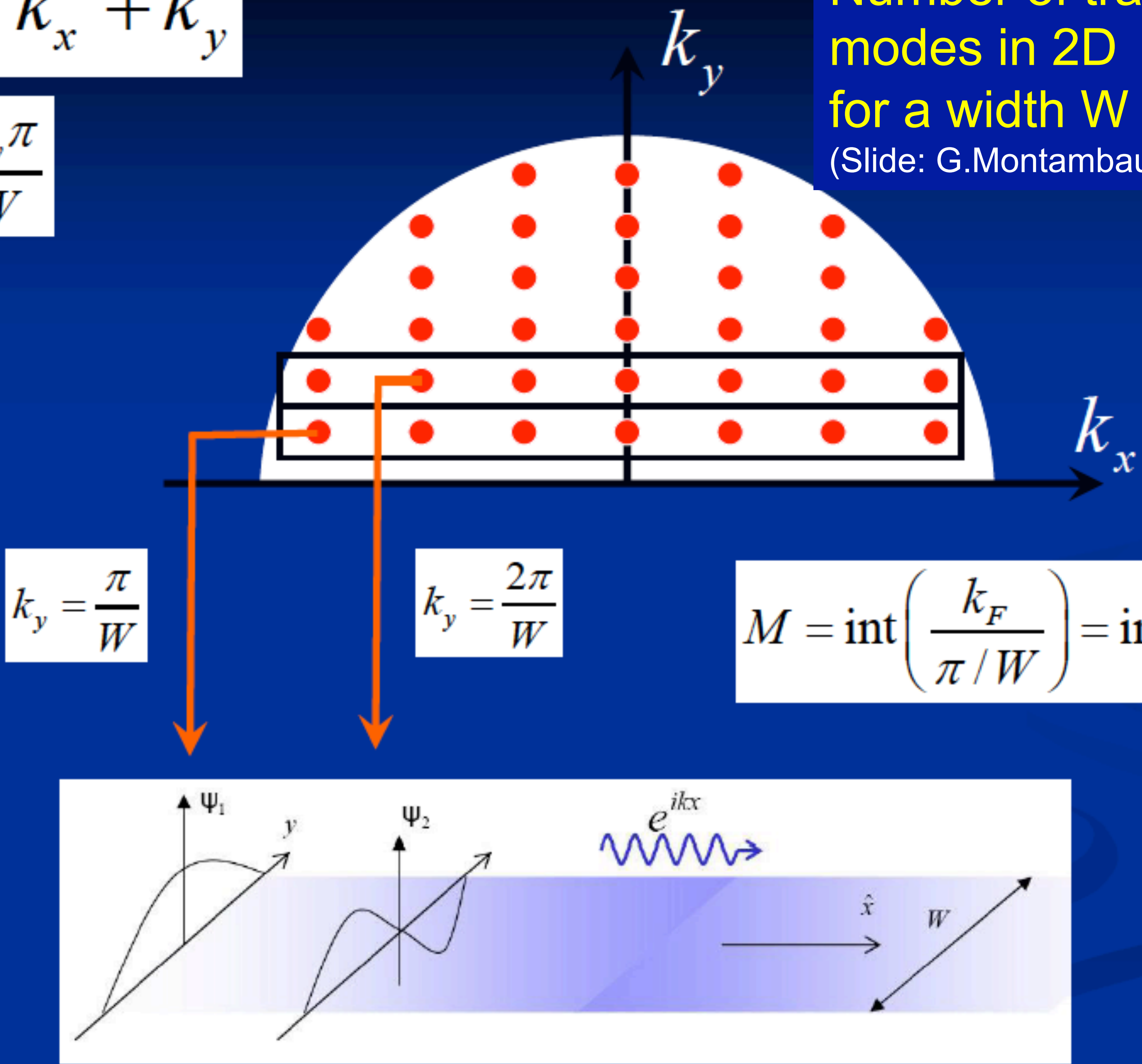
$$3D: \quad \varepsilon_{n_y,n_z}(k_x) = \frac{\hbar^2}{2m}\left[k_x^2 + n_y^2\left(\frac{\pi}{a}\right)^2 + n_z^2\left(\frac{\pi}{b}\right)^2\right] \quad (n_y, n_z > 0)$$

Number of transverse modes in 2D for a width W

(Slide: G.Montambaux)

$$k_F^2 = k_x^2 + k_y^2$$

$$k_y = \frac{n_y \pi}{W}$$



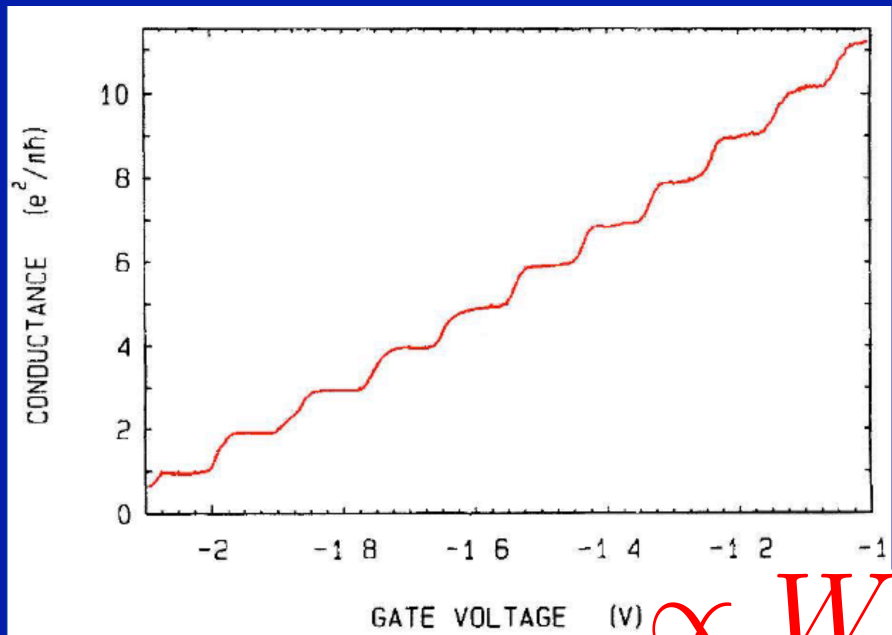
$$M = \mathrm{int}\left(\frac{k_F}{\pi / W}\right) = \mathrm{int}\left(\frac{k_F W}{\pi}\right)$$

Simplest model: only fully open or fully closed channels

(`Il faut qu’une porte soit ouverte ou fermée’, Alfred de Musset)

$$\mathcal{T}(\varepsilon) = \sum_n \theta(\varepsilon - \varepsilon_n)$$

$$G = \frac{2e^2}{h} \sum_n f(\varepsilon_n - \mu)$$



$\propto W$

Thermopower of a QPC

Theory: P.Streda J.Phys Cond Matt. 1, 1025 (1989), Proetto PRB 44, 9096 (1991)

First experiment: L.Molenkamp et al. PRL 65, 1052 (1990)

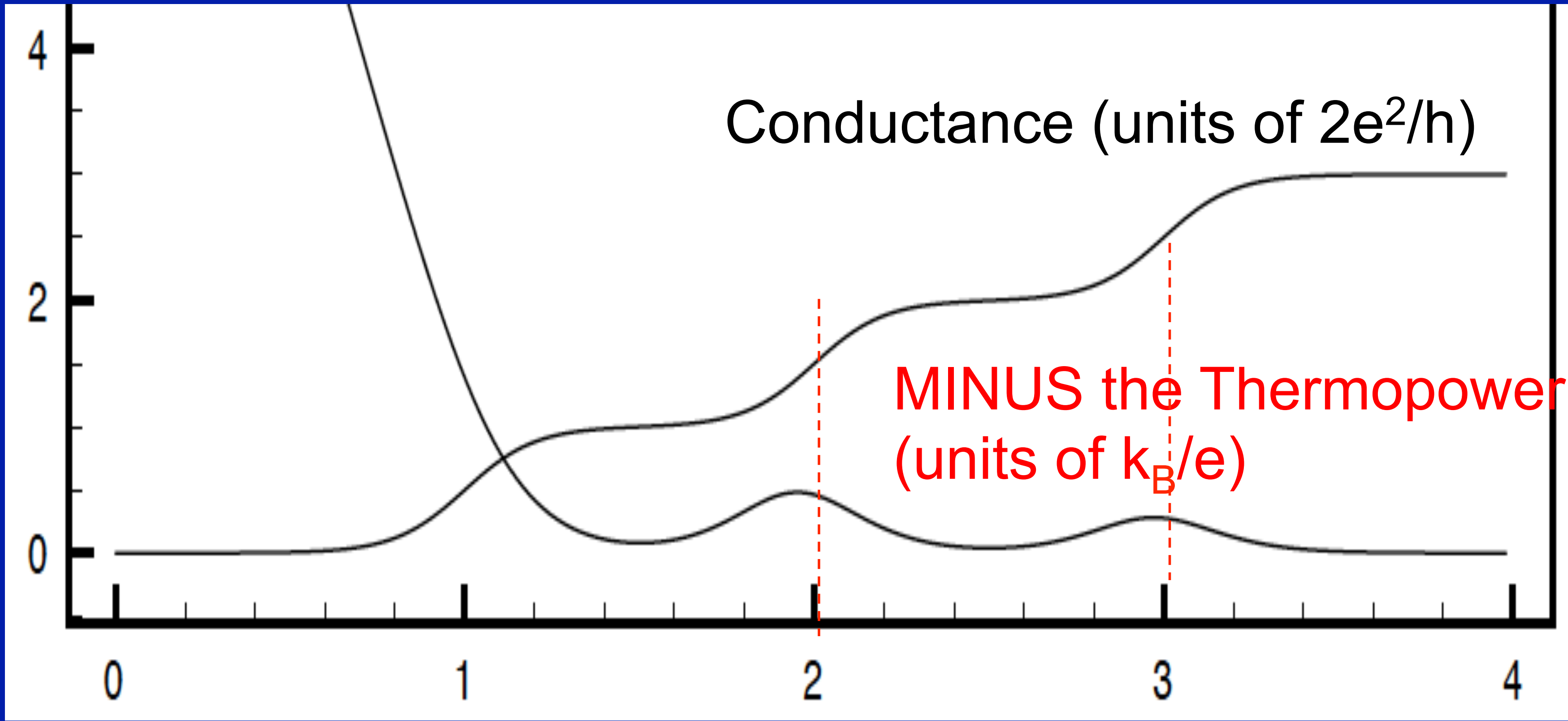
Use again simplest model (open or close channels only):

$$\mathcal{T}(\varepsilon) = \sum_{n=1}^{\infty} \theta(\varepsilon - \varepsilon_n)$$

$$x_n \equiv \frac{\varepsilon_n - \mu}{k_B T} \quad , \quad f(x) \equiv \frac{1}{1+e^x}$$

$$I_0 = \sum_n f(x_n)$$

$$I_1 = \sum_n \left[\frac{x_n}{1+e^{x_n}} + \ln(1+e^{-x_n}) \right]$$



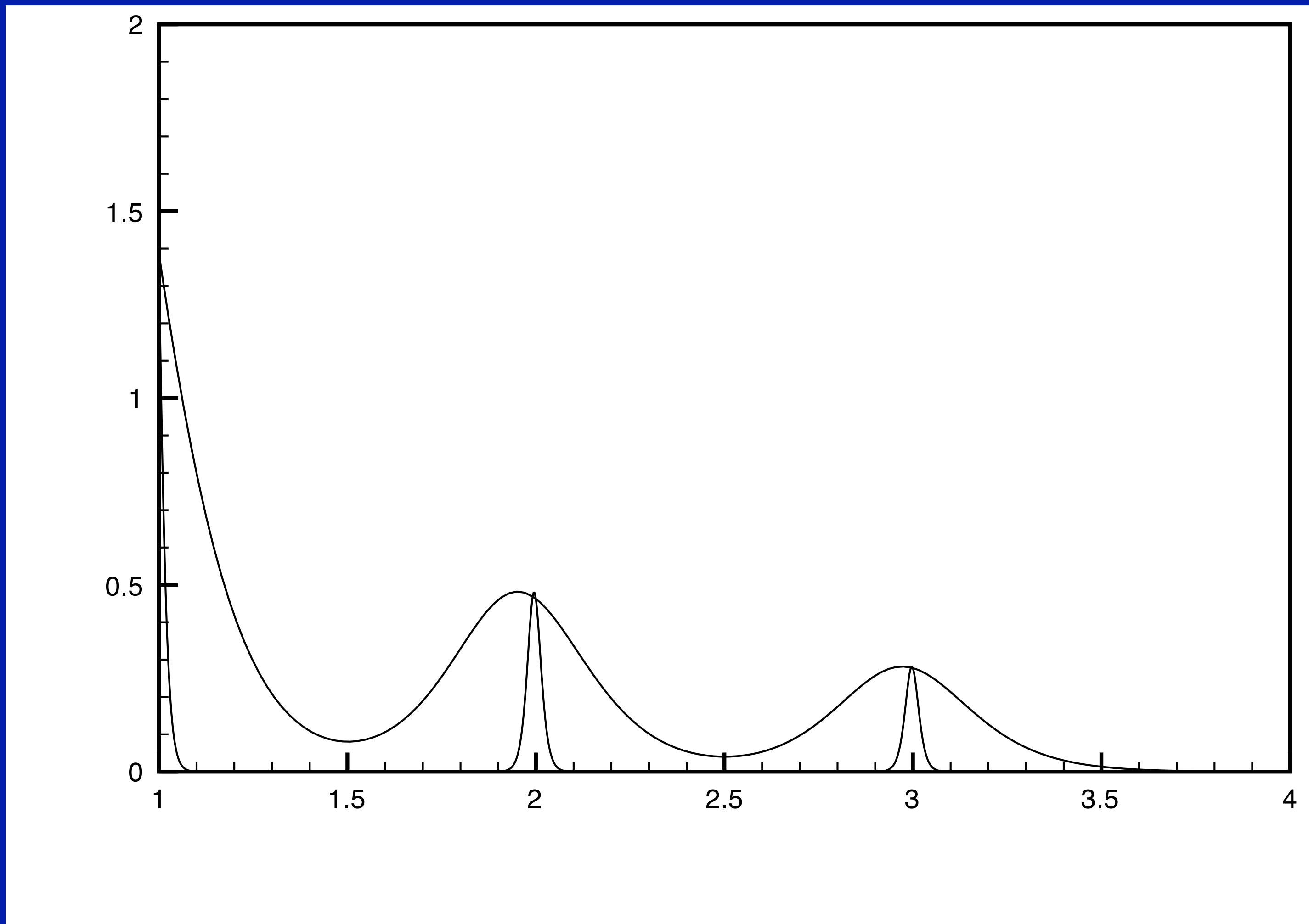
Recall at low-T: $\alpha \propto -\frac{1}{G}\frac{\partial G}{\partial \mu}$

Thermopower has a peak each time a new level becomes `active' with ~ constant height

Parabolic well: $\mu \simeq \varepsilon_n \ : \ \alpha \simeq -\frac{k_B}{e}\frac{\ln 2}{n-1/2}\ , \ G \simeq \frac{2e^2}{h}(n-\frac{1}{2})$

<u>Experimental observation: see Laurens Molenkamp's seminar</u>

Temperature dependence



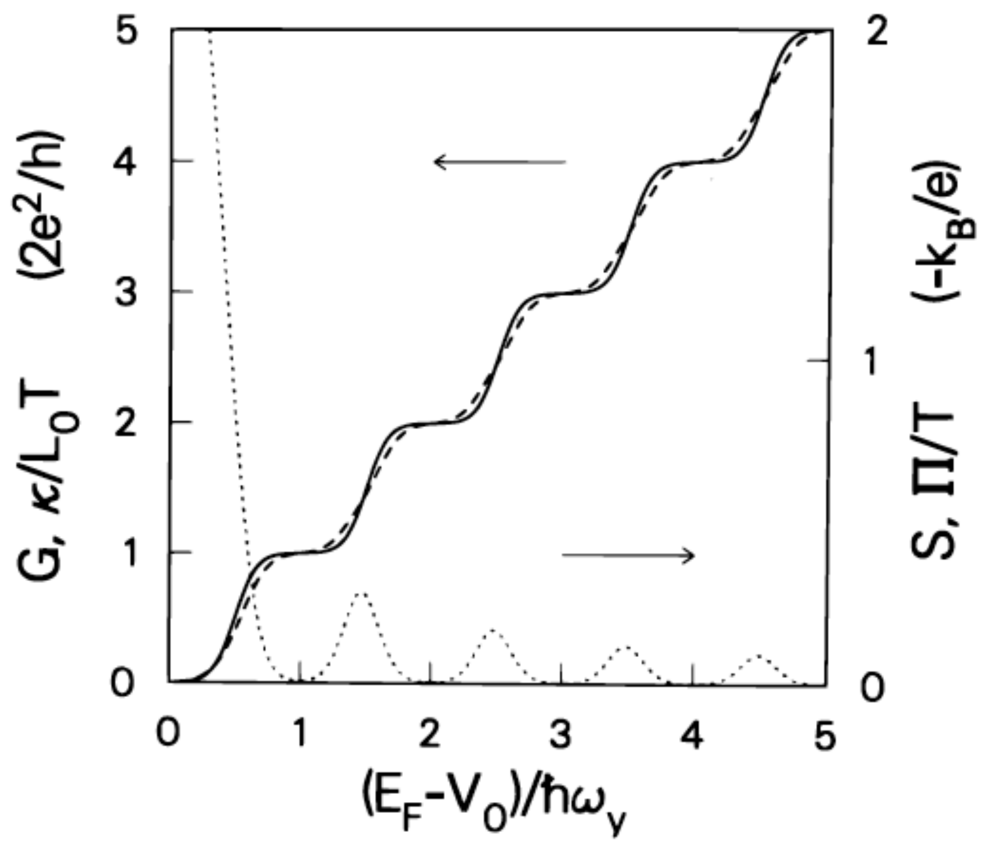


FIG. 3 Calculated conductance G (full curve), thermal conductance κ/L_0T (broken curve), and the thermopower S and Peltier coefficient $\Pi/T = T$ (same dotted curve) for a quantum point contact with a saddle shaped potential, as a function of Fermi energy at 1 K. Parameters used in the calculation are $\hbar\omega_{\mathrm{y}} = 2\,\mathrm{meV}$, $\hbar\omega_{\mathrm{x}} = 0.8\,\mathrm{meV}$.

Saddle-shape potential, van Houten et al arXiv:cond-mat 0512612

A useful observation (to be continued on Nov,19…)

cf. Mahan and Sofo, PNAS 93, 7436 (1996)

Think of:

$$p(\varepsilon) \equiv \frac{\mathcal{T}(\varepsilon)[-f'(\varepsilon)]}{\int d\varepsilon \mathcal{T}(\varepsilon)[-f'(\varepsilon)]} = \frac{g(\epsilon)}{G}$$

As a probability density, measuring the contribution to the total conductance of states around a given energy (for a given gate voltage)

The thermopower is ~ the first moment of this distribution
The thermal conductance is ~ the second moment

NOTES: CURRENTS, ETC…

Notes on Thermoelectricity of Small Systems - Collège de France - Fall 2013

Antoine Georges

(Dated: Notes complementing lectures 2 and 3 (Nov 12 - Nov 19, 2013))

Note: These are by no means intended as a self-contained set of notes. Instead, they are merely complements to the slides, covering the material presented on the blackboard during the lectures.

I. CONDUCTANCE AS TRANSMISSION: THE LANDAUER FORMULA

Useful books: Nazarov and Blanter[2], Montambaux[1].

A. Simple derivation for a single one-dimensional channel

Consider an incident wave coming from the left reservoir, which is partially reflected and partially transmitted, so that on the left side:

$$\psi_L(x) = \frac{1}{\sqrt{L}} \left[e^{+ikx} + r\, e^{-ikx}\right] \tag{1}$$

with r the reflection coefficient for the amplitude (a complex number in general). The corresponding particle current density reads:

$$\boldsymbol{j}_n \, = \, \frac{\hbar}{m} \mathrm{Re}\left[\frac{1}{i}\psi^* \partial_x \psi\right] \, = \, \frac{\hbar k}{mL}\,(1-|r|^2) \tag{2}$$

We could also have calculated the current from the transmitted wave:

$$\psi_R(x) \, = \, t\,\frac{1}{\sqrt{L}}\,e^{+ikx} \;\Rightarrow\; \boldsymbol{j}_n \, = \, \frac{\hbar k}{mL}\,|t|^2 \tag{3}$$

These two expressions are equivalent since the reflection and transmission coefficients for *probabilities* add up to unity:

$$\mathcal{R} \equiv |r|^2 \;\;,\;\; \mathcal{T} \equiv |t|^2 \;\;,\;\; \mathcal{R} + \mathcal{T} \, = \, 1 \tag{4}$$

The total current is the difference between the current originating from the left reservoir and that originating from the right reservoir (for a single-channel, the transmission coefficient in both cases is $\mathcal{T}$, see below):

$$I \, = \, 2_{spin}\,(-e)\,\frac{1}{L}\sum_{k>0} \frac{\hbar k}{m}\,\mathcal{T}(\varepsilon_k)\;[f(\varepsilon_k - \mu_L) - f(\varepsilon_k - \mu_R)] \tag{5}$$

We note that (beware of the subtleties with factors of 2: we consider only right-moving modes with $k > 0$!):

$$\frac{1}{L}\sum_{k>0}\frac{\hbar k}{m}\phi(\varepsilon_k) \to \int_0^{+\infty} \frac{dk}{2\pi}\,\frac{\hbar k}{m}\phi(\varepsilon_k) \, = \, \int d\varepsilon\,\frac{1}{2\pi\hbar}\,\phi(\varepsilon) \tag{6}$$

So that one finally gets:

$$\boxed{I \, = \, -\frac{2e}{h}\int d\varepsilon\,\mathcal{T}(\varepsilon)\;[f(\varepsilon - \mu_L) - f(\varepsilon - \mu_R)]} \tag{7}$$

This formula is actually valid for an arbitrary dispersion $\varepsilon(k_x)$, since the associated velocity reads $v_k = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k}$ and $\int \frac{dk}{2\pi}\,v_k \to \int \frac{d\varepsilon}{h}$: the density of states does not appear in the final expression !

We recall - see the lectures of spring 2013 - that the (electro-) chemical potential difference is related to the tension between the left and right reservoirs by:

$$\mu_L - \mu_R = -eV \tag{8}$$

A common chemical potential can be defined such that:

$$\mu_L = \mu + \delta\mu_L \ , \ \mu_L = \mu + \delta\mu_R \ , \ \delta\mu_L - \delta\mu_R = -eV \tag{9}$$

The linear-response conductance is thus given by ($I = GV$):

$$\boxed{G = \frac{2e^2}{h} \int d\varepsilon \, \mathcal{T}(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon}\right) \ , \ G(T=0) = \frac{2e^2}{h} \mathcal{T}(\varepsilon_F)} \tag{10}$$

Quantum of resistance:

$$\boxed{R_Q \equiv \frac{h}{e^2} = 25.812807449(86)\, k\Omega} \tag{11}$$

The remarkable point is of course that a perfect 1-channel ballistic conductor does not have infinite conductance, but rather a conductance $2e^2/h$!

B. Where does the potential drop? Contact resistance.

Let us consider a 4-probe geometry as in the slides. We are going to evaluate the electron number at point A in two possible ways. By assuming local equilibrium at a local chemical potential μ_A. Or by stating that the electrons at A are either thos coming from the left reservoir and having undergone a reflexion of those coming from the right reservoir and having been transmitted. Thus:

$$\begin{aligned} N_A &= 2\sum_{k>0} [(1+\mathcal{R}) f(\varepsilon_k - \mu_L) + \mathcal{T} f(\varepsilon_k - \mu_R)] \\ &= 2\sum_k f(\varepsilon_k - \mu_A) \end{aligned} \tag{12}$$

Beware that the first sum runs over $k > 0$ while the second one runs over all k's ! And $\sum_k = 2\sum_{k>0}$. Expanding for small departures from equilibrium, one obtains:

$$(1+\mathcal{R}+\mathcal{T}) f(\varepsilon - \mu) + [(1+\mathcal{R})\delta\mu_L + \mathcal{T}\delta\mu_R]\left(-\frac{\partial f}{\partial \mu}\right) = 2f(\varepsilon-\mu) + \delta\mu_A \left(-\frac{\partial f}{\partial \mu}\right) \tag{13}$$

Hence (similar reasoning for B):

$$2\delta\mu_A = (1+\mathcal{R})\delta\mu_L + \mathcal{T}\delta\mu_R \ , \ 2\delta\mu_B = \mathcal{T}\delta\mu_L + (1+\mathcal{R})\delta\mu_R \tag{14}$$

So that the potential drop in the channel is given by:

$$\mu_A - \mu_B = \mathcal{R}\,(\mu_L - \mu_R) \tag{15}$$

Using the Landauer formula for the whole system: $V_L - V_R = \frac{h}{2e^2}\frac{1}{\mathcal{T}} I$, we obtain the conductance of the channel as (first Landauer formula, 1957):

$$\boxed{G_{ch} = \frac{2e^2}{h}\frac{\mathcal{T}}{\mathcal{R}} = \frac{2e^2}{h}\frac{\mathcal{T}}{1-\mathcal{T}}} \tag{16}$$

Calculating the potential drops at the contact $\mu_A - \mu_L$, we obtain that they are equal on each side, and that the resistance of each contact is given by:

$$\boxed{R_c = \frac{h}{4e^2}} \tag{17}$$

We check that $R_c + R_{ch} + R_c = 1/G = \frac{h}{2e^2}$.

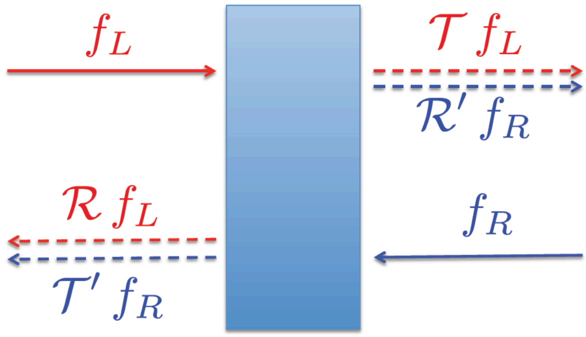


FIG. 1: Transmission and reflection from the scattering region, and probabilities of occupation of a given state.

II. GENERALIZATION OF THE LANDAUER FORMULA TO THERMOELECTRIC TRANSPORT

A. Particle, Energy and Entropy currents

We recall (lectures 2012-2013) that entropy (S) and particle number (N) are conjugate to temperature and chemical potential ($\Omega \equiv -k_B T \ln Z_{gc}$):

$$S = -\frac{\partial \Omega}{\partial T}|_\mu \ , \ N = -\frac{\partial \Omega}{\partial \mu}|_T \tag{18}$$

We consider two reservoirs at local equilibrium characterized by (T_L, μ_L) and (T_R, μ_R). The left reservoir injects particles with $k > 0$ to the left of the scattering region, while the right reservoir injects particles with $k < 0$ to the right of the scattering region. The conventions for the transmission and reflection coefficients are summarized on Fig. 1.

Let us calculate first the particle current I_N, considering e.g. the region on the left. The probability of occupation of a right-moving state with $k > 0$ there is: $f_L \equiv f(\varepsilon_k - \mu_L)$, while the probability of occupation of a left-moving state with $k < 0$ is (Fig. 1):

$$(\mathcal{R} f_L + \mathcal{T}' f_R) \tag{19}$$

In the following, we specialize to the case with time-reversal invariance, so that:

$$\mathcal{T} = \mathcal{T}' \ , \ \mathcal{R} = \mathcal{R}' \ , \tag{20}$$

and from parity: $v_{-k} = -v_k, \varepsilon(-k) = \varepsilon(k)$. Hence, we have:

$$v_k f_L + v_{-k}\,(\mathcal{R} f_L + \mathcal{T}' f_R) \ = \ v_k\, \mathcal{T}\,(f_L - f_R) \tag{21}$$

The particle current thus reads:

$$I_N \ = \ 2_{spin} \int_0^\infty \frac{dk}{2\pi}\, v_k\, \mathcal{T}\,(f_L - f_R) \tag{22}$$

As explained above $\int_0^\infty \frac{dk}{2\pi} v_k \to \int \frac{d\varepsilon}{h}$, so that the particle current I_N $(I \equiv -e I_N)$ finally reads:

$$\boxed{I_N \ = \ \frac{2}{h} \int d\varepsilon\, \mathcal{T}(\varepsilon)\ [f_L(\varepsilon) - f_R(\varepsilon)]} \tag{23}$$

We note that the particle number being a *conserved quantity*, we could equally well have calculated the current from the right side ($\dot{N}_N + \dot{N}_R = 0$), and indeed:

$$(\mathcal{T} f_L + \mathcal{R} f_R) - f_R \;=\; \mathcal{T}(f_L - f_R) \tag{24}$$

Similarly, energy is a conserved quantity, and we can calculate the energy current from either region with the result:

$$\boxed{I_E \;=\; \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\,\varepsilon\;[f_L(\varepsilon) - f_R(\varepsilon)]} \tag{25}$$

The entropy current is a more subtle issue. Indeed, *entropy is not a conserved quantity* and the entropy currents to the left and to the right of the scatterer *are not equal*, in general: dissipation takes place in the scattering region (except in the ballistic case $\mathcal{T} = 1$, see above). The discussion below follows Sivan and Imry.[3] Let us define:

$$F[X] \;\equiv\; -X\ln X - (1-X)\ln(1-X) \tag{26}$$

The entropy current on the left side reads (we use $\mathcal{R} + \mathcal{T} = 1$):

$$\boxed{I_S^L \;=\; 2\,\frac{k_B}{h}\int d\varepsilon\;\left(F[f_L] - F[(1-\mathcal{T})f_L + \mathcal{T} f_R]\right)} \tag{27}$$

while the entropy current on the right-hand side reads:

$$\boxed{I_S^R \;=\; 2\,\frac{k_B}{h}\int d\varepsilon\;\left(F\left[\mathcal{T} f_L + (1-\mathcal{T})f_R\right] - F\left[f_R\right]\right)} \tag{28}$$

It is easily checked that $I_S^L \neq I_S^R$ in general, except in linear response to first order in the gradients (as we shall see below) and, as expected, in the ballistic case where:

$$\boxed{\mathcal{T} = 1 \;\;:\;\; I_S^L = I_S^R \;=\; 2\,\frac{k_B}{h}\int d\varepsilon\;\left(F\left[f_L\right] - F\left[f_R\right]\right)} \tag{29}$$

B. Linear response

1. *Expressions of the currents in linear response*

All we have to do if we are interested in the linear response coefficient is to expand these expressions to first order in the gradients (note that I denote by $\Delta\mu$ the difference between left and right, not to be confused with the gradient $\nabla\mu = -\Delta\mu$) :

$$\Delta\mu \equiv \mu_L - \mu_R \;\;,\;\; \Delta T \equiv T_L - T_R \;\;,\;\; \Delta f \equiv f_L - f_R \tag{30}$$

The statistical factors entering the left-side entropy current is thus:

$$F[f + \Delta f] - F[(1-\mathcal{T})(f+\Delta f) + \mathcal{T} f] \;=\; \mathcal{T}\,F'[f]\,\Delta f \;+\; \frac{1}{2}(\Delta f)^2 F''[f]\,\mathcal{T}(2-\mathcal{T}) + \cdots \tag{31}$$

and for the right-side current:

$$F[f + \mathcal{T}\Delta f] - F[f] \;=\; \mathcal{T}\,F'[f]\,\Delta f \;+\; \frac{1}{2}(\Delta f)^2 F''[f]\,\mathcal{T}^2 + \cdots \tag{32}$$

Hence, up to first order in Δf (linear response), the two entropy currents coincide and read:

$$I_S \;=\; 2\,\frac{k_B}{h}\int d\varepsilon\,\mathcal{T}(\varepsilon)\,F'[f]\,\Delta f + O(\Delta f^2) \tag{33}$$

Using:

$$F'[f] \,=\, \ln\frac{1-f}{f} \,=\, \frac{\varepsilon-\mu}{k_B T} \equiv x \tag{34}$$

we recover the expected relation ($dE = TdS + \mu dN$) between the entropy, energy and particle currents *valid in linear response*:

$$I_S \,=\, \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\, \frac{\varepsilon-\mu}{T}\,\Delta f \,=\, \frac{1}{T}\left(I_E - \mu I_N\right) \tag{35}$$

We also note that, to order Δf^2, the difference between the entropy current on the right- and left- sides (related to the heat dissipated in the scattering region) read:

$$I_S^R - I_S^L \,=\, 2\,\frac{k_B}{h}\int d\varepsilon\, \frac{\mathcal{T}(1-\mathcal{T})}{f(1-f)}\,(\Delta f)^2 \tag{36}$$

where we have used $F''[f] = -1/f(1-f)$. Relationship to noise ?

2. Onsager coefficients

Using:

$$\Delta f = \left[\Delta\mu\frac{\partial}{\partial\mu} + \Delta T\frac{\partial}{\partial T}\right] f\left(\frac{\varepsilon-\mu}{k_B T}\right) \,=\, \left(-\frac{\partial f}{\partial\varepsilon}\right)\left[\Delta\mu + \frac{\varepsilon-\mu}{T}\Delta T\right] \tag{37}$$

we obtain:

$$\begin{aligned} I_N \,&=\, \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[\Delta\mu + \frac{\varepsilon-\mu}{T}\Delta T\right]\left(-\frac{\partial f}{\partial\varepsilon}\right) \\ I_S \,&=\, \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[\frac{\varepsilon-\mu}{T}\Delta\mu + \left(\frac{\varepsilon-\mu}{T}\right)^2\Delta T\right]\left(-\frac{\partial f}{\partial\varepsilon}\right) \end{aligned} \tag{38}$$

From which we immediately identify the Onsager coefficients defined as (cf 2012-2013 lectures):

$$\begin{pmatrix} I_N \\ I_S \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}\begin{pmatrix} \Delta\mu \\ \Delta T \end{pmatrix} \tag{39}$$

$$L_{11} \,=\, \frac{2}{h}\,I_0 \;\;,\;\; L_{12} = L_{21} \,=\, \frac{2}{h}\,k_B I_1 \;\;,\;\; L_{22} \,=\, \frac{2}{h}\,k_B^2 I_2 \tag{40}$$

in which the *dimensionless* integrals read ($x \equiv (\varepsilon-\mu)/k_B T$):

$$I_n \,\equiv\, \int d\varepsilon\, \mathcal{T}(\varepsilon)\left(\frac{\varepsilon-\mu}{k_B T}\right)^n\left(-\frac{\partial f}{\partial\varepsilon}\right) \,=\, \int dx\, \frac{x^n}{4\cosh^2\frac{x}{2}}\,\mathcal{T}(\mu + x\,k_B T) \tag{41}$$

We have also explicitly verified Onsager's symmetry (no magnetic field is present here, and the system is time-reversal invariant).

Let us express the corresponding linear-response coefficient in a more physical way. The electrical and heat ($\delta Q = TdS$) currents are given by:

$$I \,=\, -eI_N \;\;,\;\; I_Q = TI_S \tag{42}$$

and the tension is given by: $\Delta V = -\Delta\mu/e$, so that we obtain:

$$I = e^2 L_{11}\Delta V - eL_{12}\Delta T \;\;,\;\; I_Q = -eTL_{21}\,\Delta V + TL_{22}\,\Delta T \tag{43}$$

The (electrical) conductance is defined by the response $I = G\Delta V$ in the absence of a thermal gradient, so that:

$$\boxed{G = e^2 L_{11} = \frac{2e^2}{h} I_0} \tag{44}$$

The Seebeck coefficient α (or thermopower) is defined by the *stopping condition* (corresponding to an open circuit), i.e. $I = 0$:

$$\alpha \equiv \frac{E}{\nabla T}|_{I=0} \equiv -\frac{\Delta V}{\Delta T}|_{I=0} \tag{45}$$

so that:

$$\boxed{\alpha = -\frac{L_{12}}{eL_{11}} = -\frac{k_B}{e}\frac{I_1}{I_0}} \quad (\frac{k_B}{e} = 86.3\,\mu V K^{-1}) \tag{46}$$

The Peltier coefficient is defined by the heat current induced in the absence of a temperature gradient, as:

$$I_Q \equiv \Pi\, I|_{\Delta T=0} \tag{47}$$

so that:

$$\boxed{\Pi = -T\frac{L_{21}}{eL_{11}} = T\alpha} \tag{48}$$

which satisfies Kelvin-Onsager relation.

Finally, the thermal conductance G_{th} is also defined under open-circuit conditions, as:

$$I_Q = G_{\rm th}\,\Delta T|_{I=0} \tag{49}$$

so that:

$$\boxed{\frac{G_{\rm th}}{T} = \left[L_{22} - \frac{L_{12}L_{21}}{L_{11}}\right] = \frac{2}{h}k_B^2\left[I_2 - \frac{I_1^2}{I_0}\right]} \tag{50}$$

And the Lorenz number reads:

$$\boxed{\mathcal{L} \equiv \frac{G_{\rm th}}{TG} = \left(\frac{k_B}{e}\right)^2\left[\frac{I_2}{I_0} - \left(\frac{I_1}{I_0}\right)^2\right]} \tag{51}$$

Alternatively, we can consider a setup in which we control the current and the temperature gradient, and are interested in the resulting tension and heat current. We express ΔV as:

$$\Delta V = \frac{1}{e^2 L_{11}} I + \frac{L_{12}}{eL_{11}}\Delta T = R\,I - \alpha\,\Delta T \tag{52}$$

with the resistance $R \equiv 1/G$. Substituting into the expression of I_Q, one finally obtains:

$$\begin{pmatrix} \Delta V \\ I_Q \end{pmatrix} = \begin{pmatrix} R & -\alpha \\ \Pi & G_{\rm th} \end{pmatrix}\begin{pmatrix} I \\ \Delta T \end{pmatrix} \tag{53}$$

3. Irreversible heat dissipation in linear response

Let us finally discuss the *total* dissipated entropy. We remember (spring 2013 lectures) that the total irreversible heat production rate is the product of currents and generalized forces:

$$\frac{\partial Q}{\partial t}|_{irr} = T\frac{\partial S}{\partial t}|_{irr} = I_N\Delta\mu + I_S\Delta T = I\Delta V + I_Q\frac{\Delta T}{T} \tag{54}$$

This can be rewritten in two ways. In terms of the gradients only:

$$T\frac{\partial S}{\partial t}|_{irr} \;=\; (\Delta\mu, \Delta T)\begin{pmatrix} L_{11} & L_{21} \\ L_{21} & L_{22} \end{pmatrix}\begin{pmatrix} \Delta\mu \\ \Delta T \end{pmatrix} \tag{55}$$

In this form, we see that Onsager's matrix must be positive semi-definite to insure $\dot{Q}_{irr} \geq 0$.

Alternatively:

$$\begin{gathered}\tfrac{\partial Q}{\partial t}|_{irr} = (I, \Delta T/T)\cdot\begin{pmatrix} R & -\alpha \\ \Pi & G_{th} \end{pmatrix}\begin{pmatrix} I \\ \Delta T \end{pmatrix} \\ = RI^2 + \tfrac{G_{th}}{T}\Delta T^2 + I\Delta T\left[\tfrac{\Pi}{T} - \alpha\right] = RI^2 + \tfrac{G_{th}}{T}\Delta T^2\end{gathered} \tag{56}$$

We note that the thermoelectric effects (Seebeck and Peltier) do not contribute: they are *reversible effects.* The total irreversible heat production rate is the sum of the Joule and Fourier heating.

[1] G. Montambaux, *Conduction quantique et physique mésoscopique*, Cours de l'Ecole Polytechnique, 2013.
[2] Yu. V. Nazarov and Blanter Y., *Quantum transport - introduction to nanoscience*, Cambridge University Press, 2009.
[3] U. Sivan and Y. Imry, *Multichannel landauer formula for thermoelectric transport with application to thermopower near the mobility edge*, Phys. Rev. B **33** (1986), 551–558.