Transport Properties of a Chain of Quantum Dots with Self-Consistent Reservoirs

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Vienna, 6th June 2008

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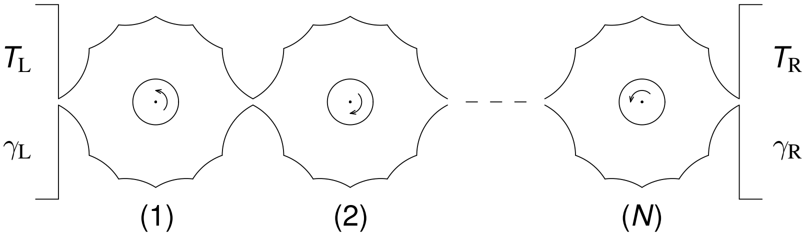
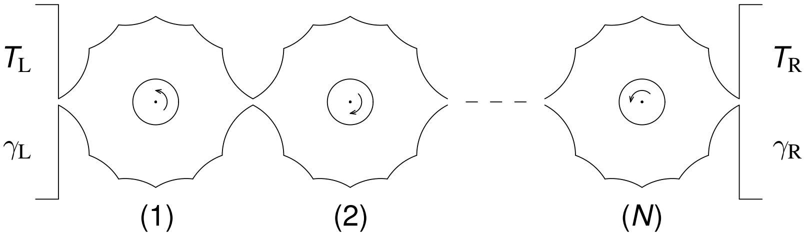
Outline

The classical EY-model



Ref. J.-P. Eckmann and L.-S. Young *Commun. Math. Phys.* **262** 237 (2006)
Ref. H. Larralde, F. Leyvraz and C. Mejía-Monasterio *J. Stat. Phys.* **113** 197 (2003)

The classical EY-model



Assumption: The system admits a stationary state

Fourier's law

$$J = -\gamma \frac{T_R - T_L}{N} \qquad (\gamma_L = \gamma_R = \gamma)$$

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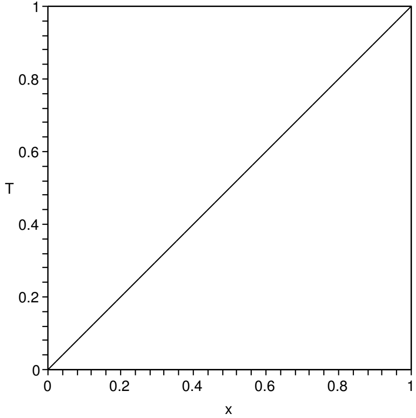
The classical EY-model

Temperature profile of the discs



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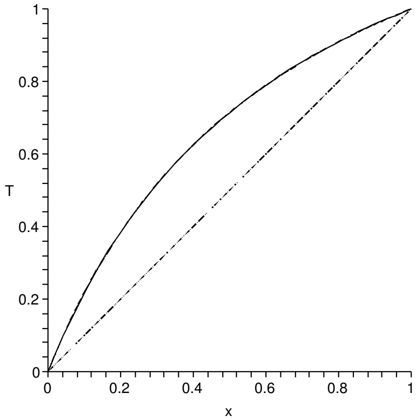

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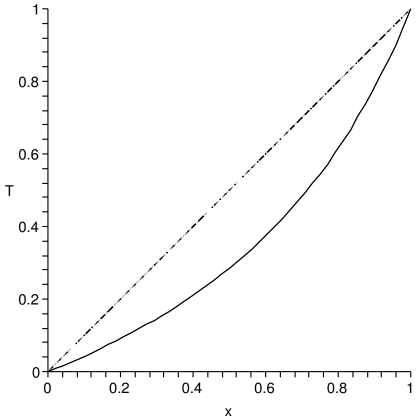
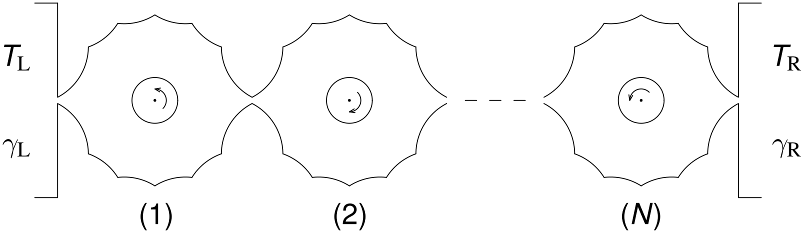


The classical EY-model



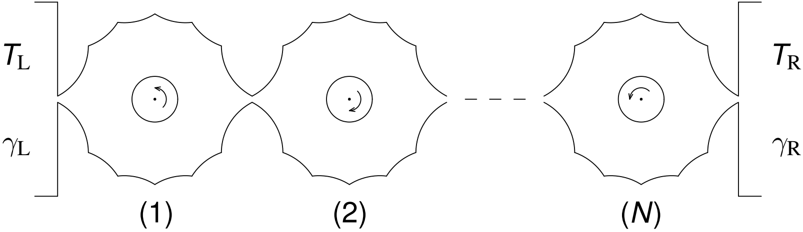
The problem

Establish a quantum version of the EY-model

Questions

1. Does Fourier's law still hold ?
2. Interference effects on the profile and current ?

The classical EY-model



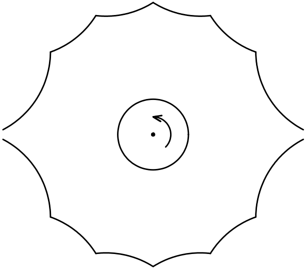
The problem

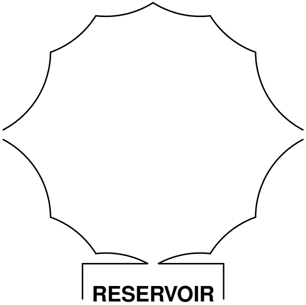
Establish a quantum version of the EY-model

Difficulty

What are quantum discs ?

An Effective Disc





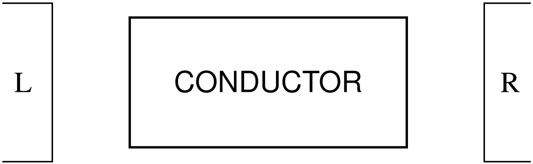
Idea

Effective disc = Particle reservoir satisfying the self-consistency condition[a]

$$I = 0 \quad \text{and} \quad J = 0$$

[a] Ref. M. Visscher and M. Rich *PRA* **12** 675 (1975)

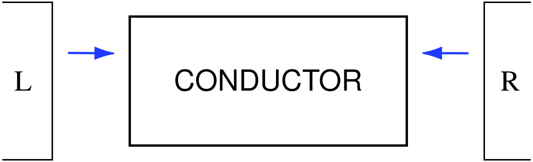
The Scattering Approach



Idea

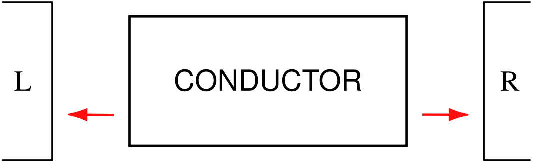
View the CONDUCTOR as a TARGET for the particles

The Scattering Approach



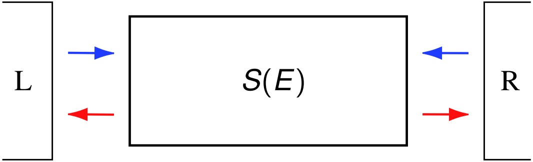
$$\psi^{\text{in}}(E)$$

The Scattering Approach



$\psi^{\text{out}}(E)$

The Scattering Approach



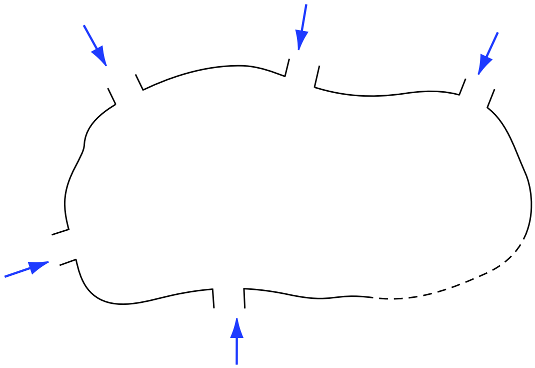
Scattering Matrix

$$\psi^{\mathrm{out}}(E) = S(E)\, \psi^{\mathrm{in}}(E)$$

Particle current conservation needs $S(E)$ to be unitary

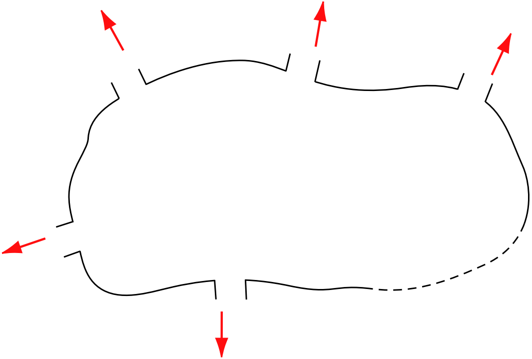
The Scattering Approach

Multi-lead system



The Scattering Approach

Multi-lead system



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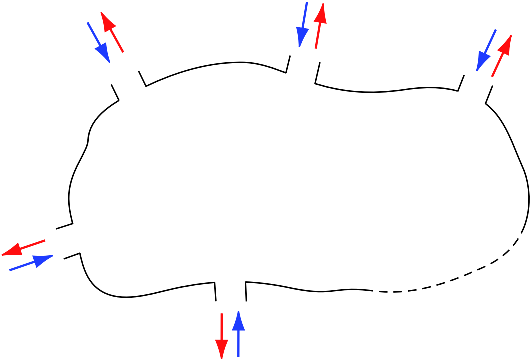
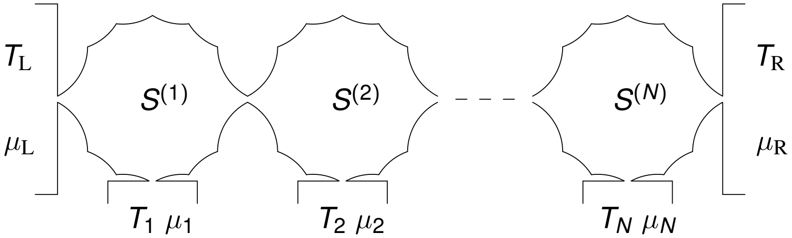


Scattering Matrix

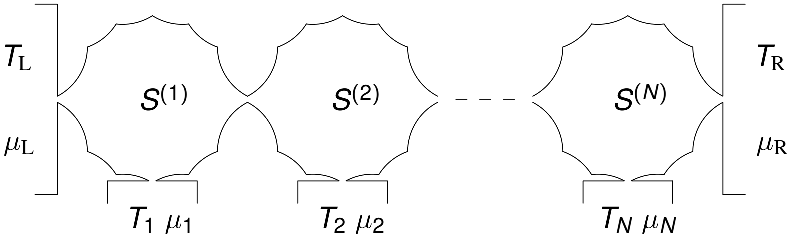
$$\psi^{\mathrm{out}}(E) = S(E)\,\psi^{\mathrm{in}}(E)$$

A Chain of Quantum Dots



1. Transport properties: Scattering matrices $S^{(1)}, \ldots, S^{(N)}$

A Chain of Quantum Dots



1. Transport properties: Scattering matrices $S^{(1)}, \ldots, S^{(N)}$
2. Effective discs = Particle reservoirs satisfying the self-consistency condition

$$I_i = 0 \quad \text{and} \quad J_i = 0 \quad \text{for} \quad i = 1, \ldots, N$$

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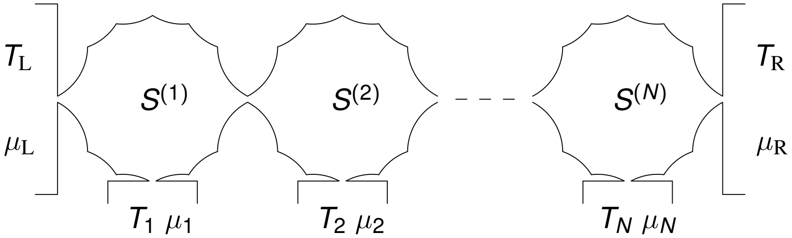

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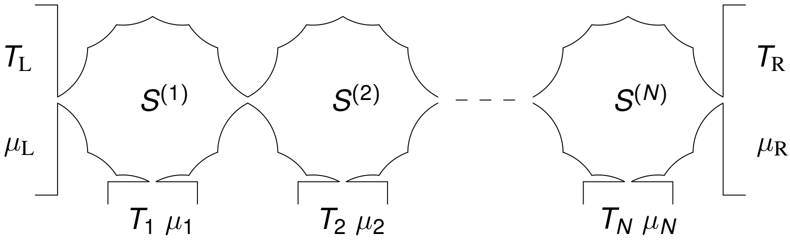
$$I_i = 0 \quad \text{and} \quad J_i = 0 \quad \text{for} \quad i = 1, \ldots, N$$

3. Reservoirs : MB, FD or BE

A Chain of Quantum Dots

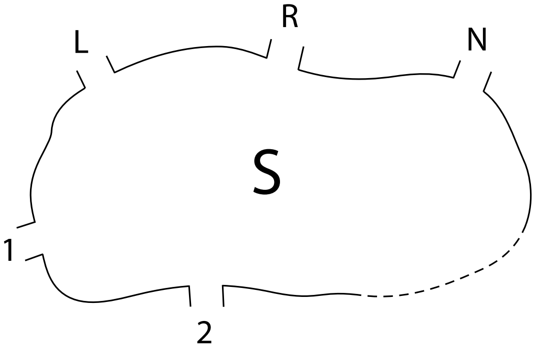


Terminology

- All expressions without a superscript (MB, FD or BE) hold in the three cases
- Universality = Independent of f (MB, FD or BE)

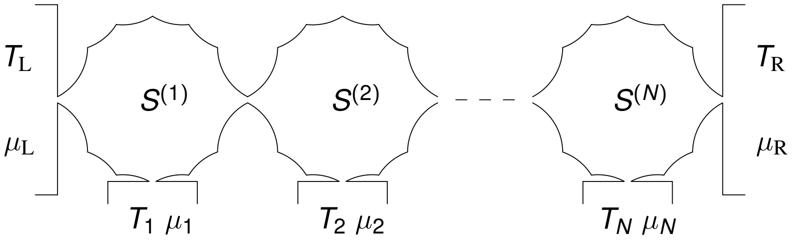
PART 1 : Any Geometry

- Multi-lead system with $N+2$ leads and **any** scattering matrix S



- Introduce the **framework** and present the **main properties** in the **linear response regime**

PART 2 : Linear Geometry



1. Given $(T_{\mathrm{L}}, \mu_{\mathrm{L}})$ and $(T_{\mathrm{R}}, \mu_{\mathrm{R}})$ we find (T_i, μ_i), for $i = 1 \ldots, N$, satisfying the self-consistency condition

$$I_i = 0 \quad \text{and} \quad J_i = 0 \quad \text{for} \quad i = 1, \ldots, N$$

2. Determine the currents: $I_{\mathrm{L}} = -I_{\mathrm{R}}$ and $J_{\mathrm{L}} = -J_{\mathrm{R}}$
3. Linear geometry : Build S from $S^{(1)}, \ldots, S^{(N)}$
   $\Longrightarrow I_{\mathrm{L}}$ and J_{L} go from left to right

The Electric Current

Notations ($i, j \in \{\mathrm{L}, 1, \ldots, N, \mathrm{R}\}$)

- The scattering matrix: S
- The transmission probability: $t_{ij} = |S_{ij}|^2$
- The distribution function

$$f_i(E) = \underbrace{\exp\left(-\frac{E-\mu_i}{k_{\mathrm{B}} T_i}\right)}_{MB} \text{ or } \underbrace{\left[\exp\left(\frac{E-\mu_i}{k_{\mathrm{B}} T_i}\right) \pm 1\right]^{-1}}_{+:FD \quad -:BE}$$

- Boltzmann and Planck constants: k_{B}, h Charge: e

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Assumption: No interaction among the particles

$$I_i = \frac{e}{h} \sum_{j \neq i} \int_0^\infty \left[f_i(E) t_{ji}(E) - f_j(E) t_{ij}(E)\right] dE$$

Ref. Electronic Transport in Mesoscopic Systems by S. Datta (1995)

The Heat Current

$$(\text{Particle Current})_i = \frac{1}{h}\sum_{j\neq i}\int_0^\infty \left[f_i(E)t_{ji}(E) - f_j(E)t_{ij}(E)\right] dE$$

$$(\text{Energy Current})_i = \frac{1}{h}\sum_{j\neq i}\int_0^\infty \left[f_i(E)t_{ji}(E) - f_j(E)t_{ij}(E)\right] E\, dE$$

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First Law of Thermodynamics: $\delta Q = dE - \mu dN$

$$J_i = \frac{1}{h}\sum_{j\neq i}\int_0^\infty \left[f_i(E)t_{ji}(E) - f_j(E)t_{ij}(E)\right] (E-\mu_i) dE$$

Ref. P. N. Butcher *J. Phys.: Condens. Matter* **2** (1990)

Summary

$$\Gamma_{ij} = \delta_{ij} - t_{ij} \qquad t_{ij} = |S_{ij}|^2$$

$$\text{Electric Current:} \quad I_i = \frac{e}{h} \sum_j \int_0^\infty f_j(E) \Gamma_{ij}(E)\, dE$$

$$\text{Heat Current:} \quad J_i = \frac{1}{h} \sum_j \int_0^\infty f_j(E) \Gamma_{ij}(E) (E - \mu_i)\, dE$$

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Conservation laws

Charge: $\sum_i I_i = 0$ Energy: $\sum_i \left(J_i + \frac{\mu_i}{e} I_i \right) = 0$

Summary

$$\Gamma_{ij} = \delta_{ij} - t_{ij} \qquad t_{ij} = |S_{ij}|^2$$

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Conservation laws

Charge: $\sum_i I_i = 0$ Heat in Linear Regime: $\sum_i J_i = 0$

Linear Response

Notations: $T_j = T + \delta T_j$ and $\mu_j = \mu + \delta\mu_j$

$$f(E; T_j, \mu_j) = f(E; T, \mu) + \frac{\partial f}{\partial T}(E; T, \mu)\, \delta T_j + \frac{\partial f}{\partial \mu}(E; T, \mu)\, \delta\mu_j$$

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For f MB, FD or BE

$$f(E;T_j,\mu_j) = f\left(\frac{E-\mu_j}{k_{\mathrm{B}} T_j}\right)$$

Linear Response

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$$f(E; T_j, \mu_j) = f\left(\frac{E - \mu_j}{k_{\mathrm{B}} T_j}\right)$$

For f MB, FD or BE

$$f(E; T_j, \mu_j) = f(E; T, \mu) - \frac{\partial f}{\partial E}(E; T, \mu) \left[\left(\frac{E - \mu}{T}\right) \delta T_j + \delta\mu_j\right]$$

Linear Response

$$
\begin{aligned}
I_i &= \frac{e}{h}\sum_j \int_0^\infty f_j(E)\Gamma_{ij}(E)\,dE \\
J_i &= \frac{1}{h}\sum_j \int_0^\infty f_j(E)\Gamma_{ij}(E)(E-\mu_i)\,dE
\end{aligned}
$$

$$
f(E;T_j,\mu_j) = f(E;T,\mu) - \frac{\partial f}{\partial E}(E;T,\mu)\ \left[\left(\frac{E-\mu}{T}\right)\delta T_j + \delta\mu_j\right]
$$

Onsager Relations

$$I_i = \sum_j L_{ij}^{(0)} \frac{\delta\mu_j}{e} + L_{ij}^{(1)} \frac{\delta T_j}{T}$$

$$J_i = \sum_j L_{ij}^{(1)} \frac{\delta\mu_j}{e} + L_{ij}^{(2)} \frac{\delta T_j}{T}$$

$$L_{ij}^{(0)} = -\frac{e^2}{h} \int_0^\infty \frac{\partial f}{\partial E}(E; T, \mu) \Gamma_{ij}(E)\, dE$$

$$L_{ij}^{(1)} = -\frac{e}{h} k_{\mathrm{B}} T \int_0^\infty \left(\frac{E-\mu}{k_{\mathrm{B}} T}\right) \frac{\partial f}{\partial E}(E; T, \mu) \Gamma_{ij}(E)\, dE$$

$$L_{ij}^{(2)} = -\frac{(k_{\mathrm{B}} T)^2}{h} \int_0^\infty \left(\frac{E-\mu}{k_{\mathrm{B}} T}\right)^2 \frac{\partial f}{\partial E}(E; T, \mu) \Gamma_{ij}(E)\, dE$$

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$$L_{ij}^{(0)} = -\frac{e^2}{h}\int_0^\infty \frac{\partial f}{\partial E}(E;T,\mu)\Gamma_{ij}(E)\,dE \qquad \Gamma_{ij} = \delta_{ij} - |S_{ij}|^2$$

$$L_{ij}^{(1)} = -\frac{e}{h}k_B T\int_0^\infty \left(\frac{E-\mu}{k_B T}\right)\frac{\partial f}{\partial E}(E;T,\mu)\Gamma_{ij}(E)\,dE$$

$$L_{ij}^{(2)} = -\frac{(k_B T)^2}{h}\int_0^\infty \left(\frac{E-\mu}{k_B T}\right)^2\frac{\partial f}{\partial E}(E;T,\mu)\Gamma_{ij}(E)\,dE$$

The Onsager relations hold: $S_{ij} = S_{ji} \Longrightarrow L_{ij} = L_{ji}$

The Main Assumption

Assumption

S does not depend on the energy

Interests

- Good approximation in some limit cases (e.g. low T in FD)
- Consequences of $S(E) = \text{Constant}$

Consequence of $S(E) = \text{Constant}$

$$L_{ij}^{(0)} = -\frac{e^2}{h}\int_0^\infty \frac{\partial f}{\partial E}(E;T,\mu)\Gamma_{ij}(E)\,dE$$

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$$L_{ij}^{(2)} = -\frac{(k_{\mathrm{B}}T)^2}{h}\int_0^\infty \left(\frac{E-\mu}{k_{\mathrm{B}}T}\right)^2\frac{\partial f}{\partial E}(E;T,\mu)\Gamma_{ij}(E)\,dE$$

Consequence of $S(E) = \text{Constant}$

$$L_{ij}^{(0)} = -\frac{e^2}{h}\int_0^\infty \frac{\partial f}{\partial E}(E;T,\mu)\,dE \cdot \Gamma_{ij}$$

$$L_{ij}^{(1)} = -\frac{e}{h}k_B T\int_0^\infty \left(\frac{E-\mu}{k_B T}\right)\frac{\partial f}{\partial E}(E;T,\mu)\,dE \cdot \Gamma_{ij}$$

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Consequence of $S(E) = \text{Constant}$

$$L_{ij}^{(0)} = \frac{e^2}{h} \underbrace{\left[-\int_0^\infty \frac{\partial f}{\partial E}(E; T, \mu)\, dE \right]}_{C(0)} \cdot \Gamma_{ij}$$

$$L_{ij}^{(1)} = \frac{e}{h} k_B T \underbrace{\left[-\int_0^\infty \left(\frac{E-\mu}{k_B T} \right) \frac{\partial f}{\partial E}(E; T, \mu)\, dE \right]}_{C(1)} \cdot \Gamma_{ij}$$

$$L_{ij}^{(2)} = \frac{(k_B T)^2}{h} \underbrace{\left[-\int_0^\infty \left(\frac{E-\mu}{k_B T} \right)^2 \frac{\partial f}{\partial E}(E; T, \mu)\, dE \right]}_{C(2)} \cdot \Gamma_{ij}$$

Consequence of $S(E) = \text{Constant}$

$$L_{ij}^{(0)} = \frac{e^2}{h} C(0) \Gamma_{ij}$$

$$L_{ij}^{(1)} = \frac{e}{h} k_{\mathrm{B}} T C(1) \Gamma_{ij}$$

$$L_{ij}^{(2)} = \frac{(k_{\mathrm{B}} T)^2}{h} C(2) \Gamma_{ij}$$

Consequence of $S(E) = $ Constant

$$L_{ij}^{(0)} = \frac{e^2}{h} C(0) \Gamma_{ij}$$

$$L_{ij}^{(1)} = \frac{e}{h} k_{\mathrm{B}} T C(1) \Gamma_{ij} = \frac{k_{\mathrm{B}} T}{e} \frac{C(1)}{C(0)} L_{ij}^{(0)}$$

$$L_{ij}^{(2)} = \frac{(k_{\mathrm{B}} T)^2}{h} C(2) \Gamma_{ij} = \frac{k_{\mathrm{B}}^2 T^2}{e^2} \frac{C(2)}{C(0)} L_{ij}^{(0)}$$

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The Coefficients $C(n)$

$$C(n) = -\int_0^\infty \left(\frac{E-\mu}{k_\mathrm{B} T}\right)^n \frac{\partial f}{\partial E}(E; T, \mu)\, dE$$

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$$\begin{aligned} C^{\mathrm{MB}}(n) &= \int_{x_0}^\infty x^n e^{-x}\, dx \\ C^{\pm}(n) &= \int_{x_0}^\infty \frac{x^n e^x}{(e^x \pm 1)^2}\, dx \end{aligned}$$

where

$$x_0 = -\frac{\mu}{k_\mathrm{B} T} \begin{cases} \in (-\infty, \infty) \text{ in MB} \\ \in (-\infty, \infty) \text{ in FD} \\ \in (0, \infty) \text{ in BE} \end{cases}$$

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$$C^{\mathrm{MB}}(n) = \int_{x_0}^\infty x^n e^{-x}\, dx$$

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where

$$x_0 = -\frac{\mu}{k_\mathrm{B}T} \begin{cases} \in (-1,\infty) \text{ in MB} \\ \in (-\infty,\infty) \text{ in FD} \\ \in (0,\infty) \text{ in BE} \end{cases}$$

We need $C(n) > 0$ for $n = 0, 1, 2$

Summary

$$I_i = \sum_j L_{ij}^{(0)} \frac{\delta\mu_j}{e} + L_{ij}^{(1)} \frac{\delta T_j}{T}$$

$$J_i = \sum_j L_{ij}^{(1)} \frac{\delta\mu_j}{e} + L_{ij}^{(2)} \frac{\delta T_j}{T}$$

Consequence of $S(E) = \text{Constant}$

$$L_{ij}^{(0)} = \frac{e^2}{h} C(0)\Gamma_{ij} \quad L_{ij}^{(1)} = \tilde{L}_0 L_{ij}^{(0)} \quad \text{and} \quad L_{ij}^{(2)} = L_0 L_{ij}^{(0)}$$

$$L_0 = \frac{k_B^2 T^2}{e^2} \frac{C(2)}{C(0)} > 0 \quad \text{and} \quad \tilde{L}_0 = \frac{k_B T}{e} \frac{C(1)}{C(0)} > 0$$

The Transport Matrix

$$L_{ij}^{(k)} \sim \Gamma_{ij} = \delta_{ij} - t_{ij} \quad (t_{ij} \in (0,1))$$

Properties

1. $$L_{ij}^{(k)} \begin{cases} > 0 & \text{if } i = j \\ < 0 & \text{if } i \neq j \end{cases}$$
2. $$\sum_i L_{ij}^{(k)} = 0 \ , \quad \forall j \qquad \text{and} \qquad \sum_j L_{ij}^{(k)} = 0 \ , \quad \forall i$$

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For f MB, FD or BE ($L_{ij}^{(1)} = \tilde{L}_0 L_{ij}^{(0)}$ and $L_{ij}^{(2)} = L_0 L_{ij}^{(0)}$)

$$\mathcal{R} \equiv \frac{\tilde{L}_0}{\sqrt{L_0}} = \frac{C(1)}{\sqrt{C(0) \cdot C(2)}} \in (0,1), \quad \forall x_0 = -\mu/(k_B T)$$

Entropy Production

Theorem

$$L = \begin{pmatrix} L^{(0)} & L^{(1)} \\ L^{(1)} & L^{(2)} \end{pmatrix}, \quad L^{(k)} = \begin{pmatrix} L^{(k)}_{\mathrm{LL}} & \mathrm{L}^{(k)}_{\mathrm{L1}} & \dots & L^{(k)}_{\mathrm{L}N} & \mathrm{L}^{(k)}_{\mathrm{LR}} \\ L^{(k)}_{1\mathrm{L}} & \mathrm{L}^{(k)}_{11} & \dots & L^{(k)}_{1N} & L^{(k)}_{1\mathrm{R}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ L^{(k)}_{N\mathrm{L}} & L^{(k)}_{N1} & \dots & L^{(k)}_{NN} & L^{(k)}_{N\mathrm{R}} \\ L^{(k)}_{\mathrm{RL}} & L^{(k)}_{\mathrm{R1}} & \dots & L^{(k)}_{\mathrm{R}N} & L^{(k)}_{\mathrm{RR}} \end{pmatrix}$$

The matrix L is real positive semi-definite:

$$\sigma_s = \sum_i \sum_j L_{ij} V_i V_j \geq 0$$

$$V_i = \begin{cases} \delta\mu_i / e & \text{if } i = 1, \dots, N+2 \\ \delta T_i / T & \text{if } i = N+3, \dots, 2N+4 \end{cases}$$

Main Trick of the Proof $\sigma_s \geq 0$

Notations: $X_i = \delta\mu_i / e$ and $Z_i = \sqrt{L_0}\, \delta T_i / T$

$$\sigma_s = \sum_{i<j} \underbrace{(-L_{ij}^{(0)})}_{>0} \; I_{ij}$$

$$I_{ij} = (X_i - X_j)^2 + (Z_i - Z_j)^2 - 2\mathcal{R} C_{ij} \,, \qquad C_{ij} = X_i Z_j + X_j Z_i - X_i Z_i - X_j Z_j$$

TRICK : $0 < \mathcal{R} < 1$

$$C_{ij} \leq 0 : I_{ij} \geq (X_i - X_j)^2 + (Z_i - Z_j)^2 \geq 0$$

$$C_{ij} > 0 : I_{ij} > (X_i - X_j)^2 + (Z_i - Z_j)^2 - 2C_{ij} = (X_i - X_j + Z_i - Z_j)^2 \geq 0$$

Ref. M. Büttiker *IBM J. Res. Dev.* **3** 317-334 (1988)

Equilibrium and Non-Equilibrium States

Definition (Equilibrium)

$$\mu_{\rm L} = \mu_1 = \cdots = \mu_N = \mu_{\rm R} \qquad \text{and} \qquad T_{\rm L} = T_1 = \cdots = T_N = T_{\rm R}$$

Equilibrium and Non-Equilibrium States

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Theorem

$$\{\textit{System is at equilibrium}\} \iff \{I_i = 0 \quad \textit{and} \quad J_i = 0, \quad \forall i\}$$

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Theorem

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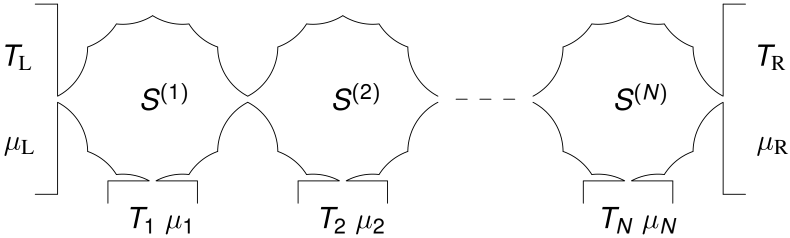
Theorem

$$\left\{ \begin{array}{c} \textit{System is at} \\ \textit{equilibrium} \end{array} \right\} \iff \sigma_s = 0$$

$$\left\{ \begin{array}{c} \textit{System is} \\ \textit{out of equilibrium} \end{array} \right\} \iff \sigma_s > 0$$

Main trick in the proofs: $0 < \mathcal{R} < 1$

The Self-Consistency Condition



The problem

Given $(T_{\rm L}, \mu_{\rm L})$ and $(T_{\rm R}, \mu_{\rm R})$, find (T_i, μ_i), for $i = 1 \ldots, N$, such that

$$I_i = 0 \quad \text{and} \quad J_i = 0 \quad \text{for} \quad i = 1, \ldots, N$$

The Self-Consistency Condition

For $i = 1, \dots, N$:

$$
\begin{aligned}
I_i &= \sum_j L_{ij}^{(0)} \frac{\delta \mu_j}{e} + L_{ij}^{(1)} \frac{\delta T_j}{T} = 0 \\
J_i &= \sum_j L_{ij}^{(1)} \frac{\delta \mu_j}{e} + L_{ij}^{(2)} \frac{\delta T_j}{T} = 0
\end{aligned}
$$

$$
\begin{aligned}
\sum_{j=1}^{N} \left(L_{ij}^{(0)} \frac{\delta \mu_j}{e} + L_{ij}^{(1)} \frac{\delta T_j}{T} \right) &= -\sum_{j=\mathrm{L,R}} \left(L_{ij}^{(0)} \frac{\delta \mu_j}{e} + L_{ij}^{(1)} \frac{\delta T_j}{T} \right) \\
\sum_{j=1}^{N} \left(L_{ij}^{(1)} \frac{\delta \mu_j}{e} + L_{ij}^{(2)} \frac{\delta T_j}{T} \right) &= -\sum_{j=\mathrm{L,R}} \left(L_{ij}^{(1)} \frac{\delta \mu_j}{e} + L_{ij}^{(2)} \frac{\delta T_j}{T} \right)
\end{aligned}
$$

The Self-Consistency Condition

Notations: $X_i = \delta\mu_i/e$, $Y_i = \delta T_i/T$, $M_{ij} = L_{ij}^{(0)}$, $(D_\ell)_i = L_{i\ell}^{(0)}$

$$M\left(X + \tilde{L}_0 Y\right) = -\sum_{\ell=\mathrm{L,R}} \left(X_\ell + \tilde{L}_0 Y_\ell\right) D_\ell$$

$$M\left(\tilde{L}_0 X + L_0 Y\right) = -\sum_{\ell=\mathrm{L,R}} \left(\tilde{L}_0 X_\ell + L_0 Y_\ell\right) D_\ell$$

TRICK: $\mathcal{R} \neq 1 \Longrightarrow L_0 \neq (\tilde{L}_0)^2$

$$MX = -\sum_{\ell=\mathrm{L,R}} D_\ell X_\ell \quad \text{and} \quad MY = -\sum_{\ell=\mathrm{L,R}} D_\ell Y_\ell$$

The profiles

Theorem ($i = 1, \ldots, N$, $\Gamma_{ij} = \delta_{ij} - t_{ij}$)

$$\mu_i = \mu_{\rm L} + A_i(\mu_{\rm R} - \mu_{\rm L})$$

$$T_i = T_{\rm L} + A_i(T_{\rm R} - T_{\rm L}) \quad \textit{with} \quad A_i = \sum_{j=1}^{N} (\Gamma^{-1})_{ij}\, t_{j\rm R}$$

Consequences of $S(E) = $ Constant

- The profiles of μ and T are decoupled $\neq$ EY-model
- The profiles are universal: they do not depend on f
- The profiles are given by $A_1, \ldots, A_N$

The profiles

Lemma ($i = 1, \ldots, N$, $\Gamma_{ij} = \delta_{ij} - t_{ij}$)

We have

$$A_i = \frac{\sum_{j=1}^{N} (-1)^{i+j} \det\left(\Gamma(j,i)\right) \; t_{j\mathrm{R}}}{\sum_{j=1}^{N} (-1)^{i+j} \det\left(\Gamma(j,i)\right) \; [t_{j\mathrm{L}} + t_{j\mathrm{R}}]}$$

where $\Gamma(j,i)$ is the (j,i) minor of Γ

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where $\Gamma(j,i)$ is the (j,i) minor of Γ

Example ($N = 1$)

$$A_1 = \frac{t_{1\mathrm{R}}}{t_{1\mathrm{L}} + t_{1\mathrm{R}}} \quad \Longrightarrow \quad \mu_1 = \frac{t_{1\mathrm{L}}\mu_\mathrm{L} + t_{1\mathrm{R}}\mu_\mathrm{R}}{t_{1\mathrm{L}} + t_{1\mathrm{R}}}$$

Ref. M. Büttiker *IBM J. Res. Dev.* **3** 317-334 (1988)

The profiles

Lemma ($i = 1, \ldots, N$, $\Gamma_{ij} = \delta_{ij} - t_{ij}$)

We have

$$A_i = \frac{\sum_{j=1}^{N} (-1)^{i+j} \det\left(\Gamma(j,i)\right)\ t_{j\mathrm{R}}}{\sum_{j=1}^{N} (-1)^{i+j} \det\left(\Gamma(j,i)\right)\ [t_{j\mathrm{L}} + t_{j\mathrm{R}}]} \in (0,1)$$

where $\Gamma(j,i)$ is the (j,i) minor of Γ

Consequence: $\mu_\mathrm{L} < \mu_i < \mu_\mathrm{R}$ and $T_\mathrm{L} < T_i < T_\mathrm{R}$

Example ($N = 1$)

$$A_1 = \frac{t_{1\mathrm{R}}}{t_{1\mathrm{L}} + t_{1\mathrm{R}}} \quad \Longrightarrow \quad \mu_1 = \frac{t_{1\mathrm{L}}\mu_\mathrm{L} + t_{1\mathrm{R}}\mu_\mathrm{R}}{t_{1\mathrm{L}} + t_{1\mathrm{R}}}$$

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The currents

Theorem ($i = 1, \ldots, N$, $\Gamma_{ij} = \delta_{ij} - t_{ij}$)

$$
\begin{aligned}
I_{\mathrm{L}} &= \sigma_0 \left(\frac{\mu_{\mathrm{R}} - \mu_{\mathrm{L}}}{e} \right) + \sigma_1 \left(\frac{T_{\mathrm{R}} - T_{\mathrm{L}}}{T} \right) \\
J_{\mathrm{L}} &= \sigma_1 \left(\frac{\mu_{\mathrm{R}} - \mu_{\mathrm{L}}}{e} \right) + \sigma_2 \left(\frac{T_{\mathrm{R}} - T_{\mathrm{L}}}{T} \right) \\
\sigma_0 &= L_{\mathrm{LR}}^{(0)} + \sum_{j=1}^{N} A_j \, L_{\mathrm{L}j}^{(0)} \,, \qquad \sigma_1 = \tilde{L}_0 \sigma_0 \quad \text{and} \quad \sigma_2 = L_0 \sigma_0
\end{aligned}
$$

Remarks

$$L_{ij}^{(1)} = \tilde{L}_0 L_{ij}^{(0)} \ \text{ and } \ L_{ij}^{(2)} = L_0 L_{ij}^{(0)} \qquad \sigma_k < 0$$

The currents

Ohm's law ($T_{\rm L} = T_{\rm R}$, $\mu = eV$):

$$I_{\rm L} = -\kappa_e \frac{V_{\rm R} - V_{\rm L}}{N}\ , \qquad \kappa_e = -N\sigma_0 > 0$$

Fourier's law ($I_{\rm L} = 0$):

$$J_{\rm L} = -\kappa_h \frac{T_{\rm R} - T_{\rm L}}{N}\ , \qquad \kappa_h = N\frac{\sigma_1^2 - \sigma_0\sigma_2}{\sigma_0 T} = -\frac{(L_0 - \tilde{L}_0^2)}{T} N\sigma_0$$

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Universal conductivity ($\Gamma_{ij} = \delta_{ij} - t_{ij}$)

$$\sigma(N) = -\frac{h}{e^2 C(0)} N\sigma_0 = N\left[t_{\mathrm{LR}} + \sum_{i,j=1}^{N} t_{\mathrm{L}j}(\Gamma^{-1})_{ji} t_{i\mathrm{R}}\right]$$

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Example ($N = 1$)

$$\sigma(1) = t_{\rm LR} + \frac{t_{\rm L1}\ t_{\rm 1R}}{t_{\rm 1L} + t_{\rm 1R}}$$

Ref. M. Büttiker *IBM J. Res. Dev.* **3** 317-334 (1988)

The currents

Ohm's law ($T_{\rm L} = T_{\rm R}$, $\mu = eV$):

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Random Matrix Theory

Question

For which $\{S_N\}_{N=1}^{\infty}$ does the limit $\lim_{N\to\infty} \sigma(N)$ exist ?

Assumption

The 3x3 complex matrices $S^{(1)}, \ldots, S^{(N)}$ are independent and identically distributed over $U(3)$ with some measure:

1. **COE** = Circular Orthogonal Ensemble
   Time-reversible $S_{ij}^{(k)} = S_{ji}^{(k)}$
2. **CUE** = Circular Unitary Ensemble
   Not time-reversal $S_{ij}^{(k)} \neq S_{ji}^{(k)}$ (e.g. magnetic field)

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1. **COE** = Circular Orthogonal Ensemble $B = 0$
   Time-reversible $S_{ij}^{(k)} = S_{ji}^{(k)}$
2. **CUE** = Circular Unitary Ensemble $B \neq 0$
   Not time-reversal $S_{ij}^{(k)} \neq S_{ji}^{(k)}$ (e.g. magnetic field)

Quantum versus Classical

Universality

$A_1, \ldots, A_N$ and $\sigma(N)$ do not depend on f

Interference effects ?

Quantum

$\varphi_1, \varphi_2 \in \mathbb{C} \Longrightarrow P = |\varphi_1 + \varphi_2|^2 = |\varphi_1|^2 + |\varphi_2|^2 +$ Interferences

Classical

$\varphi_1, \varphi_2 \in \mathbb{C} \Longrightarrow P = |\varphi_1|^2 + |\varphi_2|^2$

Quantum versus Classical

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Interference effects ?

Quantum

$$S^{(1)}, \ldots, S^{(N)} \Longrightarrow S \Longrightarrow t_{ij} = |S_{ij}|^2$$

Classical

$$S^{(1)}, \ldots, S^{(N)} \Longrightarrow P^{(1)}, \ldots, P^{(N)} \text{ where } P_{ij}^{(k)} = |S_{ij}^{(k)}|^2$$
$$\Longrightarrow P \Longrightarrow t_{ij} = P_{ij}$$

The Statistical Averages COE and CUE

1. The Average Transmission Probabilities $\langle\, t_{ij} \,\rangle$
2. The Average Universal Conductivity $\langle\, \sigma(N) \,\rangle$
3. The Average Universal Profiles $\langle\, A_1 \,\rangle, \ldots, \langle\, A_N \,\rangle$

The Average Transmission Probabilities $\langle\, t_{ij} \,\rangle$

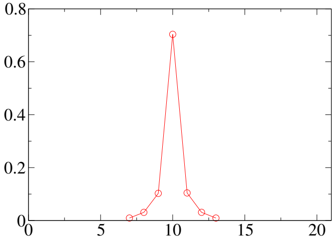
When $N \gg 1$

1. $t_{ij}^{cl} \neq t_{ij}^{qu}$ but $\langle\, t_{ij}^{cl} \,\rangle = \langle\, t_{ij}^{qu} \,\rangle$
2. $\langle\, t_{ij} \,\rangle$ do not depend on N
3. Symmetric: $\langle\, t_{ij} \,\rangle = \langle\, t_{ji} \,\rangle$
4. $\langle\, t_{ij} \,\rangle$ depend on $|i - j|$

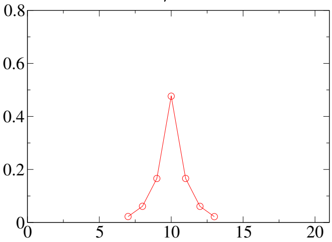
The Average Transmission Probabilities $\langle \ t_{ij} \ \rangle$

1. Short range: $\langle \ t_{ij} \ \rangle \simeq 0$ if $|i - j| > 2$
2. $\langle \ t_{i,i+1} \ \rangle_{B \neq 0} > \langle \ t_{i,i+1} \ \rangle_{B=0}$

$B = 0$



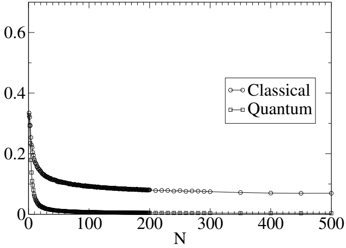
$B \neq 0$



$N = 20$: $\langle \ t_{ij} \ \rangle$ for $j = 10$ and $i = j, j \pm 1, j \pm 2$ and $j \pm 3$

The Average Universal Conductivity $\langle \sigma(N) \rangle$

$B = 0$



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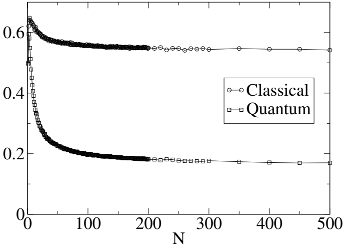
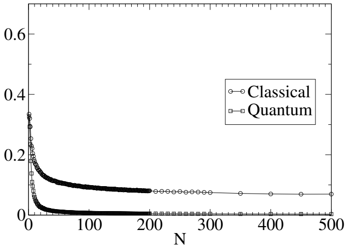


1. Good fit: $\langle \sigma^\infty \rangle + c/N$, where $\langle \sigma^\infty \rangle = \lim_{N\to\infty} \langle \sigma(N) \rangle \in (0, 1)$
2. Ohm and Fourier laws hold on average
3. Conductivity $(B \neq 0) >$ Conductivity $(B = 0)$ weak localization

The Average Universal Conductivity $\langle \sigma(N) \rangle$

$B = 0$



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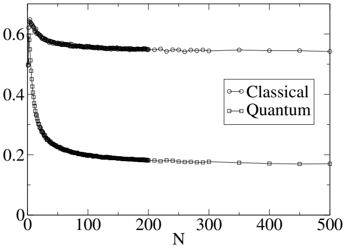
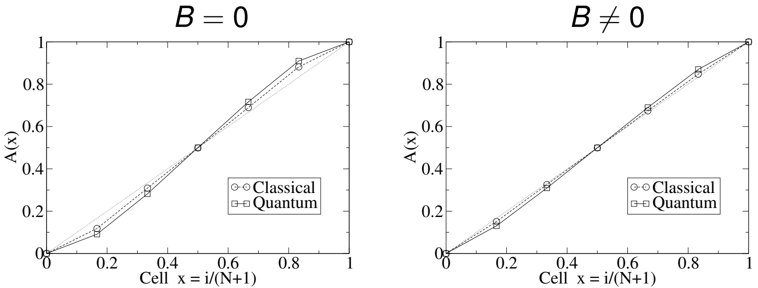


Classical conductivity $>$ Quantum conductivity weak localization

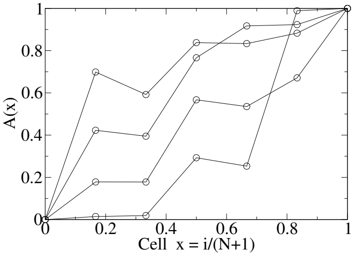
$$\langle \sigma(N) \rangle = N \left[\langle t_{\mathrm{LR}} \rangle + \sum_{i,j=1}^{N} \langle t_{\mathrm{L}j} (\Gamma^{-1})_{ji} t_{i\mathrm{R}} \rangle \right]$$

The Average Universal Profiles $\langle A(x) \rangle$ ($N = 5$)



1. Not linear/convex/concave $\neq$ EY-model
2. Linear in the limit $N \to \infty$
3. Monotone increasing
   $\to$ Heat also flows **locally** from Hot to Cold

Some Realizations ($N = 5$)



Local Negative Conductivity

The heat current may flow **locally** from Cold to Hot

Ref. M. Büttiker *PRB* **38** 17 (1988)

Summary of PART 1 (General Properties)

- Onsager relations: (I_i, J_i) and $(X_i = \delta\mu_i/e, Y_i = \delta T_i/T)$

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For f MB, FD or BE

$$f(E; T_j, \mu_j) = f(E; T, \mu) - \frac{\partial f}{\partial E}(E; T, \mu) \left[\left(\frac{E-\mu}{T} \right) \delta T_j + \delta\mu_j \right]$$

$$\mathcal{R} \equiv \frac{\tilde{L}_0}{\sqrt{L_0}} = \frac{C(1)}{\sqrt{C(0) \cdot C(2)}} \in (0,1), \quad \forall x_0 = -\mu/(k_{\mathrm{B}} T)$$

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- The self-consistency condition can be solved
- The profiles are **universal**, i.e. independent of f
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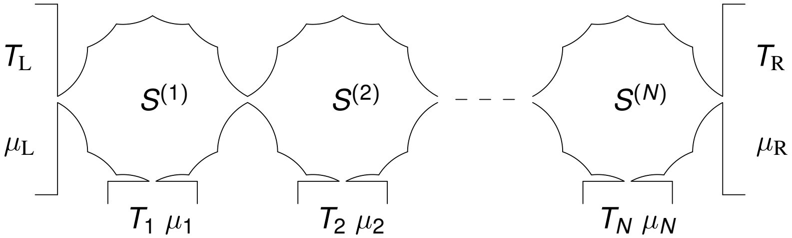
Simulation (RMT)

- On average heat also flows **locally** from Hot to Cold
- Heat may flow **locally** from Cold to Hot
- The average profiles are not convex nor concave
- The average profiles become linear as $N \to \infty$
- Ohm and Fourier laws hold on average
- Classical conductivity $>$ Quantum conductivity   weak
- Conductivity ($B \neq 0$) $>$ Conductivity ($B = 0$)   localization

Future



1. Investigate the energy dependent S-matrix situation
   $\rightarrow$ 1D crystal
2. Analyse the effects of non-linear contributions
   $\rightarrow$ thermal rectifier
3. Prove the existence of the finite limit $\sigma^\infty = \lim_{N\rightarrow\infty} \sigma(N)$