ELECTRONIC TRANSPORT in APERIODIC SOLIDS

Sponsoring

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Main References

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Content

1. Dissipation, Kubo's Formula
2. Anomalous Transport
3. Numerics

A No-Go Theorem

Let $H = H^*$ be *bounded* (*one-electron* Hamiltonian),

Let $\vec{R} = (R_1, \cdots, R_d)$ be the *position* operator (selfadjoint, commuting coordinates)

Then the electronic *current* is

$$\vec{J} = -e \frac{\imath}{\hbar} [H, \vec{R}] ,$$

Adding a force $\vec{F}$ at time $t = 0$ leads to a new evolution with Hamiltonian $H_F = H - \vec{F} \cdot \vec{R}$.

A No-Go Theorem

The 0-frequency component of the current is

$$\vec{j} = \lim_{t \to \infty} \int_0^t \frac{ds}{t} \quad e^{\imath s H_F/\hbar} \; \vec{J} \; e^{-\imath s H_F/\hbar} \, ,$$

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Simple algebra shows that (since $||H|| < \infty$)

$$\vec{F} \cdot \vec{j} = const. \lim_{t\to\infty} \frac{H(t) - H}{t} = 0,$$

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WHY ?

A No-Go Theorem

This is called *Bloch's Oscillations*. It was observed in simulations using ultracold atoms in an artificial lattice produced by lasers.

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This is called *Bloch's Oscillations*. It was observed in simulations using ultracold atoms in an artificial lattice produced by lasers.

To get a non trivial current we need

DISSIPATION !

Namely *loss of information*.

The Drude Model (1900)

Assumptions :

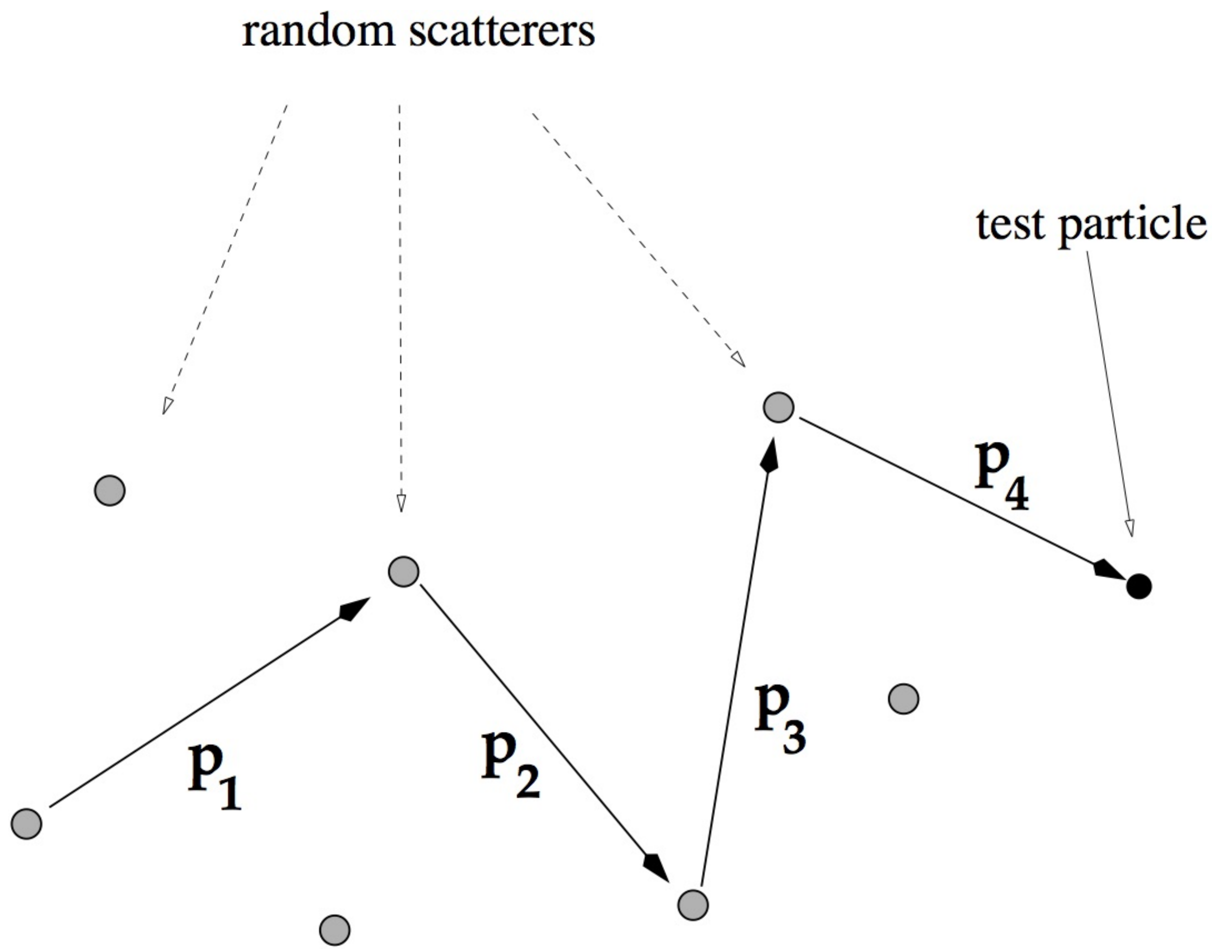
1. Electrons in a metal are *free classical particles* of mass m_* and charge q.

2. Let n denotes the *electron density*.

3. They experience collisions at *random Poissonnian times* $\cdots < t_n < t_{n+1} < \cdots$, with average relaxation time τ_{rel}.

4. If p_n is the electron momentum between times t_n and t_{n+1}, then the p_{n+1}'s is updated according to the *Maxwell distribution* at temperature T.

The Drude Model (1900)



The Drude Kinetic Model

The Drude Model (1900)

An elementary calculation leads to the *Drude formula*

$$\sigma = \frac{q^2 n}{m_*} \tau_{rel}$$

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The ratio gives the *Wiedemann-Franz Law (1853)*

$$\frac{\lambda}{\sigma} = \frac{3}{2}\left(\frac{k_B}{q}\right)^2 T$$

Aperiodicity

1. If the charges evolve in an *aperiodic environment*, their one-particle Hamiltonian is actually a *family* $(H_\omega)_{\omega\in\Omega}$ of self-adjoint operators depending on a parameter ω characterizing the degree of aperiodicity *(disorder parameter)*.

2. The aperiodicity can be *ordered* like in quasicrystals (long range order), or *disordered* like in semiconductors, glasses or liquids (short range correlations).

3. The space Ω of the disorder parameters is called the *Hull*. It is always *compact and metrizable*.

4. The *translation group* G acts on Ω by homeomorphisms $\tau^a, a \in G$.

Aperiodicity

1. **Covariance:** if G is the translation group, if $U(a)$ represents the translation by $a \in G$ in the Hilbert space of quantum states, then

$$U(a)\, H_\omega\, U(a)^{-1} = H_{T^a \omega}$$

2. **Continuity:** $\omega \in \Omega \mapsto H_\omega$ is strong resolvent continuous.

3. **Trace per Unit Volume:** if $\mathbb{P}$ is a G-invariant ergodic probability on Ω then, for $\mathbb{P}$-almost every ω

$$\mathcal{T}_{\mathbb{P}}\left(f(H)\right) = \int_\Omega d\mathbb{P}(\omega) \langle x | f(H_\omega)\, x \rangle = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \mathrm{Tr}\left(f(H_\omega) \restriction_\Lambda\right)$$

A Quantum Drude Model

Assumptions :

1. Replace the classical dynamics by the *quantum one* with *one-particle Hamiltonian* $H = (H_\omega)_{\omega\in\Omega}$.

2. Collisions occur at *random Poissonnian times* $\cdots < t_n < t_{n+1} < \cdots$, with average relaxation time τ_{rel}.

3. At each collision, the *density matrix* is updated to the equilibrium one. *(Relaxation Time Approximation)*.

4. Electrons and Holes are *Fermions*: use the *Fermi-Dirac distribution* to express the equilibrium density matrix.

A Quantum Drude Model

A straightforward calculation leads to the *Kubo formula*

(JB, Schulz-Baldes, Van Elst '94)

$$\sigma_{i,j} = \frac{q^2}{\hbar} \mathcal{T}_{\mathbb{P}} \left(\partial_j \left(\frac{1}{1 + e^{\beta(H-\mu)}} \right) \frac{1}{1/\tau_{rel} - \mathcal{L}_H} \partial_i H \right)$$

Where

A Quantum Drude Model

1. $\partial_i A = \imath[R_i, A]$ is the quantum derivative *w.r.t.* the *momentum*.

2. $\mathcal{L}_H(A) = \imath/\hbar\,[H, A]$ is called the *Liouvillian*.

3. $\beta = 1/k_B T$ and μ is the *chemical potential* fixed by the *electron density*, namely

$$n = \mathcal{T}_{\mathbb{P}}\left(\frac{1}{1 + e^{\beta(H-\mu)}}\right)$$

4. $\mathcal{T}_{\mathbb{P}}$ denotes the *trace per unit volume*, where $\mathbb{P}$ provides the way the average over the volume is defined.

The Work of E. Prodan: Numerical Results

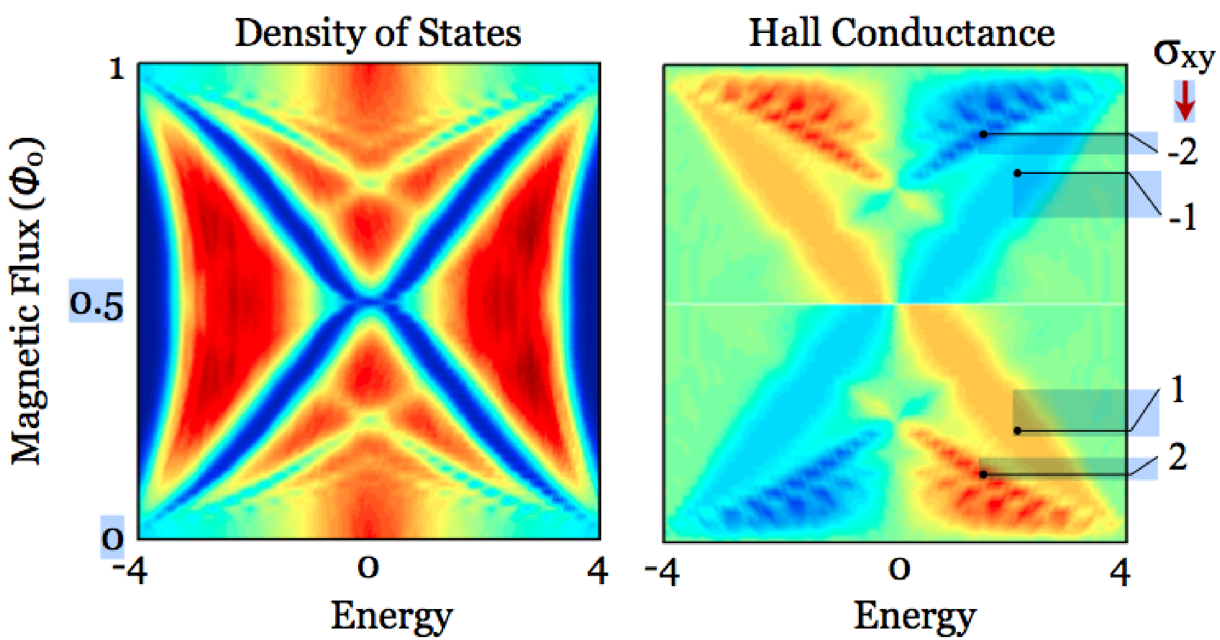
E. Prodan, "Quantum transport in disordered systems under magnetic fields: a study based on operator algebras", `arXiv:1204.6490`. *Appl. Math. Res. Express*, (2012)

Numerical implementation of the previous Kubo Formula for *disordered systems* was provided by *E. Prodan*. The formula gives an accurate algorithm which is *very stable* against disorder.

He used this algorithm to investigate more thoroughly the plateaux of conductivity in the *Quantum Hall Effect (QHE)* with his collaborators after 2012.

The Work of E. Prodan: Numerical Results

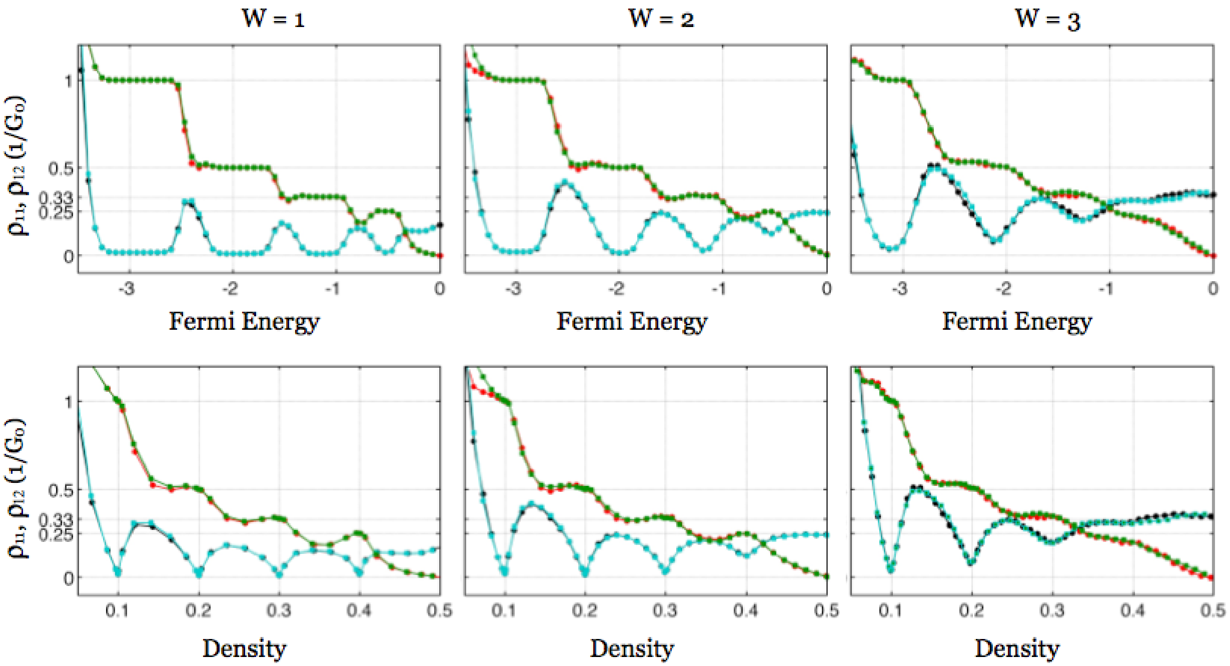
Quantum Hall Effect:



DoS (left) and colored map of the Hall conductivity (right) for W = 3. The regions of quantized Hall conductivity, which appear as well defined patches of same color, are indicated at the right.

The Work of E. Prodan: Numerical Results

Hall Plateaux:



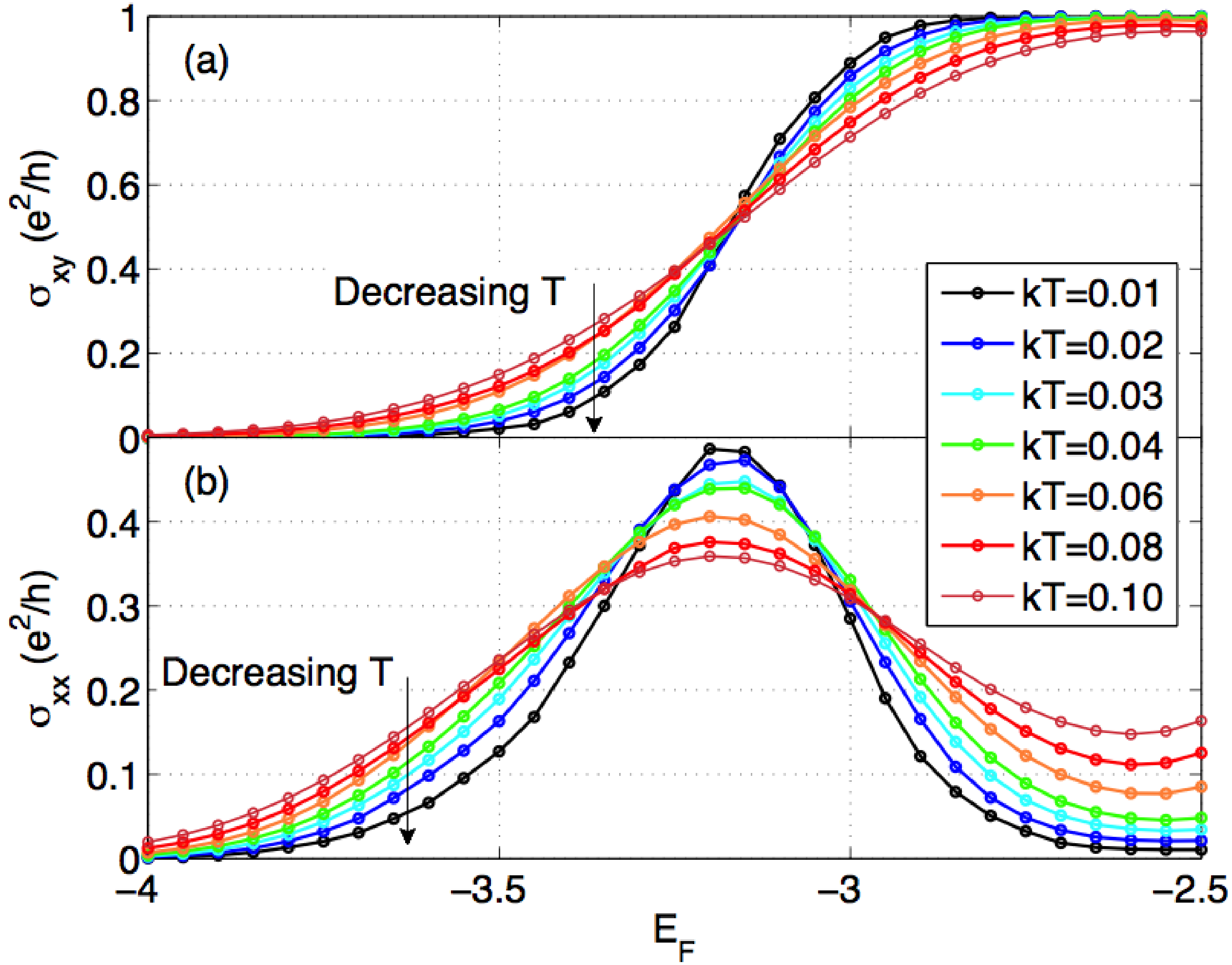
First row (Second row): The diagonal and the Hall resistivities as function of Fermi energy (density) at fixed magnetic flux ϕ, temperature T and disorder strength W

$\phi = 0.1\, h/e$
$k_B T = 1/\tau_{rel} = 0.025$
$W = 1, 2, 3.$

Each panel compares the data obtained on the 100×100 lattice (circles) and on the 120×120 lattice (squares).

The Work of E. Prodan: Numerical Results

Metal-Insulator transition between Hall plateaux



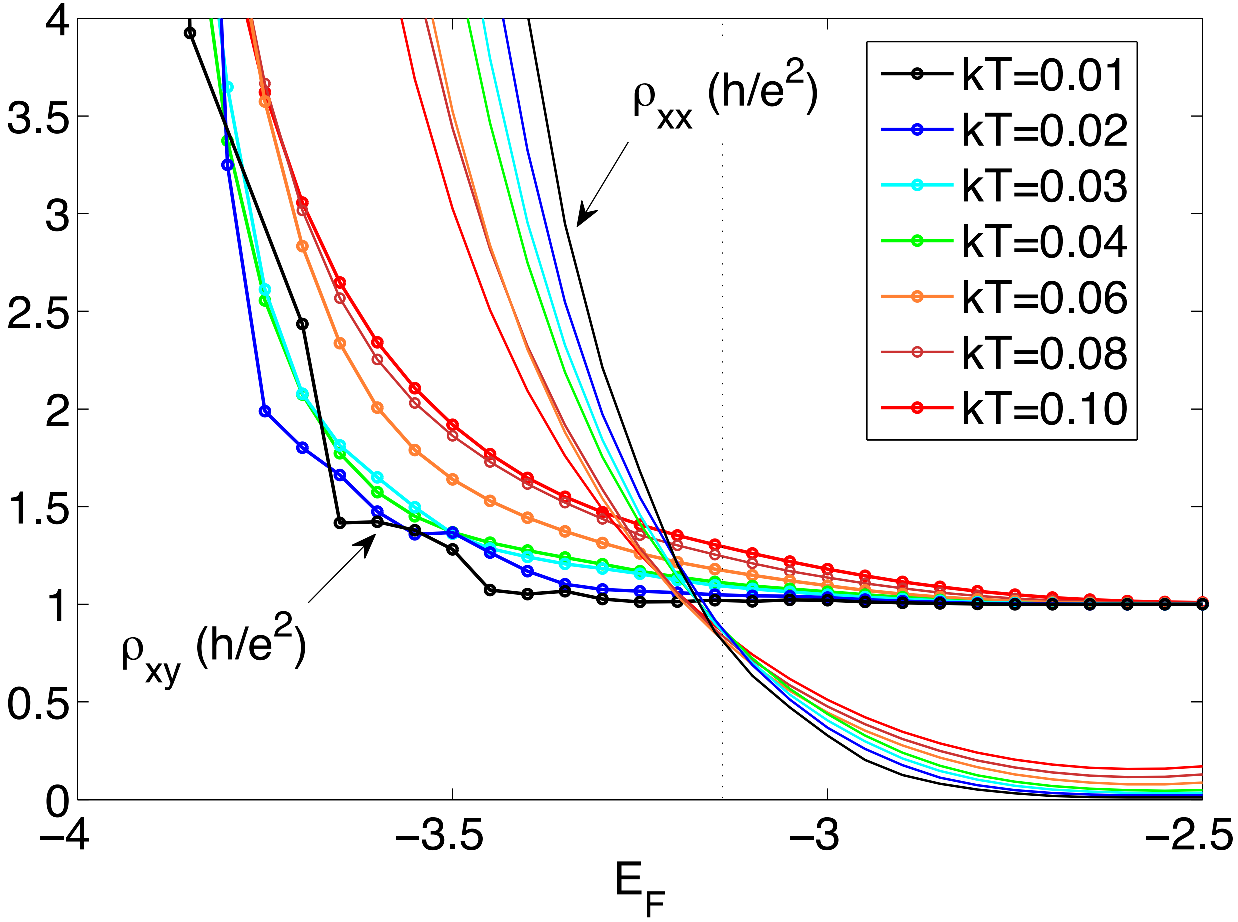
Transition from Chern(P_F) = 0 *to* Chern(P_F) = 1

The simulated (a) σ_{xy} and (b) σ_{xx}, as functions of E_F at different temperatures. *(Song & Prodan '12)*

It shows a fixed point at $E_F = E_F^c$ where $\sigma_{xx} \overset{T\downarrow 0}{\to} \sigma_{xy} = e^2/2h$

The Work of E. Prodan: Numerical Results

Metal-Insulator transition between Hall plateaux: resistivity



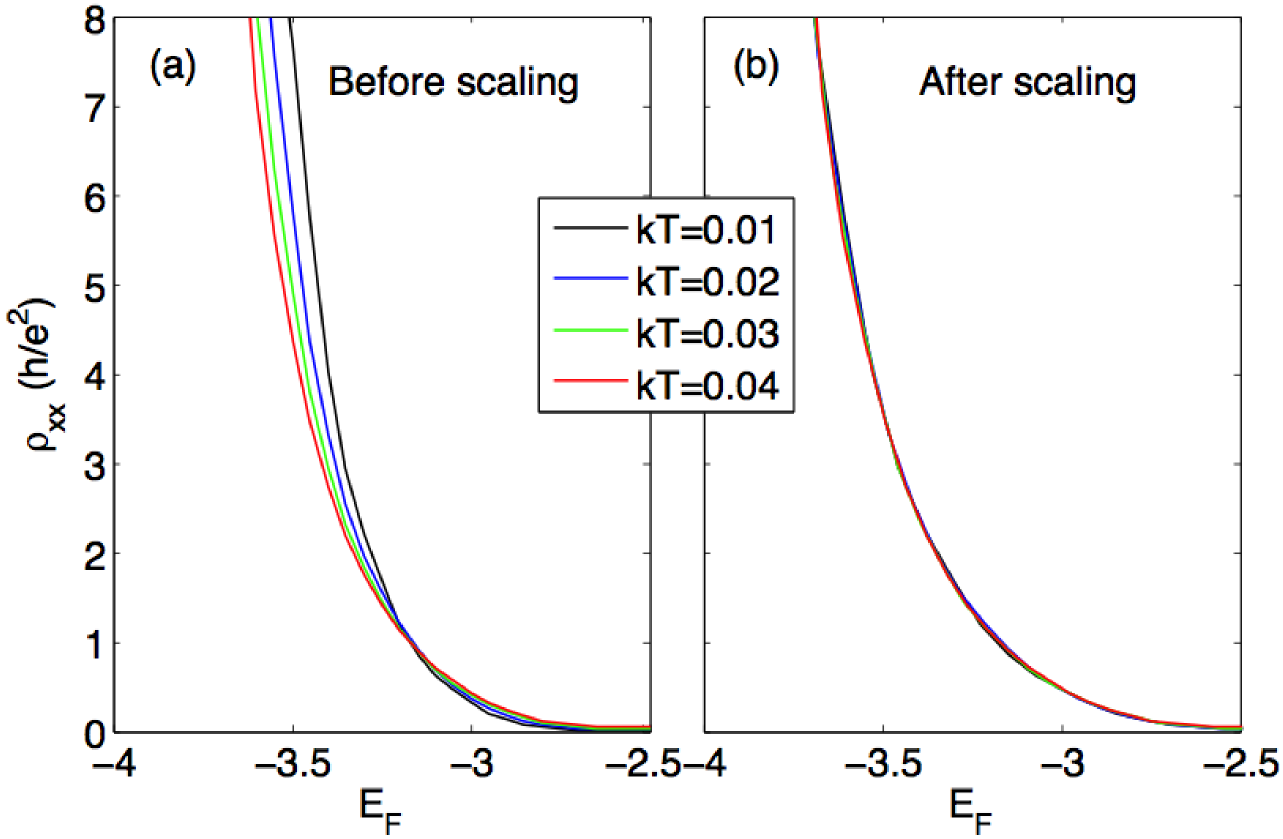
Transition from $\mathrm{Chern}(P_F) = 0$ *to* $\mathrm{Chern}(P_F) = 1$

ρ_{xy} as function of E_F at different temperatures. The curves at lower temperatures display quantized values well beyond the critical point, which is marked by the vertical dotted line. For convenience we also show the data for ρ_{xx}.

(Song & Prodan '12)

The Work of E. Prodan: Numerical Results

Metal-Insulator transition between Hall plateaux: Scaling Law



Transition from Chern(P_F) = 0 *to* Chern(P_F) = 1

The simulated ρ_{xx} as function of E_F (a) before and (b) after the horizontal axis was rescaled as:

$$E_F \to E_F^c + (E_F - E_F^c)\left(\frac{T}{T_0}\right)^{-\kappa}$$

with $E_F^c = -3.15\,,\ k_B T_0 = .08$ and $\kappa = .2$ leading to $p = 1$

(Song & Prodan '12)

What is Coherent Transport ?

Coherent transport corresponds to charge transport (*electrons* or *holes*) ignoring dissipation sources such as *electron-phonon* or *electron-electron* interactions.

1. The *independent electrons* approximation is justified.
2. The one-particle Hamiltonian $(H_\omega)_{\omega\in\Omega}$ is sufficient.
3. The wave packets *diffuses* through the medium at a rate depending upon how much *Bragg reflections* are produced *(quantum interferences)*.

What is Coherent Transport ?

WAVE DIFFUSION

but

NO CURRENT !

Spectral Measures

1. The *density of state* (DOS)

$$\int_{-\infty}^{+\infty} d\mathcal{N}_{\mathbb{P}}(E) f(E) = \mathcal{T}_{\mathbb{P}}\left(f(H)\right)$$

2. The *spectral measure* relative to a given state ψ in the Hilbert space, called *local density of state* (LDOS)

$$\int_{-\infty}^{+\infty} d\mu_{\omega,\psi}(E) f(E) = \langle \psi | f(H_\omega) \psi \rangle$$

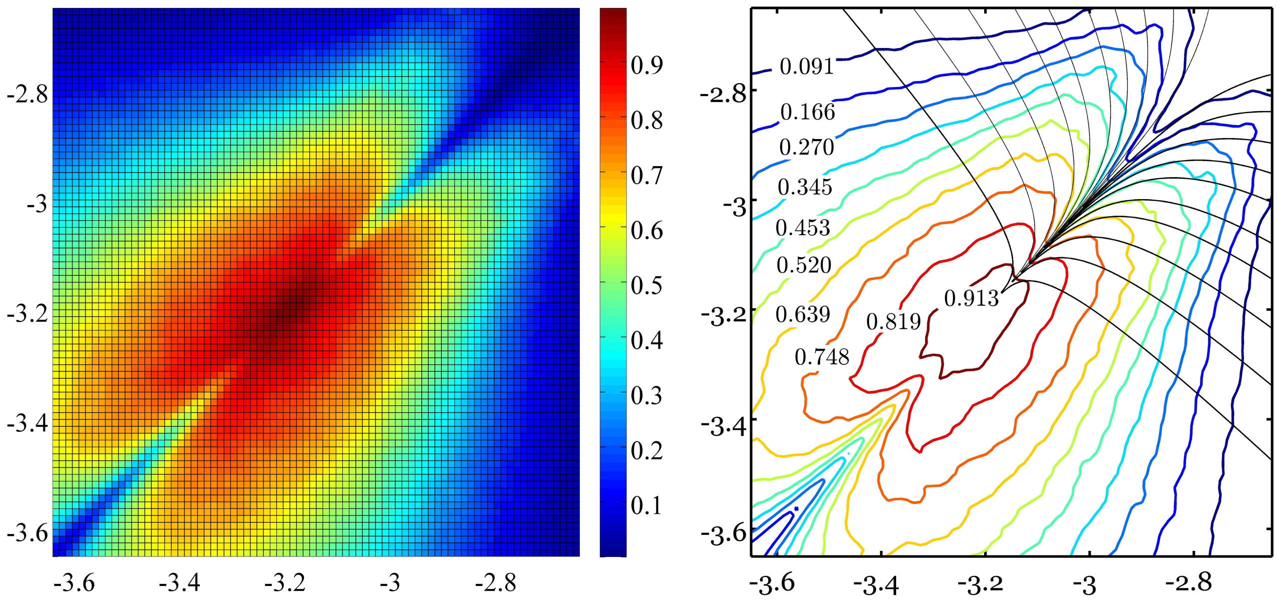
3. The *current-current correlation* (CCC) describes transport properties.

$$\int_{\mathbb{R}^2} dm(E,E') f(E) g(E') = \sum_{i=1}^{d} \mathcal{T}_{\mathbb{P}}\{f(H)\, \partial_i H \; g(H)\, \partial_i H\}$$

The Current-Current Correlation Measure: Numerics

E. Prodan, J. Bellissard, *Ann. of Phys.*, **368**, 1-15, (2016).

The QHE scaling laws come from a singularity in the Current-Current Measure. Here $dm(E,E') = f(E,E')dEdE'$



Left: intensity plot of the current-current correlation distribution $f(E,E')$.
Right: level sets of $f(E,E')$
The calculation was made on a 120×120 lattice and the adta were averaged over 100 random configurations.
(Prodan & Bellissard '16)

The Current-Current Correlation Measure: Numerics

The *scaling law* observed in the *QHE resistivity* at the metal-insulator transition E_c can be explained by an expression of the form:

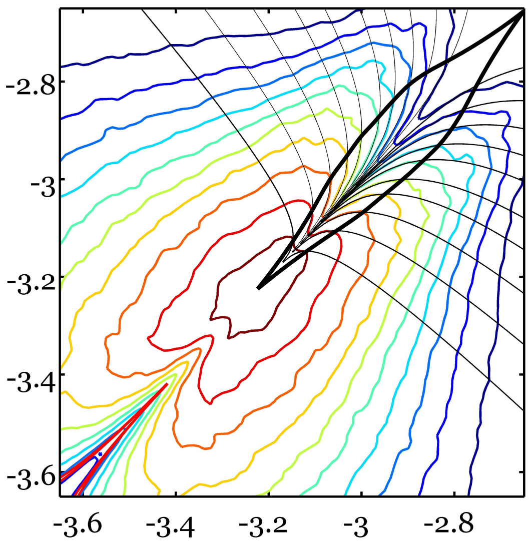
$$f(E,E') = g\left(\frac{E+E'-2E_c}{|E-E'|^{\kappa/p}}\right), \qquad E,E' \simeq E_c\,.$$

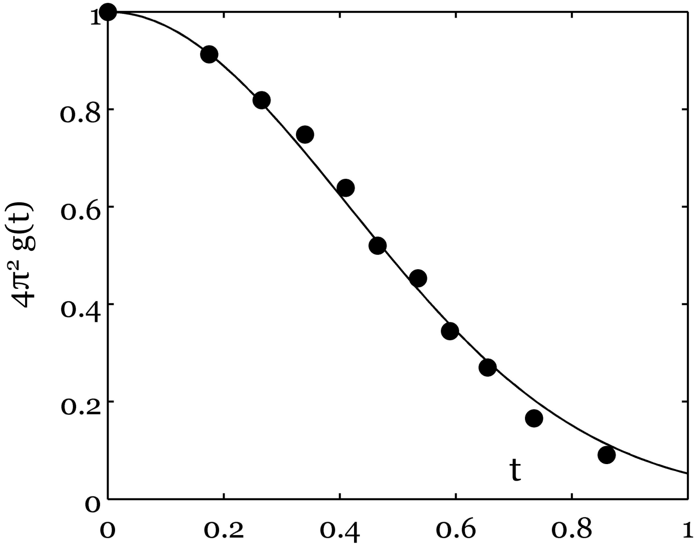
It leads to

$$\sigma_{ii} = \frac{e^2}{h}\int_0^\infty \frac{4\pi}{1+y^2}\, g\left(\frac{E_F}{(\Gamma|E-E'|)^{\kappa/p}}\right)\,dy\,, \qquad \Gamma = \frac{1}{\tau_{rel}}\,.$$

The Current-Current Correlation Measure: Numerics

The function $g(t)$ can be computed also and fits well with a Gaussian curve.





Left: The trace of the asymptotic region where the scaling invariance of the current-current correlation function occurs.
Right: Plot of 10 values of the function $g(t)$, together with a Gaussian fit. *(Prodan & Bellissard '15)*

Local Exponents

Given a positive measure μ on $\mathbb{R}$:

$$\alpha_\mu^\pm(E) = \lim \left\{ \begin{matrix} \sup \\ \inf \end{matrix} \right\}_{\varepsilon \downarrow 0} \frac{\ln \int_{E-\varepsilon}^{E+\varepsilon} d\mu}{\ln \varepsilon}$$

For Δ a Borel subset of $\mathbb{R}$:

$$\alpha_\mu^\pm(\Delta) = \mu\text{-ess} \left\{ \begin{matrix} \sup \\ \inf \end{matrix} \right\}_{E \in \Delta} \alpha_\mu^\pm(E)$$

Local Exponents

Properties:

1. For all E, $\alpha_\mu^\pm(E) \geq 0$. In addition, $\alpha_\mu^\pm(E) \leq 1$ for μ-almost all E.

2. If μ is *ac* on Δ then $\alpha_\mu^\pm(\Delta) = 1$, if μ is *pp* on Δ then $\alpha_\mu^\pm(\Delta) = 0$.

3. If μ and ν are equivalent measures on Δ, then $\alpha_\mu^\pm(E) = \alpha_\nu^\pm(E)$ μ-almost surely.

4. α_μ^+ coincides with the *packing dimension*.
   α_μ^- coincides with the *Hausdorff dimension*.

Local Exponents

1. The *LDOS exponent* $\alpha^{\pm}_{\text{LDOS}}$ is defined as the maximum over the state ψ of the local exponent associated with μ_ψ.

2. The *DOS exponents* $\alpha^{\pm}_{\text{DOS}}$ is the local exponent associated with $\mathcal{N}_{\mathbb{P}}$.

3. It follows that

$$\alpha^{\pm}_{\text{LDOS}}(\Delta) \leq \alpha^{\pm}_{\text{DOS}}(\Delta)$$

Transport Exponents

1. For $\Delta \subset \mathbb{R}$ a Borel subset, let $P_{\Delta,\omega}$ be the corresponding *spectral projection* of H_ω. Set

$$\vec{R}_\omega(t) \;=\; e^{\imath t H_\omega}\, \vec{R}\, e^{-\imath t H_\omega}$$

2. The *averaged spread* of a typical wave packet with energy in Δ is measured by

$$L_\Delta^{(p)}(t) \;=\; \left(\int_0^t \frac{ds}{t} \int_\Omega d\mathbb{P}\, \langle x | P_{\Delta,\omega} | \vec{R}_\omega(t) - \vec{R}|^p P_{\Delta,\omega} | x \rangle \right)^{1/p}$$

3. Define $\beta = \beta_p^{\pm}(\Delta)$ similarly so that $L_\Delta^{(p)}(t) \sim t^\beta$

Transport Exponents

Properties:

- $\beta_p^-(\Delta) \leq \beta_p^+(\Delta)$ and $\beta_p^\pm(\Delta)$ are *non decreasing* in p.
- The transport exponent is the *spectral exponent* of the Liouvillian $\mathcal{L}_H$ localized around energies in Δ near the eigenvalue 0 (diagonal of the current-current correlation).

Transport Exponents

Heuristic:

1. $\beta = 0 \to$ absence of diffusion: (*ex: localization*)

2. $\beta = 1 \to$ ballistic motion: (*ex: in crystals*)

3. $\beta = 1/2 \to$ quantum diffusion: (*ex: weak localization*)

4. $\beta < 1 \to$ subballistic regime

5. $\beta < 1/2 \to$ subdiffusive regime: (*ex: in quasicrystals*)

Transport Exponents

Guarneri's Inequality:

$$\beta_p^{\pm}(\Delta) \;\geq\; \frac{\alpha^{\pm}_{\mathrm{LDOS}}(\Delta)}{d}$$

Heuristics: *ac spectrum*

1. *ac* spectrum implies $\beta \geq 1/d$.
2. *ac* spectrum implies ballistic motion in $d = 1$.
3. *ac* spectrum is compatible with quantum diffusion in $d \geq 2$. Expected to hold in *weak localization* regime.
4. *ac* spectrum is compatible with *subdiffusion* for $d \geq 3$. Expected to hold in *quasicrystals*.

The Anomalous Drude Formula

(Mayou '92, Sire '93, Bellissard, Schulz-Baldes '95)

In the Relaxation Time Approximation, it can be proved that

$$\sigma \overset{\tau_{rel} \uparrow \infty}{\sim} \tau_{rel}^{2\beta_F - 1}$$

where $\beta_F = \beta_2(E_F)$ is the transport exponent at Fermi level.

The Anomalous Drude Formula

1. In practice, $\tau_{rel} \uparrow \infty$ as $T \downarrow 0$.
2. If $\beta_F = 1$ (*ballistic motion*), $\sigma \sim \tau_{rel}$ (*Drude*). The system behaves as a conductor.
3. For $1/2 < \beta_F \leq 1$, $\sigma \uparrow \infty$ as $T \downarrow 0$: the system behaves as a conductor.
4. If $\beta_F = 1/2$ (*quantum diffusion*), $\sigma \sim const.$: residual conductivity at low temperature.
5. For $0 \leq \beta_F < 1/2$, $\sigma \downarrow 0$ as $T \downarrow 0$: the system behaves as an insulator.

Transport in Quasicrystals

Lectures on Quasicrystals,
F. Hippert & D. Gratias Eds., Editions de Physique, Les Ulis, (1994),

S. Roche, D. Mayou and G. Trambly de Laissardière,
Electronic transport properties of quasicrystals, J. Math. Phys., **38**, 1794-1822 (1997).

Quasicrystalline alloys :

Metastable QC's: **AlMn**

(Shechtman D., Blech I., Gratias D. & Cahn J., PRL **53***, 1951 (1984))*

AlMnSi

AlMgT $(T = Ag, Cu, Zn)$

Defective stable QC's: **AlLiCu** *(Sainfort-Dubost, (1986))*

GaMgZn *(Holzen et al., (1989))*

Transport in Quasicrystals

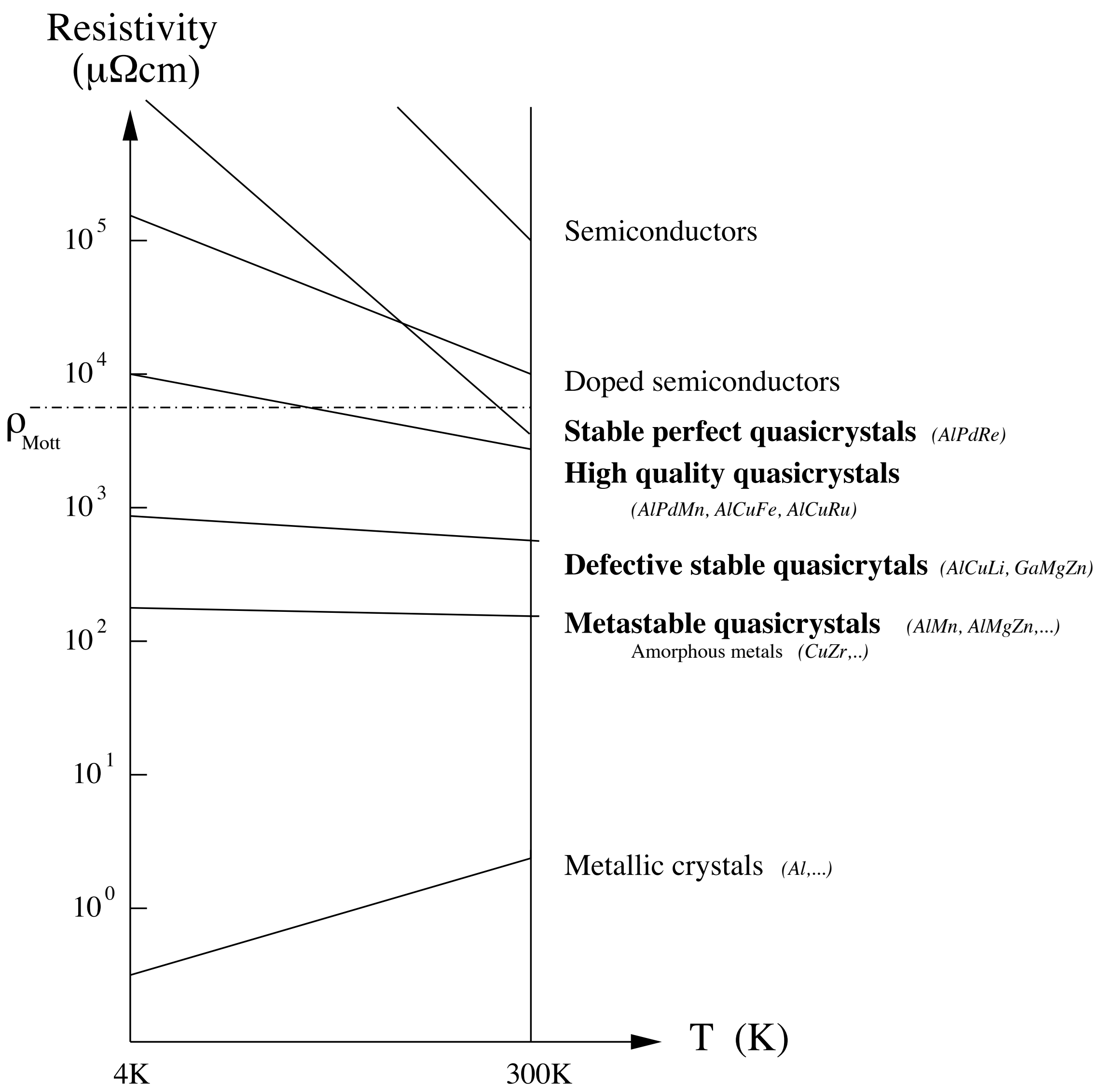
High quality QC's: **AlCuT** $(T = Fe, Ru, Os)$

(Hiraga, Zhang, Hirakoyashi, Inoue, (1988); Gurnan et al., Inoue et al., (1989); Y. Calvayrac et al., (1990))

"Perfect" QC's: **AlPdMn**

AlPdRe

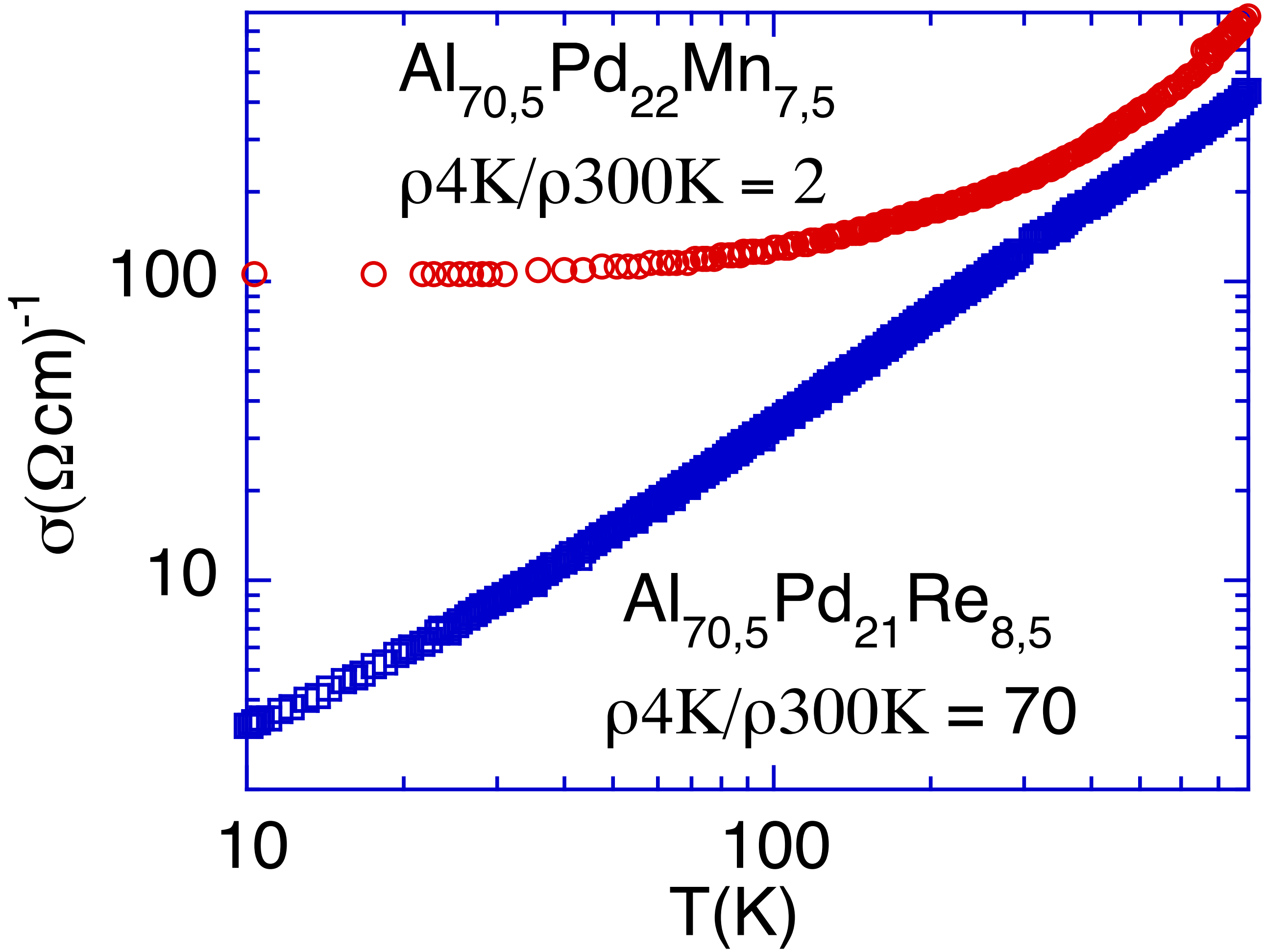
Transport in Quasicrystals



Typical values of the resistivity

(C. Berger in Lectures on Quasicrystals*)*

Transport in Quasicrystals



Conductivity of Quasicrystals vs Temperature vs. Temperature

$\sigma \approx \sigma_0 + a\,T^\gamma$ *with* $1 < \gamma < 1.5$

for $.01\,K \leq T \leq 1000\,K$

Transport in Quasicrystals

1. Numerical simulations for the icosahedral phase of *AlCuCo* suggest $\beta_F \sim 0.375 = 3/8$ *(S. Roche & Fujiwara, Phys. Rev.,* **B58***, 11338-11396, (1998))* and using Bloch's Law $\tau_{rel} \sim T^{-5}$, gives

$$\sigma \overset{T\downarrow 0}{\sim} T^{5/4}$$

   a result compatible with experiments.

2. Numerical simulations performed for the octagonal lattice exhibit level repulsion and Wigner-Dyson's distribution *(M. Schreiber, U. Grimm, R. A. Roemer, J. -X. Zhong,* Comp. Phys. Commun.*,* **121-122***, 499-501 (1999).)*

Transport in Quasicrystals

Thouless Argument

1. For a sample of size L in dimension d :
   Mean level spacing $\Delta \sim L^{-d}$.
   Thus Heisenberg time $\tau_H \sim L^d$.

2. Time necessary to reach the boundary (*Thouless*) $L \sim \tau_{Th}^{\beta_F}$. Thus $\tau_{Th} \sim L^{1/\beta_F}$.

Transport in Quasicrystals

Comparing these estimate gives two regimes.

1. if $\beta_F > 1/d$ level repulsion dominates implying
   - quantum diffusion $\langle x^2 \rangle \sim t$
   - *residual conductivity*
   - absolutely continuous spectrum at Fermi level;

2. if $\beta_F < 1/d$ level repulsion can be ignored and
   - anomalous diffusion dominates $\langle x^2 \rangle \sim t^{2\beta_F}$
   - insulating behaviour with scaling law
   - *singular continuous* spectrum near Fermi level.

Aalborg Seal and Coat of Arm

Thanks for listening !