COMPUTATIONAL NONCOMMUTATIVE GEOMETRY

The work of E. Prodan

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Happy Birthday Henri !

Noncommutative Geometry Festival

Noncommutative Geometry Festival

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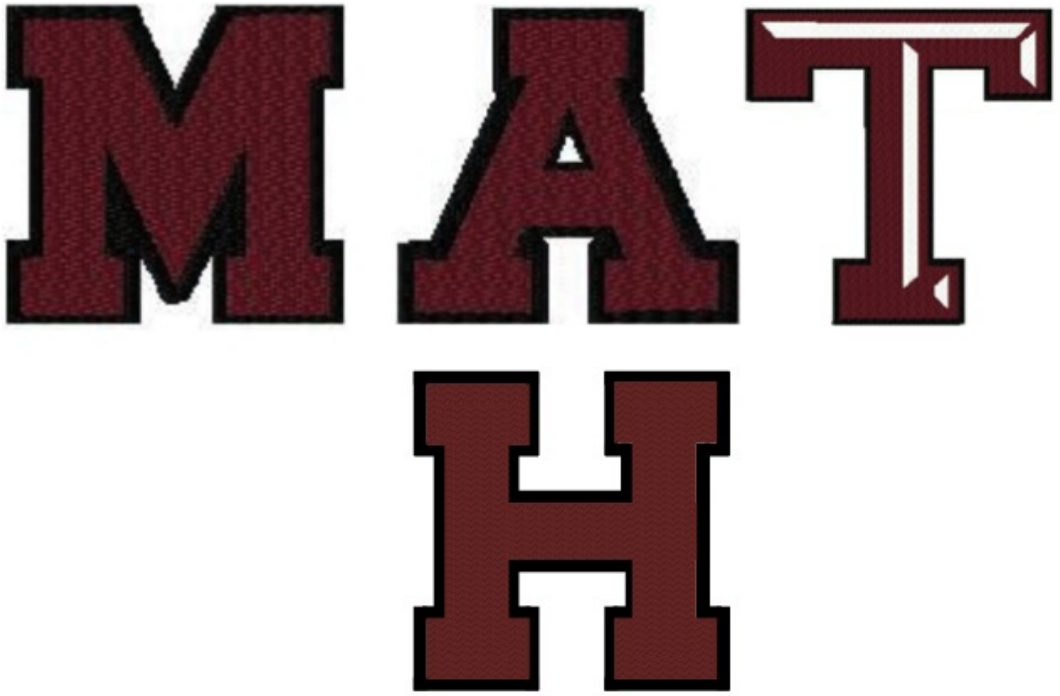

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J. Bellissard, *Coherent and dissipative transport in aperiodic solids*,
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When simulation meets experiment", `arXiv:1301.5305`.

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Content

1. The Noncommutative Brillouin Zone
2. Kubo's formula: the Relaxation Time Approximation
3. The Quantum Hall Effect: numerical Study
4. Conclusion

I - The Noncommutative Brillouin Zone

J. Bellissard, *Gap Labeling Theorems for Schrödinger's Operators*, in *From Number Theory to Physics*, Springer (1993), pp. 538-630.

J. Bellissard, D. Herrmann, M. Zarrouati, *Hull of Aperiodic Solids and Gap Labeling Theorems*, in *Directions in Mathematical Quasicrystals*, CRM Monograph Series **13**, (2000), pp. 207-259.

Aperiodicity

- In a solid, periodic or not, the basic object is its *Hull* Ω: it is a *compact metrizable space* endowed with an action of the *translation group* $\mathbb{R}^d$ by homeomorphisms.
- The *Hamiltonian* describing the electronic motion is a *strong-resolvent continuous* family $H = (H_\omega)_{\omega\in\Omega}$ of self adjoint operators, acting on a common Hilbert space $\mathcal{H} \simeq L^2(\mathbb{R}^d) \otimes \mathbb{C}^N$ and *affiliated* to the C^*-algebra $\mathcal{A} = C(\Omega) \rtimes \mathbb{R}^d$.
- There is a *unitary representation* U of the translation group in $\mathcal{H}$. The family H is *covariant*

$$U(a)H_\omega U(a)^{-1} = H_{\mathrm{T}^a\omega} \qquad\qquad a \in \mathbb{R}^d$$

The Noncommutative Brillouin Zone

- The C^*-algebra $\mathcal{A} = C(\Omega) \rtimes \mathbb{R}^d$ is the aperiodic analog of the space of *continuous functions* over the *Brillouin Zone*, which is a torus in the periodic case.
- $\mathcal{A}$ is represented in $\mathcal{H}$ through a *covariant* family of $*$-representations

$$\pi_\omega(A)\psi(x) = \int_{\mathbb{R}^d} d^d y \; A(\tau^{-x}\omega, y - x) \; e^{\imath B \cdot x \wedge y} \; \psi(y)$$

  if B is a uniform magnetic field added.
- The Hull comes naturally with a *translation invariant ergodic* probability measure $\mathbb{P}$ associated with the Gibbs measure describing the atomic equilibrium.

Calculus

- The volume form of the Brillouin zone is given by the *trace per unit volume*

$$\mathcal{T}_{\mathbb{P}}\{A\} = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \operatorname{Tr}\{\pi_\omega(A)\chi_\Lambda\} = \int_\Omega d\mathbb{P}(\omega)\, A(\omega, 0)$$

- The group dual to the translation group acts on $\mathcal{A} = C(\Omega) \rtimes \mathbb{R}^d$ by duality, defining a family $(\partial_i)_{i=1}^d$ of $*$-derivations of $\mathcal{A}$, aperiodic analog of $\partial/\partial k_i$, such that

(Connes-Takai-Takesaki duality)

$$\pi_\omega(\partial_i A) = -\imath\, [X_i, A]$$

where $\vec{X} = (X_1, \cdots, X_d)$ denotes the position operators.

Thermodynamics for Electrons

- If $A \in \mathcal{A}$ is a *one-electron observable*, its thermal average is given by

$$\langle A \rangle_{T,\mu} = \mathcal{T}_{\mathbb{P}} \left\{ A \, \frac{1}{1 + e^{\beta(H-\mu)}} \right\} \qquad \beta = \frac{1}{k_{\mathrm{B}} T}, \quad \mu = \text{chemical potential}$$

- In particular the *electron density* is given by

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

II - Kubo's Formula

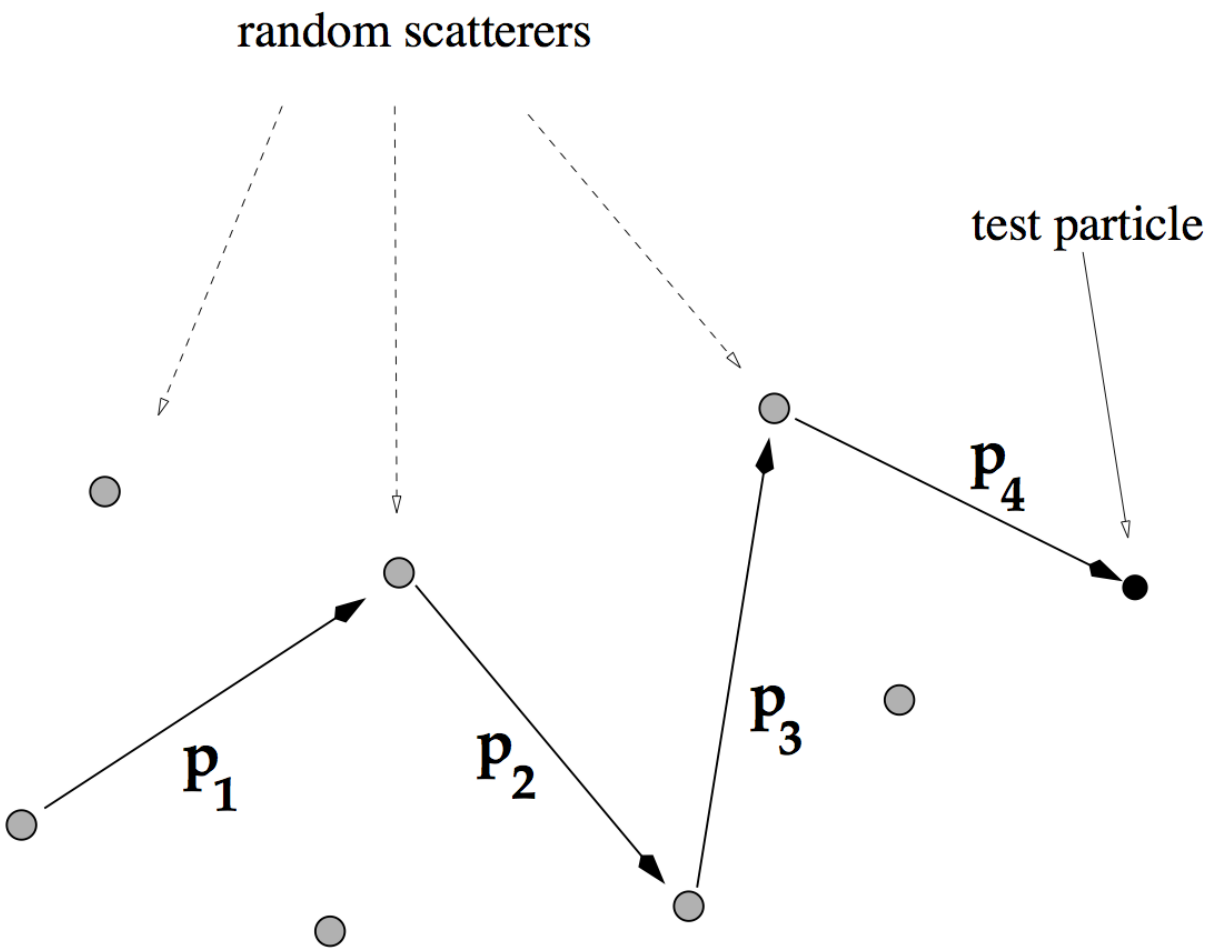
(Relaxation Time Approximation)

H. Schulz-Baldes, J. Bellissard, *Rev. Math. Phys.*, **10**, (1998), 1-46.

H. Schulz-Baldes, J. Bellissard, *J. Stat. Phys.*, **91**, (1998), 991-1026.

J. Bellissard, *Coherent and dissipative transport in aperiodic solids*, Lecture Notes in Physics, **597**, Springer (2003), pp. 413-486.

The Drude Model



The Drude Model

P. Drude, *Ann. Phys.*, **1**, (1900), 566-613; *Ann. Phys.*, **3**, (1900), 369-302.

- Electrons in a metal are *free classical particles* of mass m_* and charge q.
- They experience collisions at random *Poissonnian times* $\cdots < t_n < t_{n+1} < \cdots$, with average relaxation time τ_{rel}.
- If p_n is the electron momentum between times t_n and t_{n+1}, then the $p_{n+1} - p_n$'s are *independent random variables* distributed according to the *Maxwell distribution* at temperature T.
- The conductivity is then given by

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

The Relaxation Time Approximation

- Replace the classical dynamics by the *quantum one-electron dynamic* in the aperiodic solid.
- At each collision, force the *density matrix* to come back to equilibrium. (*Relaxation time Approximation* or RTA).
- There is only one *relaxation time* τ_{rel}. The electric conductivity is then given by Kubo's formula:

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

Here q is the charge of the carriers, $\beta = 1/k_B T$, μ is the chemical potential and $\mathcal{L}_H = \imath/\hbar\,[H,.]$.

Models for the Electronic Motion

E. Prodan, "Quantum transport in disordered systems under magnetic fields: a study based on operator algebras", arXiv:1204.6490.

- *Disorder* occurs in *semiconductors* at very low temperature or in many *topological insulators*.
- It is convenient to use the *tight-binding representation*: electrons are located on a lattice $\mathbb{Z}^d$. The kinetic term is given by a sum of hopping terms with magnetic field

$$H_{kin}\psi(x) = \sum_{|a|\leq r} t(a)\, e^{-\imath B\cdot x\wedge a}\, \psi(x-a)$$

- H_{kin} commutes with the *magnetic translation* *(Zak '64)*

Models for the Electronic Motion

Example: the Harper model

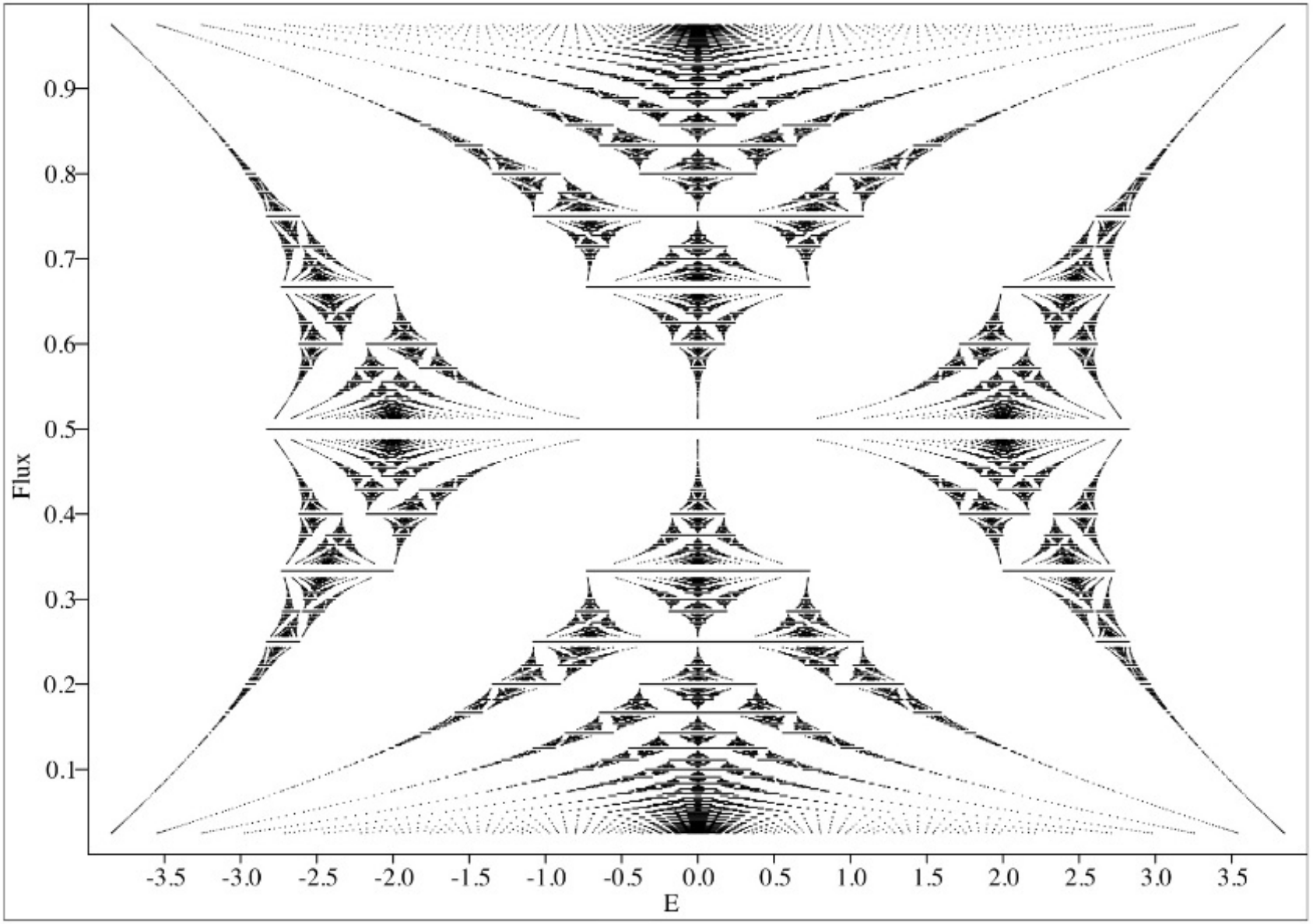
if $t(a) = 0$ for $|a| \neq 1$ and $t(\pm e_i) = 1$ for $i = 1, 2$ *(nearest neighbors hopping)* then

$$H_{kin} = U_1 + U_1^{-1} + U_2 + U_2^{-1}$$

with

$$U_1 U_2 = e^{2\imath\pi\phi/\phi_0}\, U_2 U_1 \qquad\qquad \phi_0 = \frac{h}{e}$$

and ϕ is the *the unit cell magnetic flux*.


Flux
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
E

Models for the Electronic Motion

- The disorder potential $V_\omega = W\omega$ with $\omega = (\omega_x)_{x\in\mathbb{Z}^d}$ where the ω_x's are *i.i.d. uniformly* distributed on $[-1/2, 1/2]$ *(Anderson)*

- The Hull is then $\Omega = [-1/2, 1/2]^{\mathbb{Z}^d}$. The probability $\mathbb{P}$ becomes

$$d\mathbb{P}(\omega) = \prod_{x\in\mathbb{Z}^d} d\omega_x \restriction_{[-1/2,1/2]}$$

- The observable algebra becomes $\mathcal{A} = C(\Omega) \rtimes \mathbb{Z}^d$ where $\mathbb{Z}^d$ acts like a shift on Ω.

Numerical Computations for Disordered Solids

- **Step 1:** The space is divided into cubes of size $2N+1$ for N large enough. The disorder is changed into *periodic configurations* of period N: Ω is replaced by $\Omega_N \subset \Omega$ with

$$\Omega_N \simeq [-1/2, 1/2]^{C_N} \qquad C_N = \{-N, \cdots, N\}^d$$

- The observable algebra becomes $\mathcal{A}_N = C(\Omega_N) \rtimes \mathbb{Z}^d$ and the Hamiltonian H is approximated by H_{per}
- The trace becomes

$$\mathcal{T}_{\mathbb{P},N}\{A\} = \frac{1}{(2N+1)^d} \int_{\Omega_N} \prod_{x \in C_N} d\omega_x \, \mathrm{Tr}\left\{\pi_\omega(A)\chi_{C_N}\right\}$$

Numerical Computations for Disordered Solids

Result 1 *(E. Prodan '12) The error made with the previous replacement is exponentially small in* N.

More precisely, if $f_1, \cdots, f_L$ *are functions of the form* $f = \partial_i \Phi(H)$ *where* Φ *is analytic in* $\mathrm{dist}(z, \sigma(H)) \leq \kappa$, *then for any* $0 < \xi$ *with* $\sinh(\xi) < \kappa/2d$, *the following bound hold*

$$\left| \mathcal{T}_{\mathbb{P}} \left\{ \prod_j f_j \right\} - \mathcal{T}_{\mathbb{P},\mathrm{N}} \left\{ \prod_j f_j \right\} \right| \leq D(i_1, \cdots, i_L; \xi) \prod_{j=1}^{L} \|\Phi_j\| \, e^{-2\sqrt{2}/3 \, \xi N}$$

with $D(i_1, \cdots, i_L; \xi)$ *uniform in* N *and independent of the* Φ_j*'s.*

Numerical Computations for Disordered Solids

- **Step 2:** The periodicity introduced in step 1 allows to use Bloch theory to restrict the volume to C_N with *Bloch boundary conditions* labeled by the *quasi-momentum* $\vec{k} \in \mathbb{T}^d$.
- Such a reduction is possible only if the *magnetic fluxes* through the 2-faces of a unit cell of period are *rational multiples* of the flux quantum h/e.
- The next step consists in *discretizing* $\mathbb{T}^d$ so that only quasi-momenta of the form below are kept in the calculation

$$\vec{k} \in \mathbb{T}^d_N \quad \Leftrightarrow \quad \vec{k} = 2\pi \frac{\vec{m}}{2N+1} \quad \vec{m} \in (\mathbb{Z}_N)^d \quad \mathbb{Z}_N = \mathbb{Z}/(2N+1)\mathbb{Z}$$

Numerical Computations for Disordered Solids

- To illustrate the way to *estimate the error* made during this discretization process, let $f(\theta) = \sum_{n\in\mathbb{Z}} a_n e^{\imath n\theta}$ be analytic in k, so that its Fourier coefficients *decay exponential fast*.
- Sampling f on the values $\theta = 2\pi m/M$ gives a *finite* Fourier expansion

$$f\left(2\pi\frac{m}{M}\right) = \sum_{n=0}^{M-1} \hat{a}_n e^{\imath 2\pi nm/M} \qquad \hat{a}_n = \sum_{p\in\mathbb{Z}} a_{n+Mp}$$

- It follows that $|\hat{a}_n - a_n| \leq Ce^{-c_2 M}$ uniformly *w.r.t.* $0 \leq n \leq M-1$.

Numerical Computations for Disordered Solids

- *Discretization* leads to the algebra $\mathcal{B}_N = C(\Omega_N \times \mathbb{T}_N^d) \rtimes \mathbb{Z}_N^d$. Then there is an *isometric* $*$-endomorphism $J : \mathcal{B}_N \to \mathcal{A}_N$ and a *conditional expectation* $P : \mathcal{A}_N \to \mathcal{B}_N$ with

$$P \circ J = I_{\mathcal{B}_N} \qquad\qquad J \circ P = \chi_{C_N}$$

- It follows that the *spectrum* of the discretized Hamiltonian H_N is included in the *spectrum* of the periodic approximation H_{per}

- **Result 2** *(E. Prodan '12) The error made with the previous replacement is exponentially small in N. This method allows to compute efficiently various physical quantities numerically, including the conductivity.*

III - The Quantum Hall Effect

(A Numerical Study)

J. Bellissard, A. van Elst, H. Schulz-Baldes, *J. Math. Phys.*, **35**, (1994), 5373-5451.

E. Prodan, "Quantum transport in disordered systems under magnetic fields:
a study based on operator algebras", arXiv:1204.6490.

J. Song, E. Prodan, "The plateau-insulator transition in the Integer Quantum Hall Effect"
When simulation meets experiment", arXiv:1301.5305.

A List of Rigorous Results

- In the limit $T \downarrow 0$, at constant electron density n_{el}, the *chemical potential* $\mu(T)$ converges to the Fermi Energy E_F.
- The *Fermi projection* $P_F = \chi(H \leq E_F)$ is obtained as a (weak) limit (with $\beta = 1/k_B T$)

$$P_F = w - \lim_{T \downarrow 0} \frac{1}{1 + e^{\beta(H - \mu(T))}} \qquad \lim_{T \downarrow 0} \mathcal{T}_{\mathbb{P}} \left\{ \frac{1}{1 + e^{\beta(H - \mu(T))}} \right\} = n_{el}$$

- The *density of states* (DoS) is the positive Borel measure on $\sigma(H)$ defined by

$$\int_{\sigma(H)} \mathcal{N}(dE)\ f(E) = \mathcal{T}_{\mathbb{P}} \{ f(H) \}$$

A List of Rigorous Results

- The *current-current correlation function* is the positive Borel measure on $\sigma(H)^{\times 2}$ defined by

$$\int_{\sigma(H)\times\sigma(H)} m(dE, dE')\ f(E)\, g(E') = \sum_{i=1}^{d} \mathcal{T}_{\mathbb{P}}\{f(H)\ \partial_i H\ g(H)\ \partial_i H\}$$

- The *localization length* $\xi(E)$ can be expressed as

$$\int_{\Delta} d\mathcal{N}(E)\xi(E)^2 = \int_{\Delta\times\sigma(H)} \frac{m(dE, dE')}{|E - E'|^2}$$

- If E_F lies in an energy interval of *localized states* with finite *localization length* then

$$\sum_{i=0}^{d} \mathcal{T}_{\mathbb{P}}\left\{(\partial_i P_F)^2\right\} < \infty$$

A List of Rigorous Results

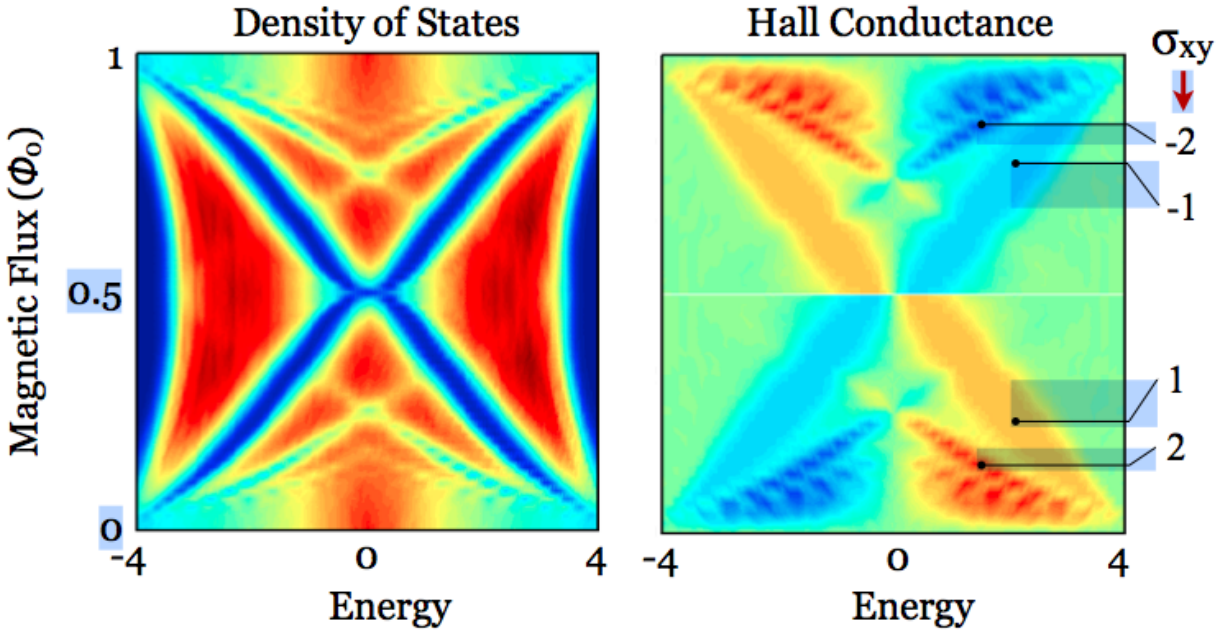
- Under the following assumptions
  1. the dimension is $d = 2$,
  2. the magnetic field is *uniform*,
  3. the *Fermi energy* lies in a region of localized states with *finite localization length*
  4. the *relaxation time* $\tau_{rel} \uparrow \infty$ as $T \downarrow 0$,

$$\lim_{T\downarrow 0} \sigma_{xx} = \lim_{T\downarrow 0} \sigma_{yy} = 0 \quad \lim_{T\downarrow 0} \sigma_{xy} = \frac{e^2}{h}\,\mathrm{Chern}(P_F) \quad \mathrm{Chern}(P_F) \in \mathbb{Z}$$

- The *Chern number* is given by

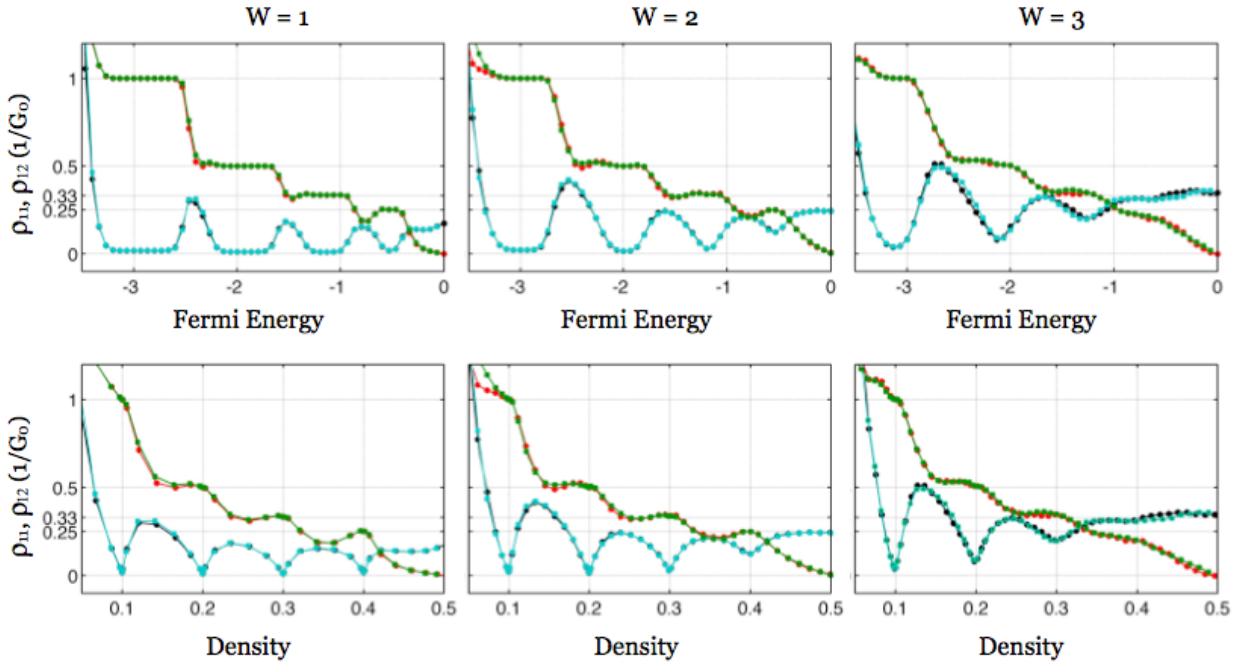
$$\mathrm{Chern}(P_F) = \frac{1}{2\imath\pi}\mathcal{T}_{\mathbb{P}}\{P_F\ [\partial_1 P_F, \partial_2 P_F]\}$$

DoS and Hall Conductivity



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 Hall Plateaux

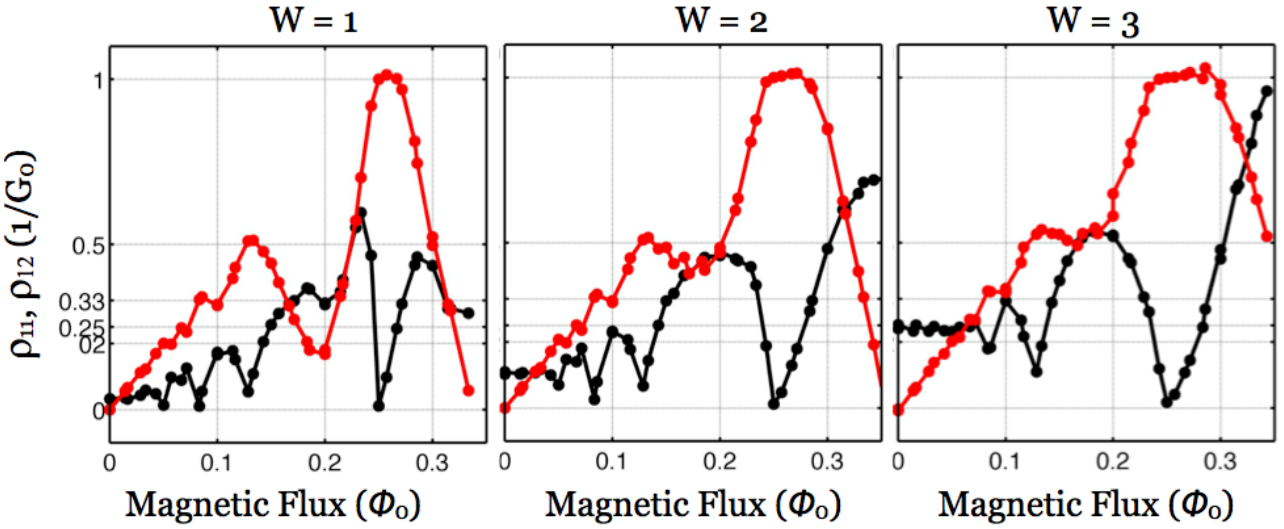


First row (Second row): The diagonal and the Hall resistivities as function of Fermi energy (density) at fixed magnetic flux ϕ, temperature T and disorder strength W

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

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

The Hall Plateaux

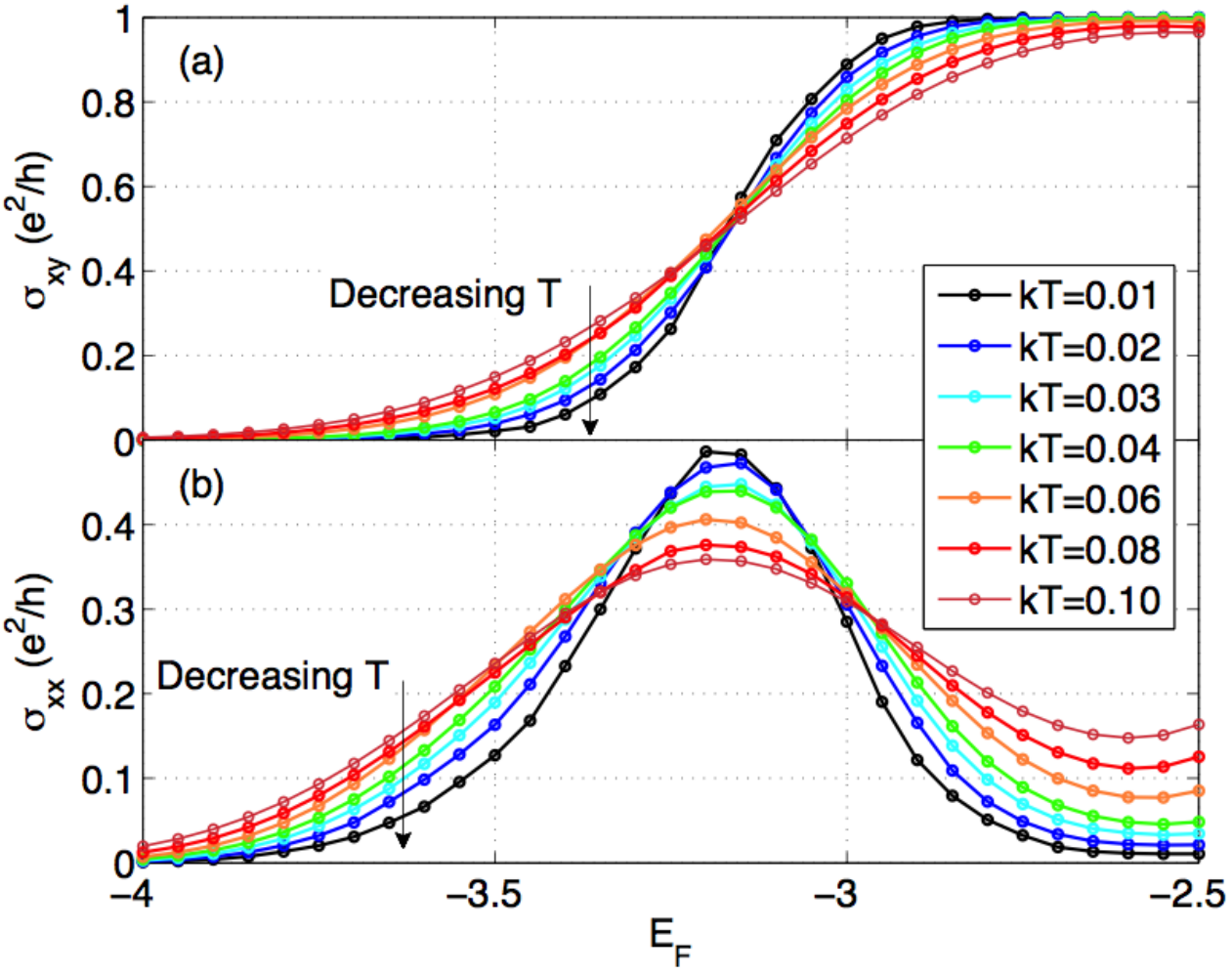


The diagonal and the Hall resistivities as function of magnetic flux

$k_{\mathrm{B}}T = 1/\tau_{rel} = 0.025$
$n_{el} = .25$
$W = 1, 2, 3.$

The data obtained on the 100×100, 120×120 *and* 140×140 *lattices are joined together.*
This is the first set of numerical data showing the transverse conductivity as a function of the magnetic field and exhibiting the appearance of the first plateau

Transition between 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* $\sigma_{xx} \overset{T\downarrow 0}{\rightarrow} \sigma_{xy} = e^2/2h$

Transition between Plateaux

- Between two plateaux of the QHE, the localization length *must diverge* at some critical Fermi energy E_F^c. It has been shown, using a *semiclassical analysis* that *(Chalker, Coddington '88)*

$$\xi(E_F) \sim |E_F - E_F^c|^{-\nu} \qquad \nu = \frac{8}{3} \simeq 2.6$$

- If $\tau_{rel} \overset{T \downarrow 0}{\sim} T^{-p}$, using a *scaling approach* *(Thouless '77)*, the *resistivity* is given by

$$\rho(E_F, T) = F\left((E_F - E_F^c)\left(\frac{T}{T_0}\right)^{-\kappa}\right) \qquad \kappa = \frac{p}{\nu}$$

- Many *experiments confirm* these predictions with *ambiguities* about the values of p, ν.

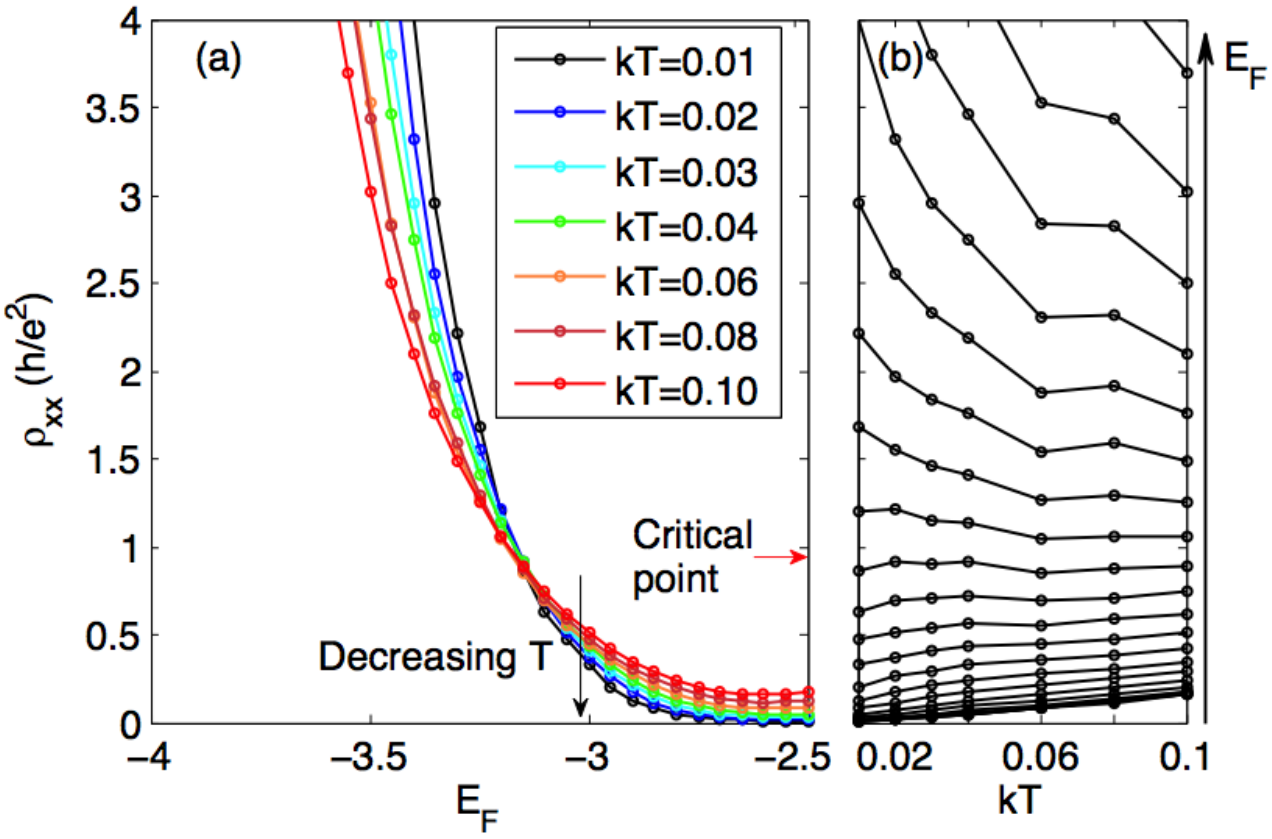
Transition between Plateaux

- The *resistivity* tensor ρ is the *inverse* of the *conductivity* tensor σ

$$\rho = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{bmatrix}^{-1} \quad \Rightarrow \quad \rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} \quad \rho_{xy} = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

- The transition between the plateaux $\text{Chern}(P_F) = 0$ (*plateau insulator* or PI) and $\text{Chern}(P_F) = 1$ (*Hall plateau* or PH) can be investigated with *high precision* using the previous numerical method. On plateaux, $\sigma_{xx} \overset{T \downarrow 0}{\to} 0$, so that $\rho_{xx} \to \infty$ on the *PI side*, and $\rho_{xx} \to 0$ on the *PH side*.

Transition between Plateaux

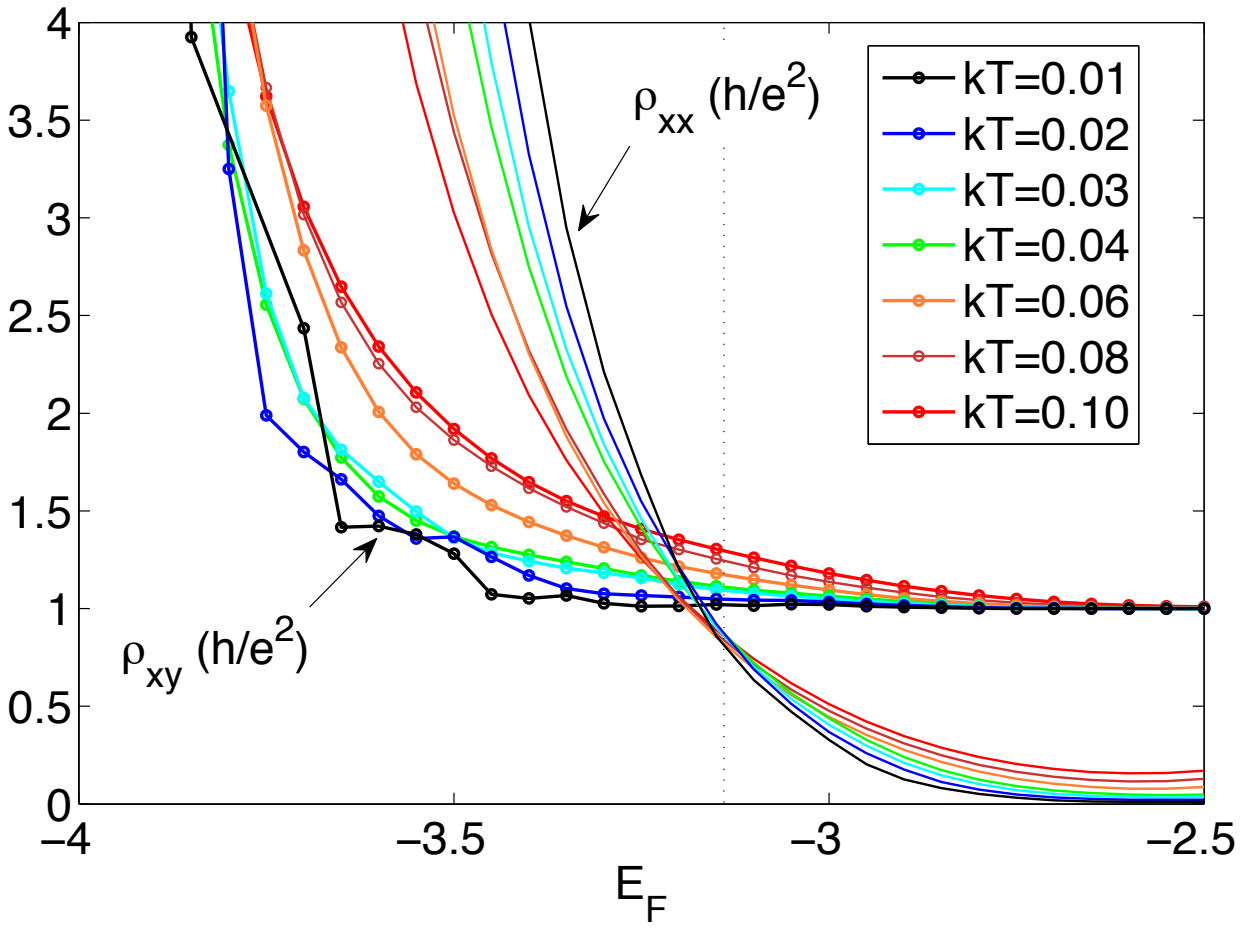


Transition from Chern(P_F) = 0 *to* Chern(P_F) = 1

(a) The simulated ρ_{xx} as function of E_F at different temperatures. (b) ρ_{xx} as function of temperature for various E_F values. The arrow indicates the PH-PI transition.

(Song & Prodan '12)

Transition between Plateaux

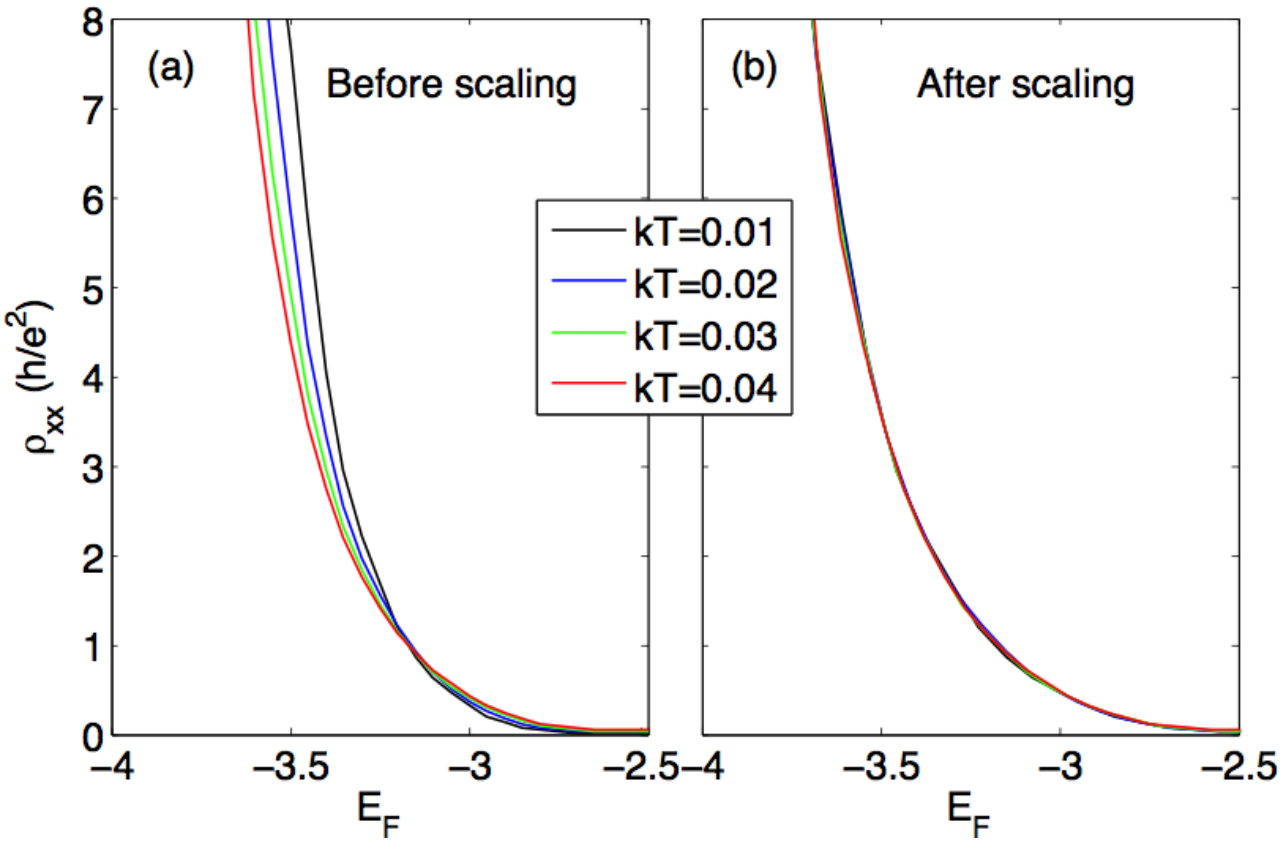


Transition from Chern(P_F) = 0 *to* Chern(P_F) = 1

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)

Transition between Plateaux



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)

Transition between Plateaux

- The numerical results of *Prodan* and *Song-Prodan*, show that
  1. there is no need to introduce the *interactions*
  2. the prediction of the *scaling theory* and of *Chalker & Coddington* are confirmed
  3. the temperature dependence of the relaxation time scale like $\tau_{rel} \sim T^{-1}$ at low temperature.
- However, the RTA does not provide with a mechanism to explain the *extreme experimental precision* of the plateau: with the RTA $\delta\sigma_{xy}/\sigma_{xy} \sim 10^{-4} - 10^{-5}$ *(JB, van Elst, Schulz-Baldes '94)* while experimentally $\delta\sigma_{xy}/\sigma_{xy} \leq 10^{-8} - 10^{-10}$!
  This fact requires to introduce the *variable range hoping* in the theory. *(recent progress in Androulakis, JB, Sadel J. Stat. Phys. '12)*

To Conclude

- The formalism inspired by Connes's *Noncommutative Geometry* has been used successfully to describe rigorously various properties of *aperiodic solids*.

- The *Quantum Hall Effect* is among the most spectacular application. *(JB, van Elst, Schulz-Baldes '94)*

- The derivation of *Kubo's formula* in the relaxation time approximation for aperiodic solids has provided also important applications in the past, such as the conduction properties of *quasicrystals*. *(JB '02)*

- Thanks to the hard work of *Emil Prodan* and his *collaborators*, it is now possible to use this formalism efficiently in *numerical* calculations for *disordered systems* as well.
  This is probably the first step towards making this formalism accessible to a wider public of users.

Thanks for listening !