Identifying Topology in Mesoscopic Quantum Transport using Thouless Conductance

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I. Abstract

The dependence of quantum transport properties upon topological features is studied numerically. To that purpose, we use the Thouless formula as a measure of quantum conductance. Different types of disorder which preserve chiral symmetry (e.g. graphene) are considered. We present numerics for the $\beta(g)$ function which support the well accepted scaling assumption. Comparison is made with existing results obtained using the non linear σ-model and analytical calculations of weak localization corrections.

II. Introduction

Scaling

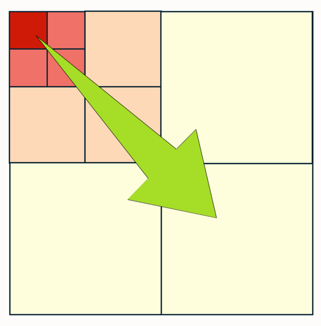
Consider a system of size L and a quantity $g(L)$. It displays a scaling behaviour if it satisfies

$$g(\lambda L) = f(\lambda, g(L))$$

which means that the change of g with respect to L depends only on g:

$$\frac{d \ln g}{d \ln L} \equiv \beta(g)$$

The sign of β determines the flow of $g(L)$ as L increases.



Knowing $g(L)$ at any scale L, we can predict it for all scales.

Scaling of electrical conductance

The electrical conductance g of disordered systems displays a scaling behaviour both in the Drude limit:

$$g(L) = \sigma L^{d-2}, \qquad g(\lambda L) = \lambda^{d-2} g(L), \qquad \beta(g) = d-2$$

and in the strong localized regime:

$$g(L) \sim e^{-L/\xi}, \qquad g(\lambda L) = g^{\lambda}(L), \qquad \beta(g) = \ln g$$

These results are universal i.e. independent of material properties. We consider two phases:

$$\beta(g) > 0 \implies g \xrightarrow{L\to\infty} \infty \text{ (Metal)}$$

$$\beta(g) < 0 \implies g \xrightarrow{L\to\infty} 0 \text{ (Insulator)}$$

Metal-Insulator transition

Quantum corrections to the classical Drude limit are obtained in the metallic regime by means of the Kubo formula. The conductivity then depends on the system size L,

$$g(L) = \sigma(L)\, L^{d-2}$$

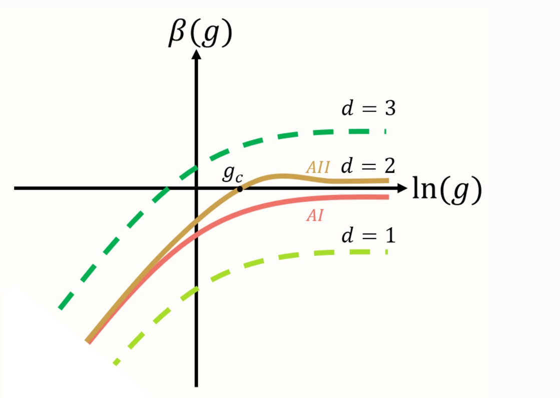
while preserving scaling of $g(L)$ so that $\beta(g)$ can be computed

$$\beta(g) = d - 2 + \frac{\alpha}{g} + O(1/g^2)$$

The gang of 4 scaling theory assumes continuity of $\beta(g)$ in between the Drude and localized limits. Since $\beta < 0$ for $g \sim 0$, the sign of the first non vanishing correction is very important at $d = 2$.

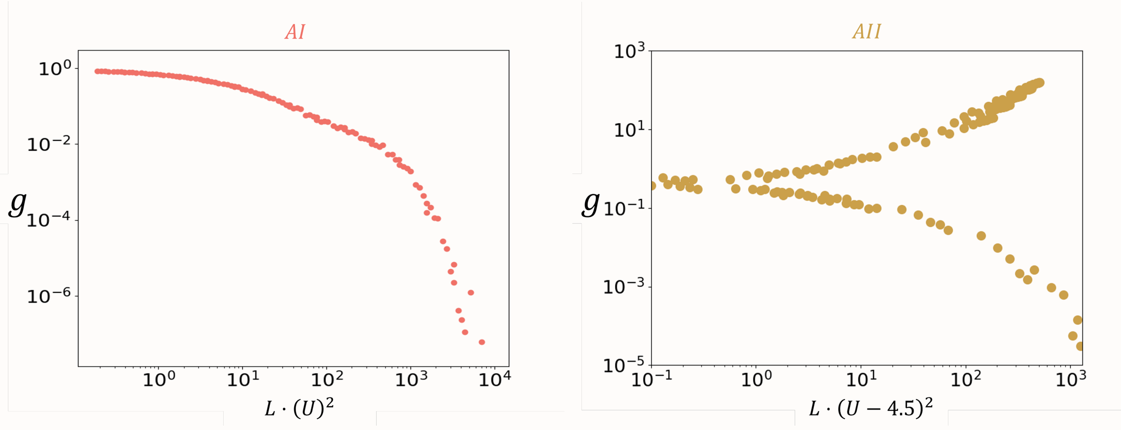
Weak localization $\alpha < 0$
$\beta(g)$ stays negative
No transition

Weak anti-localization $\alpha > 0$
$\beta(g)$ changes sign
Metal-Insulator transition



The sign of α **depends on the symmetry class** of the disordered system.

Numerically, we have checked these scaling behaviours:



III. Symmetry and Topology

Quantum corrections to the Kubo formula depend on the anti-unitary symmetries of the system: time reversal, particle-hole, and (unitary) chirality. The combination of these symmetries leads to 10 symmetry classes presented by Altland and Zirnbauer (AZ) and associated topology via the periodic table.

	Symmetry			Dimension		
	T	C	S	0	1	2
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	0	$\mathbb{Z}$	0
AI	1	0	0	$\mathbb{Z}$	0	0
BDI	1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
DIII	-1	1	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
AII	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
CII	-1	-1	1	0	$\mathbb{Z}$	0
C	0	-1	0	0	0	$\mathbb{Z}$
CI	1	-1	1	0	0	0

$0, \mathbb{Z}_2, \mathbb{Z}$ indicate the allowed topological invariants of the system.

Classes A, AI, and AII correspond to the unitary, orthogonal and symplectic Wigner-Dyson classes.

α is positive for the symplectic class AII and negative for the orthogonal AI. It vanishes for the unitary A, however the second order is negative so the behaviour is similar to AI.

Vanishing of $\beta(g)$ in Chiral classes

Using the non-linear σ-model in $d = 2$, it can be shown that in the three classes AIII, BDI, and CII, **all** corrections to the Drude conductivity vanish. Hence there is no localization even at strong disorder. This behaviour of localization in $d = 2$ seems to apply to $d = 1$ as well (yellow).

IV. Thouless conductance

The electrical conductance is, in a way, a measure of the de-localization of the wavefunctions. We can also achieve this measure by sensing sensitivity to boundary conditions (BC). The logic is that localized states in the bulk will tend to be insensitive to BC changes.

We change the BC by applying phase change ϕ to periodic BC. We define the Thouless conductance

$$g_T = \frac{1}{\Delta}\left\langle \left| \frac{\partial^2 E}{\partial \phi^2} \right|_{\phi=0} \right\rangle$$

where Δ is the average nearest energy level spacing and $\langle \ldots \rangle$ denotes average over disorder.

The energy curvature is the Thouless energy, and in the diffusive regime it is equal to

$$\left| \frac{\partial^2 E}{\partial \phi^2} \right|_{\phi=0} = \frac{2d\hbar}{\tau_L}$$

where τ_L is the system diffusion time. We can associate it with the width of the energy spectrum.

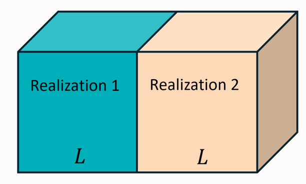
Relation to the Kubo formula

For a large (finite) system and in the diffusive regime, we can relate the Thouless (g_T) and Kubo (g_d) conductances using Random Matrix Theory (RMT),

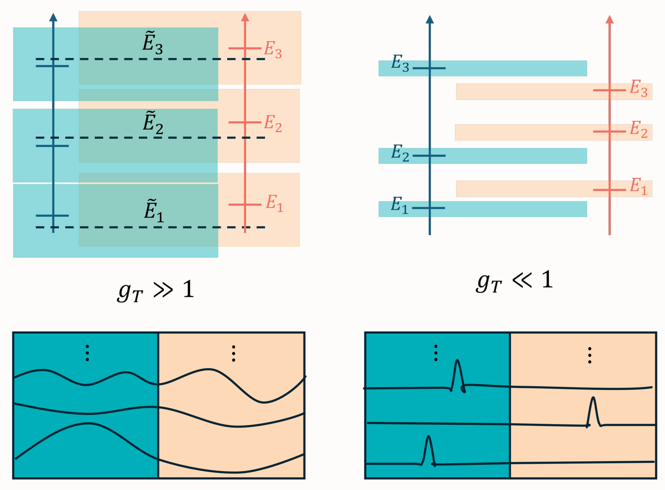
$$g_T = 2\pi g_d$$

This relation also holds beyond RMT.

Consider a system made of two subsystems, each with a different disorder realization



The broader the Thouless energy as compared to the mean level spacing, the more we can construct wavefunctions which span over the entire new system.



In contrast to local Kubo formula, both g_T and g_d depend on the spectrum only, not on the wavefunctions. It's a very useful property in numerical calculations.

V. Lattices and disorder models

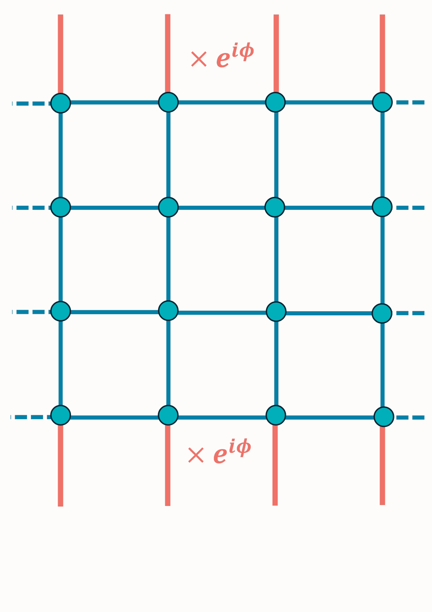
We tested the behaviour of the Thouless conductance on four tight binding models with different random disorder types, which belong to the AI, AII and BDI symmetry classes.

Classes AI, AII

Here, i, j are sites on a square lattice with lattice constant 1. We set $t, \lambda = 1$. ε_i is random uniform on-site disorder, $\langle \varepsilon_i \rangle = 0$, $\langle \varepsilon_i^2 \rangle = U^2/12$. Spin-orbit coupling via Rashba effect is used for AII.

$$H_{AI} = \sum_i \varepsilon_i c_i c_i^\dagger + t \sum_{\langle i,j \rangle} c_i c_j^\dagger$$

$$H_{AII} = \sum_{i,\sigma} \varepsilon_i c_{i\sigma} c_{i\sigma}^\dagger + i\lambda \sum_{\sigma\sigma', \langle i,j \rangle} c_{i\sigma}^\dagger \left(\mathbf{r} \times \boldsymbol{\sigma} \right)_z^{\sigma\sigma'} c_{j\sigma'}$$

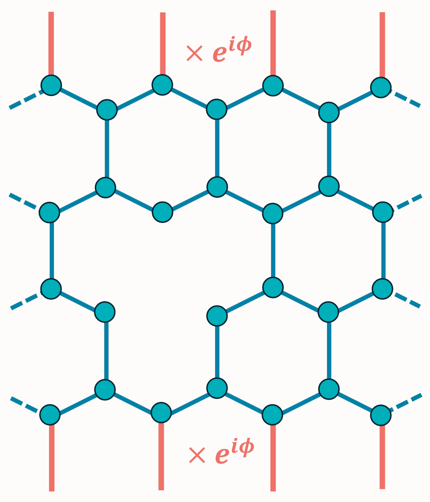


BDI Class

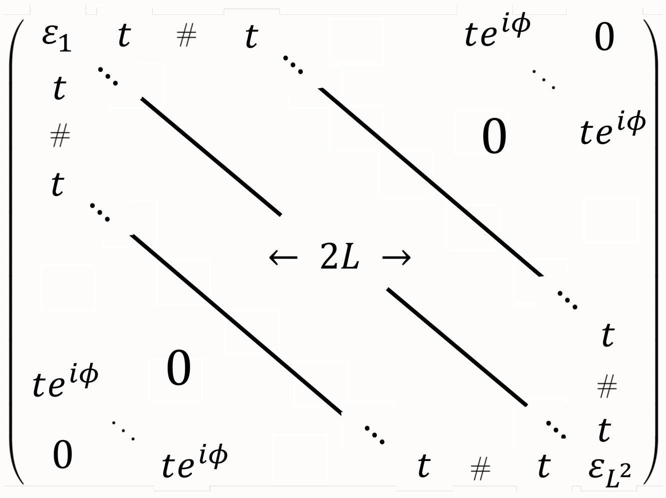
We discuss two models of disorder - hopping and random vacancy density. i, j are sites on a honeycomb lattice. $t = 1$, δt are uniformly distributed $\langle \delta t_i \rangle = 0$, $\langle \delta t_i^2 \rangle = U^2/12$. For vacancy disorder, I contains a random sampling of all N atoms, and $|I|/N = U$.

$$H_{BDI}^{hop} = \sum_{\langle i,j \rangle} (t + \delta t)\, c_i c_j^\dagger$$

$$H_{BDI}^{V} = t \sum_{\langle i,j \rangle} c_i c_j^\dagger - t \sum_{i \in I} \sum_{\langle j,i \rangle} c_i c_j^\dagger$$

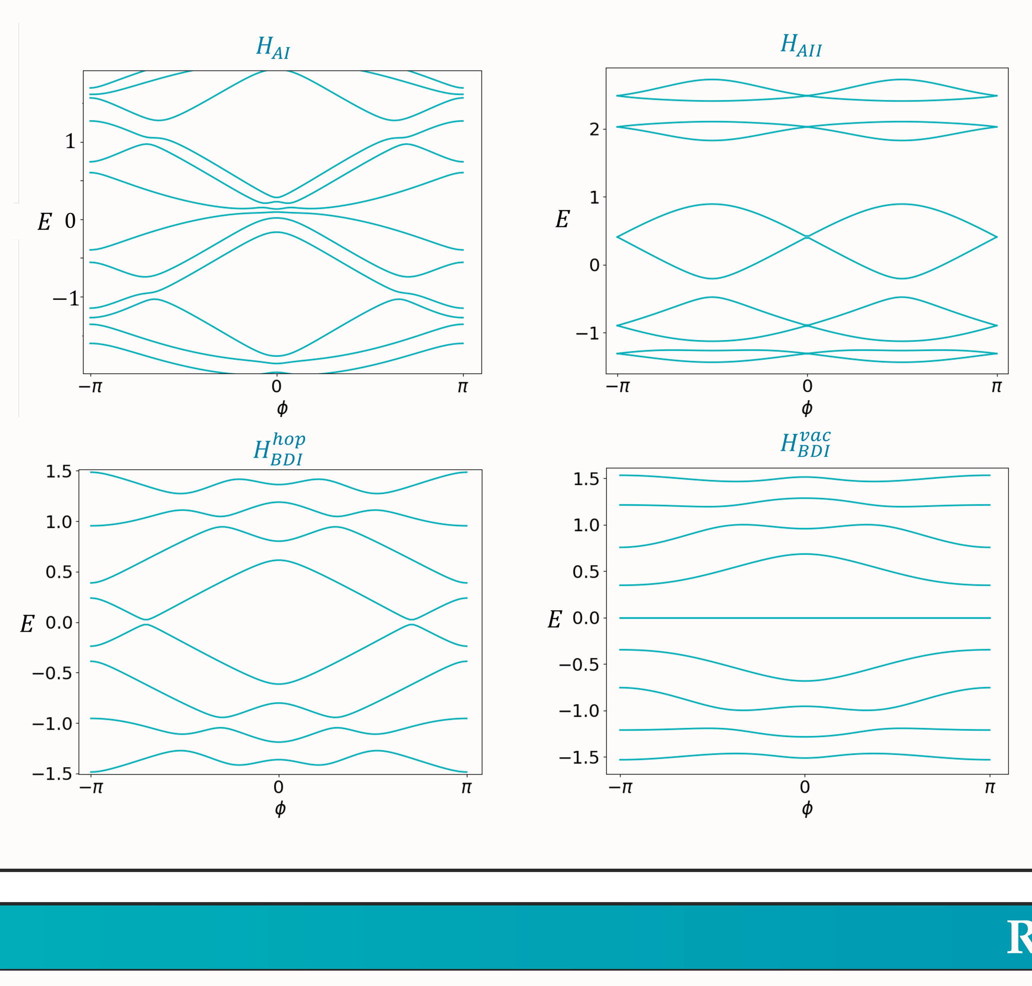


All models have periodic BC in one axis while the other axis' BC are multiplied by a phase $e^{i\phi}$ (twisted boundary conditions).



For $d = 2$, the Hamiltonian has the following structure. In RMT, all matrix elements are independently Gaussian distributed. Here, we are not in the RMT limit, and g_T can be related to g_d only in the diffusive regime.

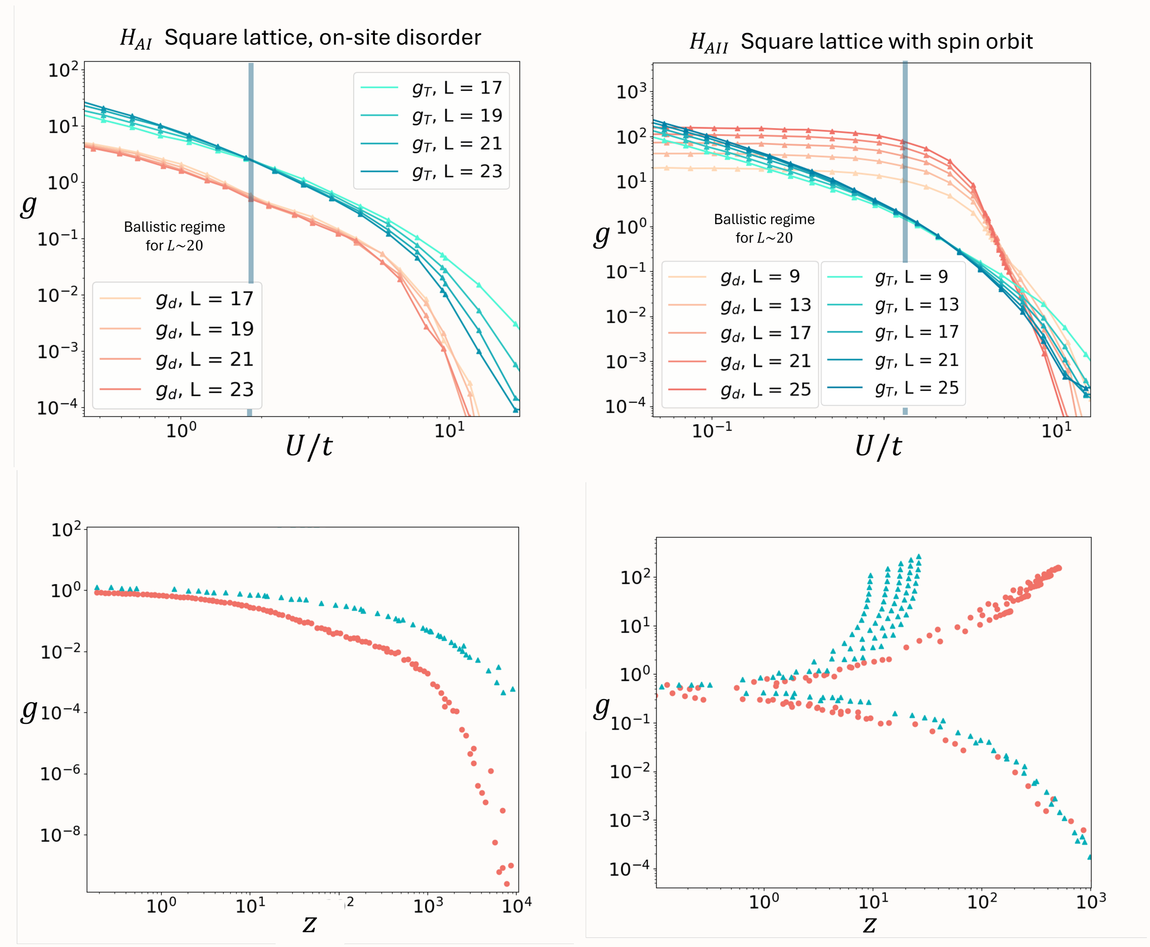
The spectrum $E(\phi)$ looks as follows. Disorder lifts the degeneracies, except for Kramers degeneracies in AII. A flat band appears at the center of the spectrum for the vacancy disorder model, indicating a spatially localized zero mode.



VI. Results

Classes AI, AII

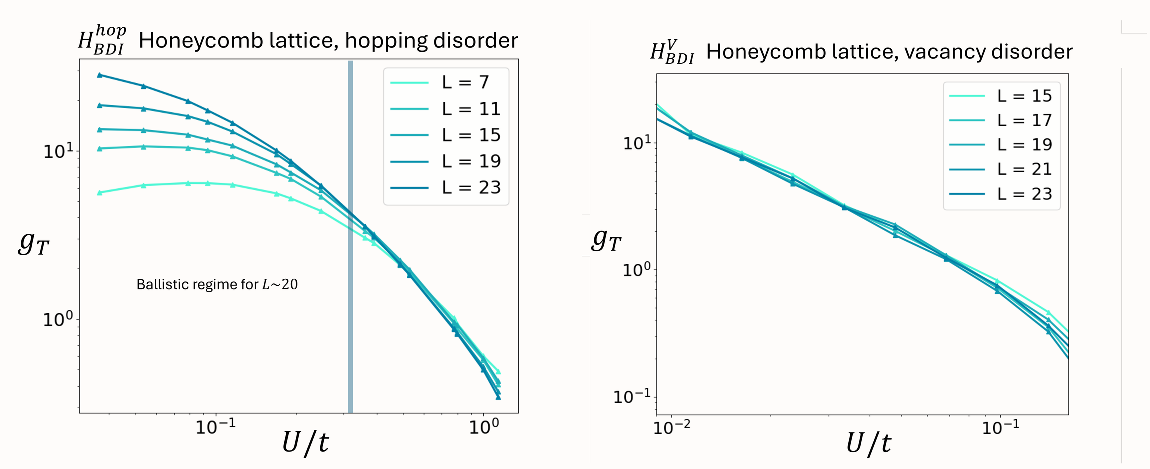
For the square lattice with (AII) or without spin-orbit (AI) coupling, we calculated the Thouless conductance g_T as well as g_d.



The mean free path l_e is calculated using Fermi golden rule, and the diffusive regime is determined. g_T seems not to have scaling at the ballistic regime.

Class BDI

g_T does not depend on L in the diffusive regime, i.e $\beta(g) = 0$ there.



VII. Discussion and future plans

We have shown, using Thouless conductance, that $\beta(g)$ vanishes in BDI in $d = 2$. The three chiral classes displaying this behaviour do not have an interesting topology in $d = 2$, but they do all have the $\mathbb{Z}$ group at $d = 1$, which is related to the fundamental group (π_1) of their non-linear σ-model manifold. We wish to relate the vanishing of the corrections of β to this group.

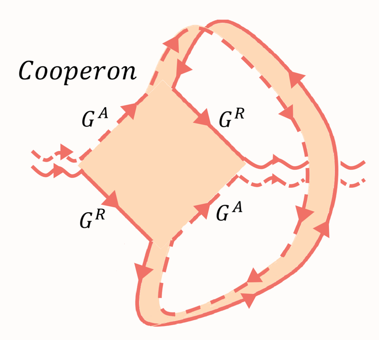
Analytical Computation

We study an analytical model of graphene with a random potential that preserves chiral symmetry. We perform a perturbative computation of the first order correction α (weak localization) using Kubo formula,

$$\sigma_{xx} = \frac{1}{\pi} \int d^2 r \, \mathrm{Tr}\left(j^x G^R j^x G^A - \frac{1}{2} j^x G^R j^x G^R - \frac{1}{2} j^x G^A j^x G^A \right)$$

where G^R (G^A) are the retarted (advanced) resolvant operators of our model. Chirality implies that

$$\sigma_z G^R \sigma_z = -G^A$$



giving

$$\sigma_{xx} = -\frac{1}{\pi} \int d^2 r \, \mathrm{Tr}\left(j^x G^R(r) j^x G^R(r) + j^y G^R(r) j^y G^R(r) \right)$$

Hence contributions from disorder-averaged $\overline{G^R G^R}$ ($\overline{G^A G^A}$) should be taken into account. They cancel out exactly the contribution from $\overline{G^R G^A}$ causing α to vanish.

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