Graphene: Quantum Transport via Evanescent Waves

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(slides from the talk with additional notes added in some places)

Overview

Quantum Transport: Landauer Formula

Graphene:

- Introduction
- Eigenfunctions
- Transmission through a E = 0 'barrier'
- Conductivity
- Other Geometries
- Magnetic Field: Aharonov-Bohm effect

Summary and Literature

Landauer Formula

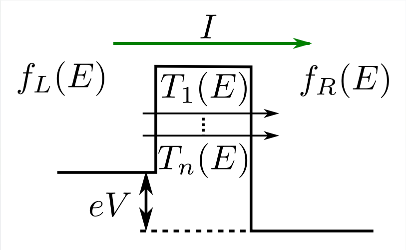
$\psi_{n,E}$: Eigenstate with energy E

$$T_n(E) = \frac{j_{\text{out}}(\psi_{n,E})}{j_{\text{in}}(\psi_{n,E})}$$

T: temperature, V: applied voltage, I: current

$$I = \frac{e}{h}\int_{-\infty}^{\infty} \mathsf{d}E \sum_n T_n(E)[f_L(E) - f_R(E)]$$

$$f_L(E) = f_R(E - eV)$$



Use $T \to 0, V \to 0$:

$$I = \frac{e}{h} \cdot eV \cdot \sum_n T_n(E_F)$$

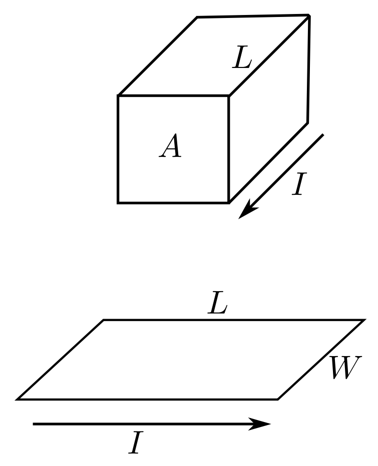
$$I = GV \quad \Rightarrow \quad G = \frac{e^2}{h}\sum_n T_n(E_F)$$

'multi-channel Landauer formula'

Fano factor:

$$F = \frac{\sum_n T_n(1 - T_n)}{\sum_n T_n}$$

2D: Conductance and Conductivity



G: conductance, σ: conductivity

3D: $G = \sigma \cdot \frac{A}{L}$ A: cross section area, L: length

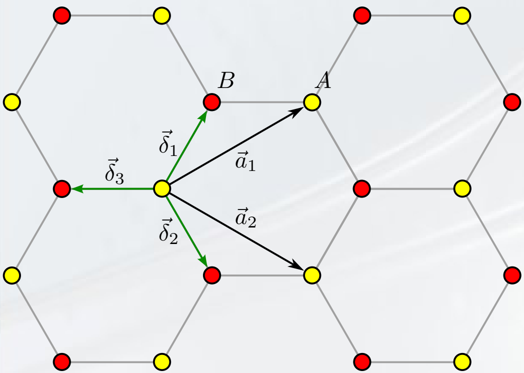
2D: $G = \sigma \cdot \frac{W}{L}$ W: width, L: length

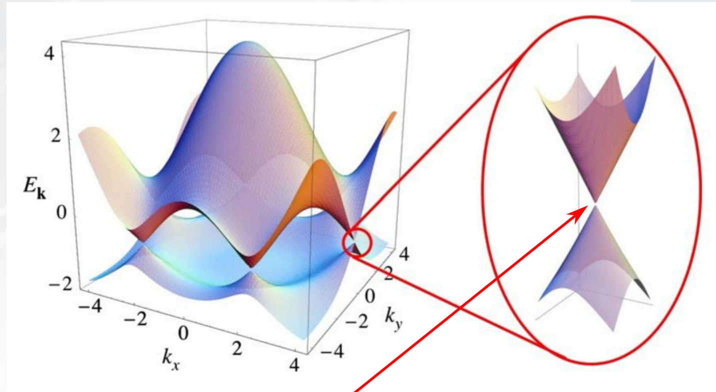
2D: one complex variable $z = x + \mathrm{i}y$ instead of two real variables x, y

$\psi(z) := \psi(\operatorname{Re} z, \operatorname{Im} z)$ with wave function $\psi(x, y)$

Graphene

Castro Neto 2009, Rev Mod Phys 81 109, arXiv:0709.1163





$$n(E) \propto E$$

What is $G(E=0)$

Low energy limit, valley K only:

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$H_K(\vec{r}) = v_{\mathsf{F}} \begin{pmatrix} 0 & p_x - \mathrm{i}p_y \\ p_x + \mathrm{i}p_y & 0 \end{pmatrix}$$

$$\vec{p} = -\mathrm{i}\hbar\vec{\nabla} \qquad v_{\mathsf{F}} \approx 10^6\,\frac{\mathrm{m}}{\mathrm{s}}$$

$$\vec{p} = -\mathrm{i}\hbar\vec{\nabla}$$

Schrödinger

Hamiltonian:

$$H = \frac{\vec{p}^2}{2m}$$

Eigenstates:

$$\psi(\vec{r}) = \exp(\mathrm{i}\vec{k}\cdot\vec{r})$$

Eigenvalues: $E = \dfrac{\hbar^2\vec{k}^2}{2m}$

Probability current:

$$\vec{j}(\vec{r}) = \mathrm{Re}(\psi^* \frac{\vec{p}}{m}\psi)$$
$$= \frac{\hbar}{2m\mathrm{i}}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*)$$

Dirac 2D

(= valley K of graphene, used from here on)

$$H = v_\mathsf{F}\vec{p}\cdot\vec{\sigma}$$
$$= v_\mathsf{F}\begin{pmatrix} 0 & p_x - \mathrm{i}p_y \\ p_x + \mathrm{i}p_y & 0 \end{pmatrix}$$

$$\psi(\vec{r}) = \begin{pmatrix} 1 \\ s\exp(\mathrm{i}\phi_{\vec{k}}) \end{pmatrix}\cdot\exp(\mathrm{i}\vec{k}\cdot\vec{r})$$

$$E = s\hbar v_\mathsf{F}|\vec{k}| \qquad s \in \{-1, 1\}$$

$$\vec{j}(\vec{r}) = \psi^\dagger\, v_\mathsf{F}\vec{\sigma}\,\psi$$

Dirac 2D Zero Energy Modes

$$H = v_\mathsf{F}\vec{p}\cdot\vec{\sigma}$$
$$= -\mathrm{i}\hbar v_\mathsf{F}\begin{pmatrix} 0 & \partial_x - \mathrm{i}\partial_y \\ \partial_x + \mathrm{i}\partial_y & 0 \end{pmatrix}$$

$\vec{r} \in \mathbb{R}^2$ (infinite plane)

and $E \neq 0$:

$$\psi(\vec{r}) = \begin{pmatrix} 1 \\ s\exp(\mathrm{i}\phi_{\vec{k}}) \end{pmatrix} \cdot \exp(\mathrm{i}\vec{k}\cdot\vec{r})$$

$$E = s\hbar v_\mathsf{F}|\vec{k}| \qquad s \in \{-1, 1\}$$

$E = 0:$

$$H\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0$$

$$\Leftrightarrow$$

$$(\partial_x + \mathrm{i}\partial_y)\psi_1 = 0$$
$$(\partial_x - \mathrm{i}\partial_y)\psi_2 = 0$$

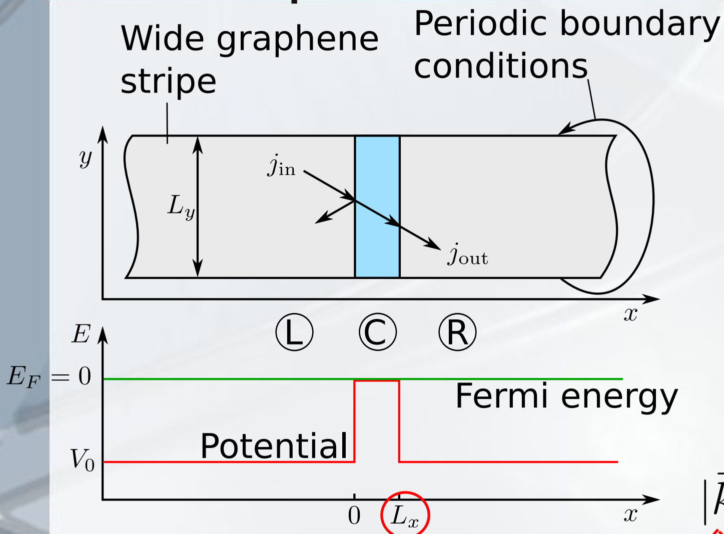
analytic

Solutions:

$$\psi_1(x, y) = \psi_1(x + \mathrm{i}y)$$
$$\psi_2(x, y) = \psi_2(x - \mathrm{i}y)$$

c.c. analytic

Transport: Piecewise Wave Function



$$\psi^L(x=0,y) = \psi^C(x=0,y)$$

$$\Rightarrow$$

$$\psi_1^C(x,y) = c_1 \cdot \mathrm{e}^{\mathrm{i}k_y y + k_y x}$$
$$\psi_2^C(x,y) = c_2 \cdot \mathrm{e}^{\mathrm{i}k_y y - k_y x}$$

Evanescent waves

$$|\vec{k}|\hbar v_{\mathrm{F}} = E = |V_0|$$

$$\psi^L = \left[\begin{pmatrix} 1 \\ \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{ik_x x} + r \begin{pmatrix} 1 \\ \mathrm{e}^{-\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{-ik_x x}\right] \cdot \mathrm{e}^{\mathrm{i}k_y y}$$

$$\psi^C = \begin{pmatrix} \psi_1^C \\ \psi_2^C \end{pmatrix}$$

analytic

c.c. analytic

$$\psi^R = t \cdot \begin{pmatrix} 1 \\ \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{ik_x x + \mathrm{i}k_y y}$$

$$\psi^L(x=0) = \psi^C(x=0)$$
$$\psi^C(x=L_x) = \psi^R(x=L_x)$$

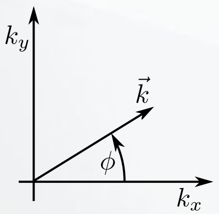
4 equations for t, r, c_1, c_2

Transport: Transmission Probability

For the conductance, we want the transmission probability T:

$$T = \frac{j_{\text{out}}}{j_{\text{in}}} \quad \Rightarrow \quad T = |t|^2$$

Solving the linear system gives:



$$T = \frac{\cos^2(\phi)}{\cosh^2(k_y L_x) - \sin^2(\phi)} \approx \frac{1}{\cosh^2(k_y L_x)}$$

$$|k_y L_x| \leq |k_F L_x| \gg 1$$

Energy of the plane wave:

$$|V_0| = E = \hbar v_F |\vec{k}|$$

Use:

$$k_F := |\vec{k}|$$

Assume:

$$k_F L_x \gg 1$$

Use $\phi \approx 0$ and calculate T again:

$$T = 4 \cdot \left| \frac{\psi_1^C(x=0,y)}{\psi_1^C(x=L_x,y)} + \frac{\psi_2^C(x=0,y)}{\psi_2^C(x=L_x,y)} \right|^{-2}$$

Transport: Conductivity

Periodic boundary conditions:

$$\psi(y=0)=\psi(y=L_y) \quad \Rightarrow \quad k_y=\frac{2\pi}{L_y}\cdot n \quad \text{with } n\in\mathbb{Z}$$

Total transmission: $|k_y L_x| \leq |k_F L_x| \gg 1$

$$T=\sum_{n=-n_0}^{n_0}\frac{1}{\cosh^2(k_y L_x)} \approx \sum_{n=-\infty}^{\infty}\frac{1}{\cosh^2(k_y L_x)} \approx \underbrace{\int_{-\infty}^{\infty}\frac{1}{\cosh^2(x)}\,\mathrm{d}x}_{=2}\cdot\frac{L_y}{2\pi L_x}$$

$L_y \gg L_x$

Conductance:

$$G=\frac{e^2}{h}T=\underbrace{\frac{e^2}{h\pi}}_{\text{this might be } \sigma \text{ (conductivity)}}\cdot\frac{L_y}{L_x}$$

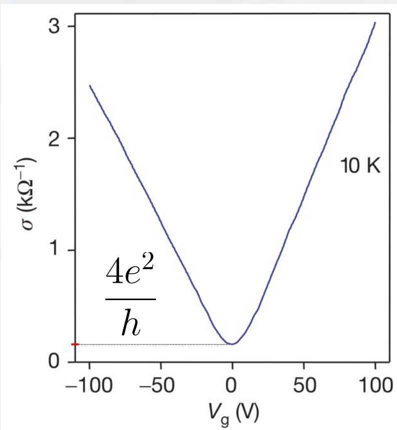
$F=\frac{1}{3}$

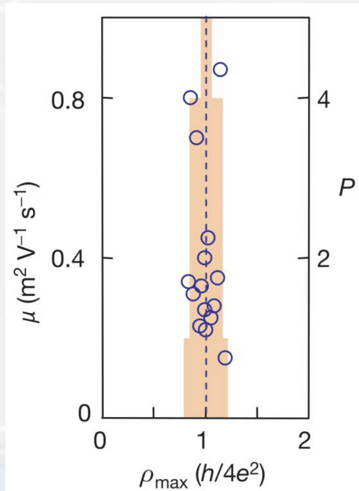
Transport: Conductivity

Conductivity at the Dirac point: $\sigma = \dfrac{e^2}{h\pi}$

2 spin and 2 valley states (neglected) $\Rightarrow$ factor 4: $\sigma = \dfrac{4e^2}{h\pi}$

Measurement:





Novoselov et al. 2005,
Nature 438 p. 197,
arXiv:cond-mat/0509330

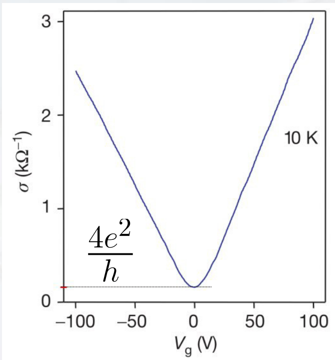
Quantum transport through evanescent waves!

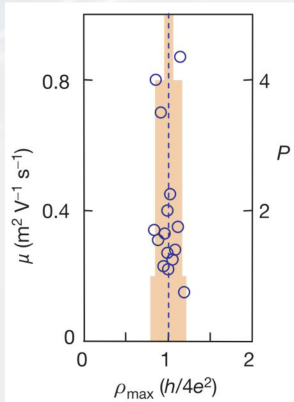
Conductivity $\sigma > 0$ at Dirac point confirmed, order of magnitude agrees

The Missing Pi

Theory: $\sigma = \dfrac{4e^2}{h\pi} \qquad \dfrac{1}{\sigma} = 20\,\mathrm{k}\Omega$

Graphene on Silicon Oxide substrate



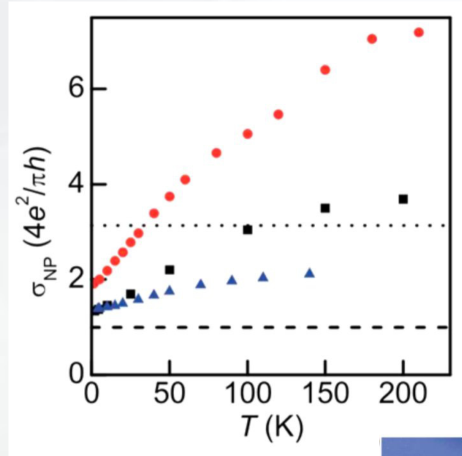


Novoselov et al. 2005, Nature 438 p. 197, arXiv:cond-mat/0509330

Coupling to substrate

Charge inhomogeneities

Graphene with Substrate Etched Away

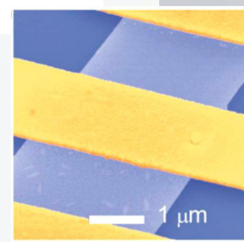


Mayorov et al 2012, Nano Letters 12 p. 4629, arXiv:1206.3848

$E \sim 1\,\mathrm{meV}$

$\Delta n \sim 10^8\,\mathrm{cm}^{-2}$

$= 1\,\mu\mathrm{m}^{-2}$



Corbino Geometry

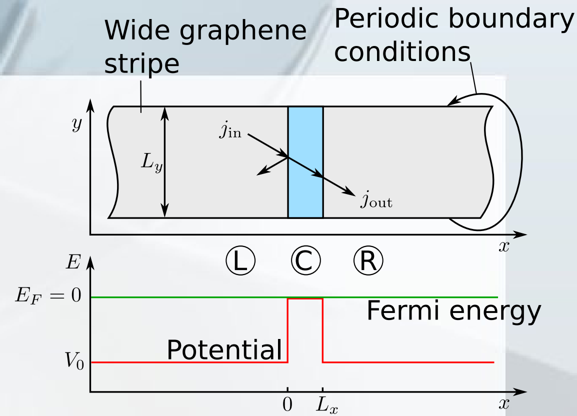
$$\psi^C = \begin{pmatrix} \psi_1^C \\ \psi_2^C \end{pmatrix}$$

analytic

c.c. analytic

$\psi_1^C(z)$ analytic and $w(z)$ analytic

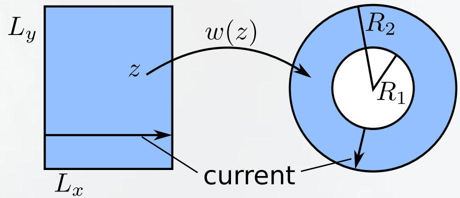
$\Rightarrow \psi_1^C(w(z))$ analytic



$\Rightarrow$ use $w(z)$ to map geometry:

$$w(z) = R_1 \cdot \exp\left(\frac{2\pi z}{L_y}\right)$$

with $\dfrac{L_x}{L_y} = \dfrac{1}{2\pi} \cdot \ln\left(\dfrac{R_2}{R_1}\right)$



$\phi \approx 0$

Boundary conditions:

$$\Rightarrow \psi^L(x=0,y) = \begin{pmatrix} 1+r \\ 1+r \end{pmatrix} \cdot \mathrm{e}^{\mathrm{i}k_y y}$$

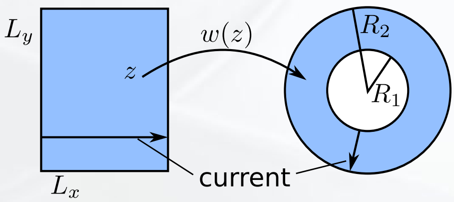
$$\psi^L = \left[\begin{pmatrix} 1 \\ \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{ik_x x} + r \begin{pmatrix} 1 \\ \mathrm{e}^{-\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{-ik_x x}\right] \cdot \mathrm{e}^{\mathrm{i}k_y y}$$

$$\psi^R = t \cdot \begin{pmatrix} 1 \\ \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{ik_x x + \mathrm{i}k_y y} \qquad \Rightarrow \psi^R(x = L_x, y) = \begin{pmatrix} t \\ t \end{pmatrix} \mathrm{e}^{\mathrm{i}k_y y}$$

Corbino Geometry: Conductance

$$w(z) = R_1 \cdot \exp\left(\frac{2\pi z}{L_y}\right)$$

with $\frac{L_x}{L_y} = \frac{1}{2\pi} \cdot \ln\left(\frac{R_2}{R_1}\right)$



$$T_n = \frac{1}{\cosh^2(k_y L_x)} = \frac{1}{\cosh^2(n \cdot \ln(R_2/R_1))}$$

$$k_y = \frac{2\pi}{L_y} \cdot n$$

with $n + \frac{1}{2} \in \mathbb{Z}$

$|R_2 - R_1| \ll R_1$:

$$G \approx \frac{2e^2}{h} \cdot \frac{1}{\ln(R_2/R_1)}$$

$F \approx \frac{1}{3}$

$R_1 \ll R_2$:

$$G \approx \frac{8e^2}{h} \cdot \frac{R_1}{R_2}$$

$F \approx 1 - G \cdot \frac{h}{8e^2}$

$\psi(y = 0)$
$= -\psi(y = L_y)$

Berry's phase

Magnetic field

$$\vec{B} = \begin{pmatrix} 0 \\ 0 \\ B_z(x,y) \end{pmatrix}$$

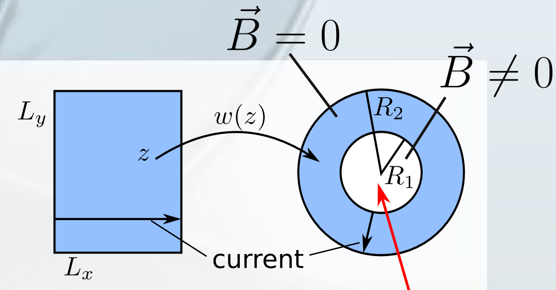
see ch. 2.3 from Katsnelson, 2012

$$B_z = \vec{\nabla}^2 \phi(x,y)$$

$$\psi^C_{1,2} = \exp(\mp q\phi)\bar{\psi}^C_{1,2}$$

$$H(B)\psi^C = 0 \quad \Leftrightarrow$$

$$H(B=0)\bar{\psi}^C = 0$$



$$w(z) = R_1 \cdot \exp\left(\frac{2\pi z}{L_y}\right)$$

$$\phi(R_2) - \phi(R_1) = \Phi \cdot \ln\left(\frac{R_2}{R_1}\right)$$

Boundary Conditions:

$$\psi^L(x=0,y) = \begin{pmatrix} 1+r \\ 1+r \end{pmatrix} \cdot \mathrm{e}^{\mathrm{i}k_y y}$$

$$\psi^R(x=L_x,y) = \begin{pmatrix} t \\ t \end{pmatrix} \mathrm{e}^{\mathrm{i}k_y y}$$

0 $\quad R_1$

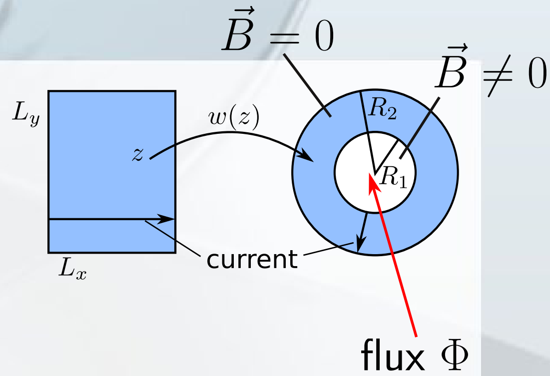
$$\psi^C_1(x,y) = \mathrm{e}^{-q\phi(R)}\mathrm{e}^{-\mathrm{i}k_y y}\mathrm{e}^{k_y x}$$

$$T = 4 \cdot \left| \frac{\psi^C_1(x=0,y)}{\psi^C_1(x=L_x,y)} + \frac{\psi^C_2(x=0,y)}{\psi^C_2(x=L_x,y)} \right|^{-2}$$

$\phi \approx 0$

$$\mathrm{e}^{-q(\phi(R_1)-\phi(R_2))}\mathrm{e}^{k_y L_x}$$

Aharonov-Bohm effect



$$w(z) = R_1 \cdot \exp\left(\frac{2\pi z}{L_y}\right)$$

$$\phi(R_2) - \phi(R_1) = \Phi \cdot \ln\left(\frac{R_2}{R_1}\right)$$

$$T = 4 \cdot \left| \frac{\psi_1^C(x=0,y)}{\psi_1^C(x=L_x,y)} + \frac{\psi_2^C(x=0,y)}{\psi_2^C(x=L_x,y)} \right|^{-2}$$

$$\mathrm{e}^{-q(\phi(R_1)-\phi(R_2))}\mathrm{e}^{k_y L_x}$$

Final result:

$$G = \frac{e^2}{h} \cdot \left[1 - f_1(R_2/R_1) \cdot \cos\left(\frac{e\Phi}{\hbar}\right)\right]$$

$$F = \frac{1}{3} + f_2(R_2/R_1) \cdot \cos\left(\frac{e\Phi}{\hbar}\right)$$

$R_2/R_1 = 5$:
Effects of $5\,\%$
and $42\,\%$

see ch. 3.1 of Katsnelson, 2012 for 'intrinsic disorder' related to zitterbewegung

Summary

Minimal conducitivity at $E = 0$ is $\sigma = \frac{4e^2}{h\pi}$ (no (external) disorder or scattering at impurities)

Analytic functions (='conformal maps') for $\sigma(E = 0)$ in different geometries

Aharonov-Bohm effect in a Magnetic field at $E = 0$ predicted

Literature

This talk:	Katsnelson: Graphene (2012, Cambridge University Press) (ch. 2.3 and 3)
Landauer formula:	Cuevas, Scheer: Molecular Electronics (2010, World Scientific Publishing) (ch. 4)
	Datta: Electronic Transport in Mesoscopic Systems, (1995, Cambridge University Press)
Berry's Phase:	Böhm: The Geometric Phase in Quantum Systems (2003, Springer) (esp. ch. 2 together with ch. 2.4 from Katsnelson, 2012; ch. 12)