MAX-PLANCK-GESELLSCHAFT

mpipks

What can graphene teach us about the bridge between QFT and kinetic theory?

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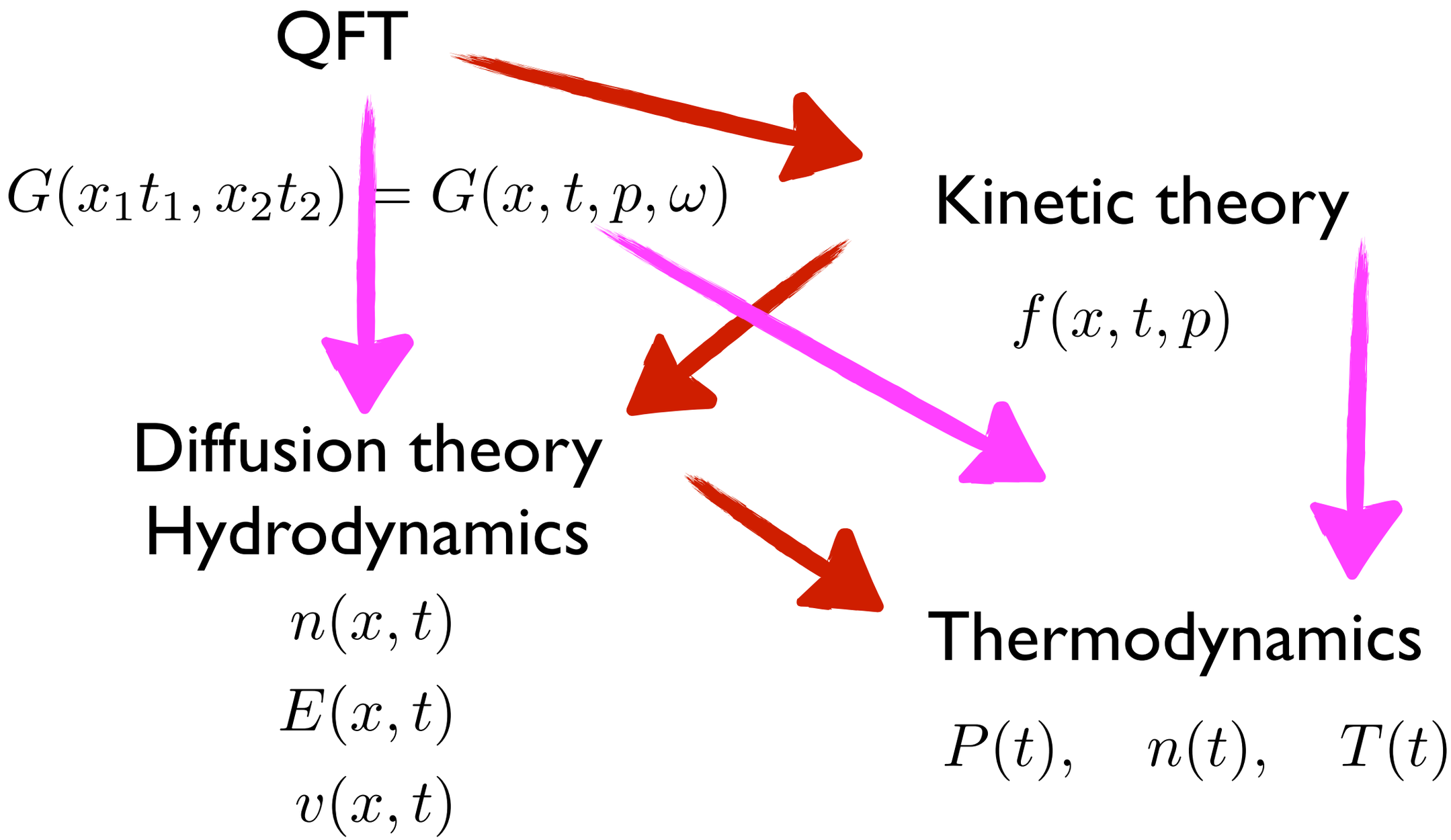
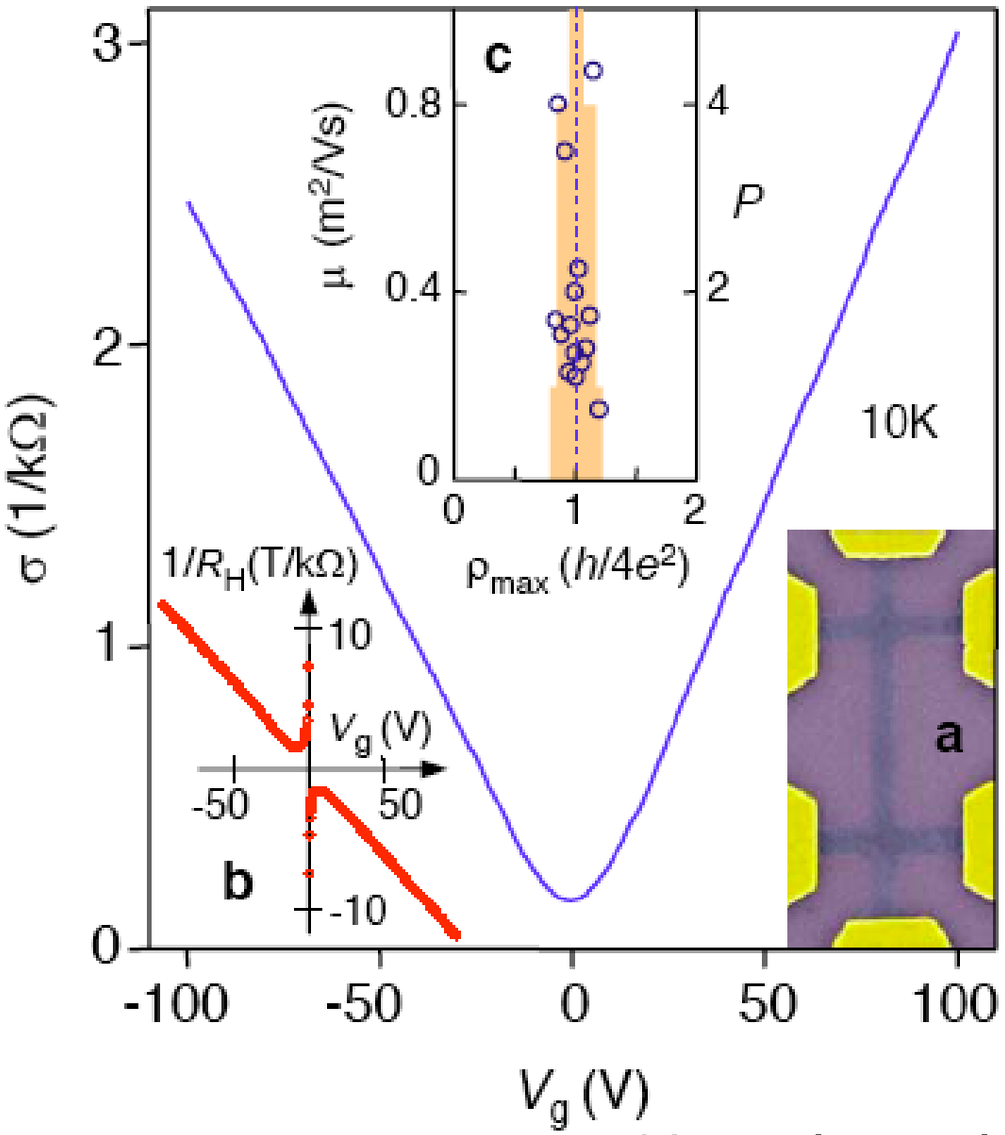
Reduced descriptions

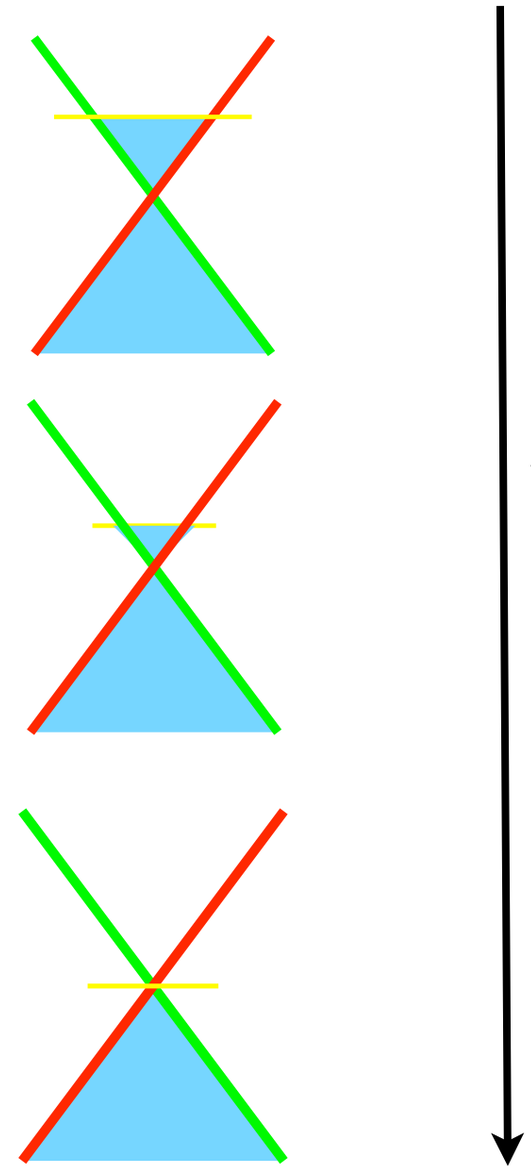


Conductivity in graphene

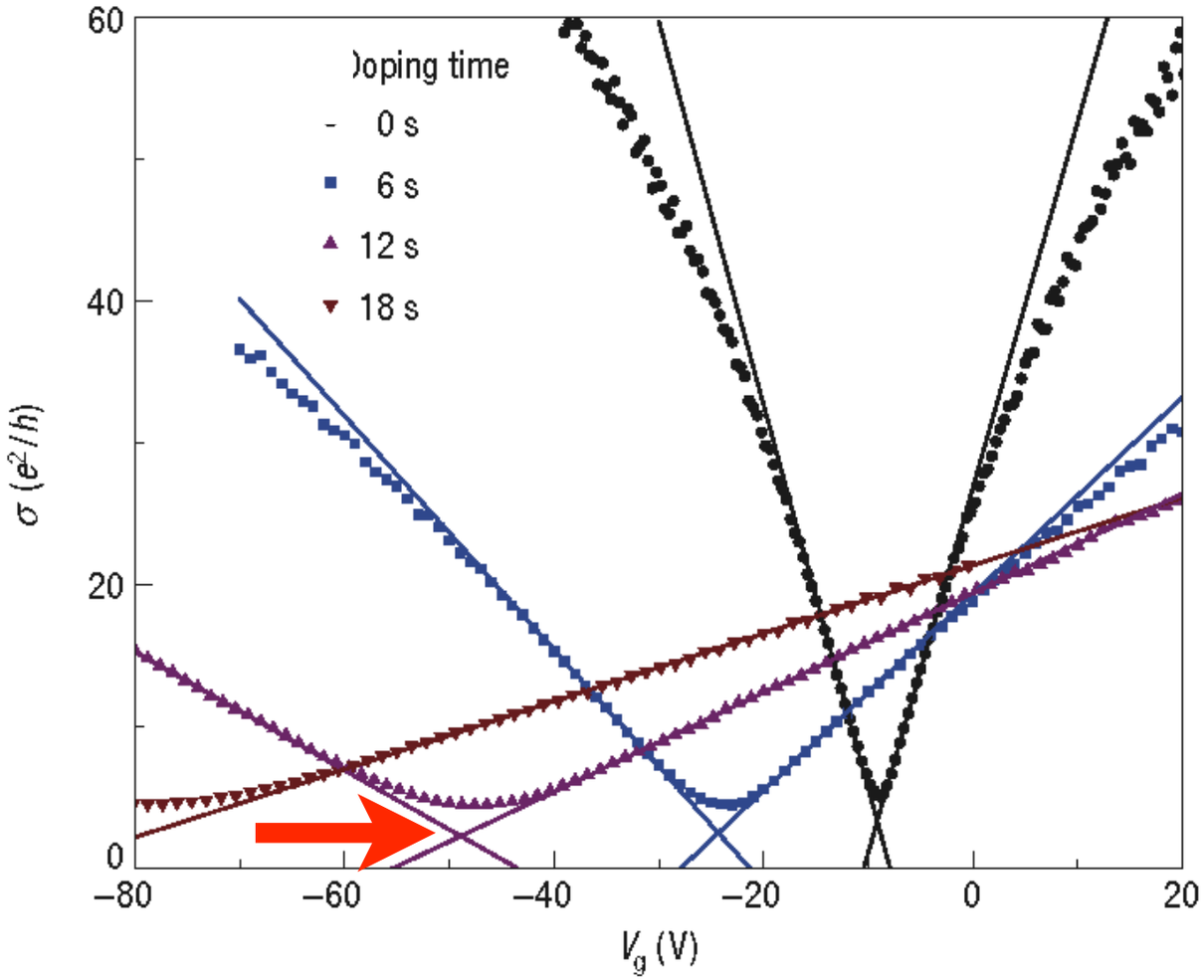


Novoselov et al., Nature 2005

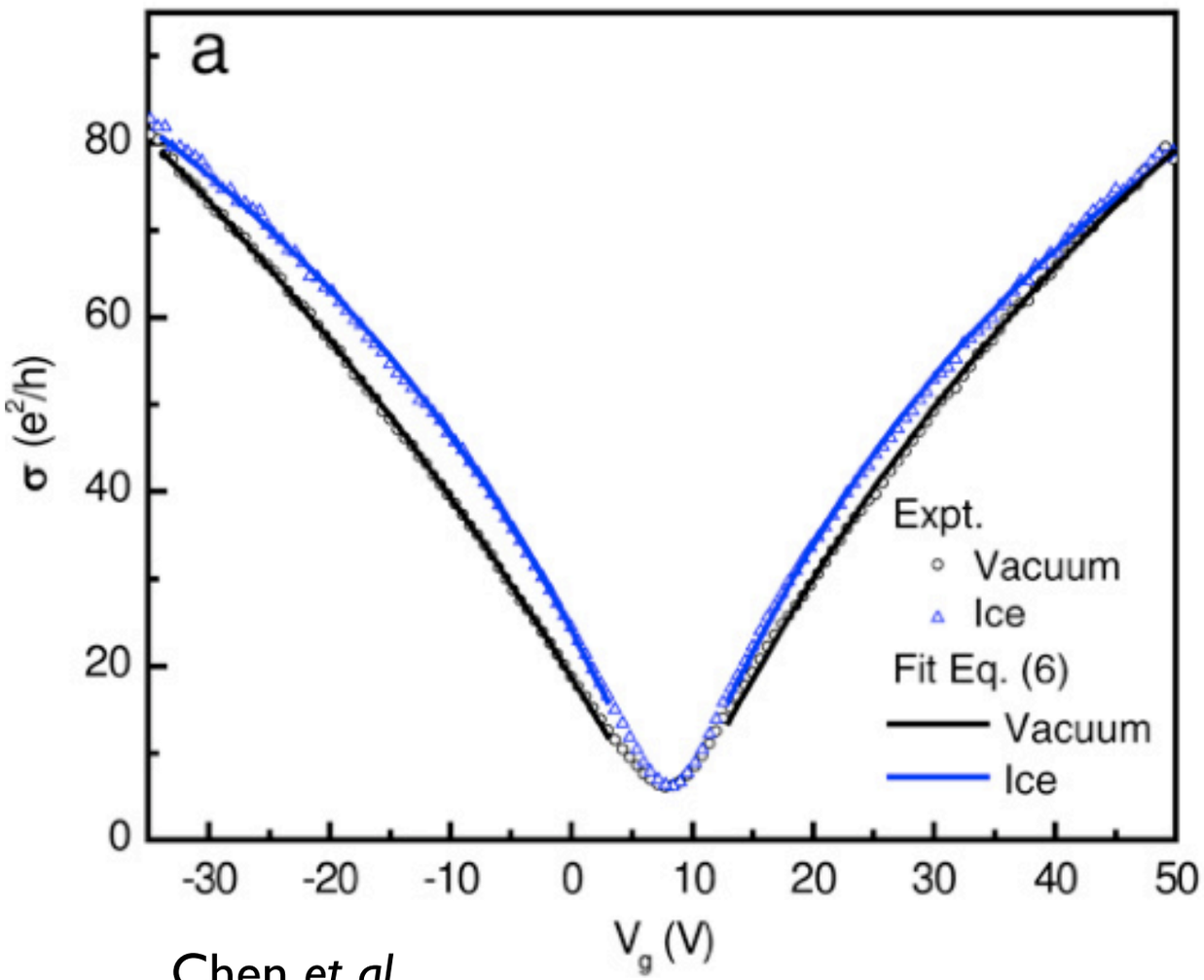
~~Universal~~ conductivity minimum?



Residual conductivity



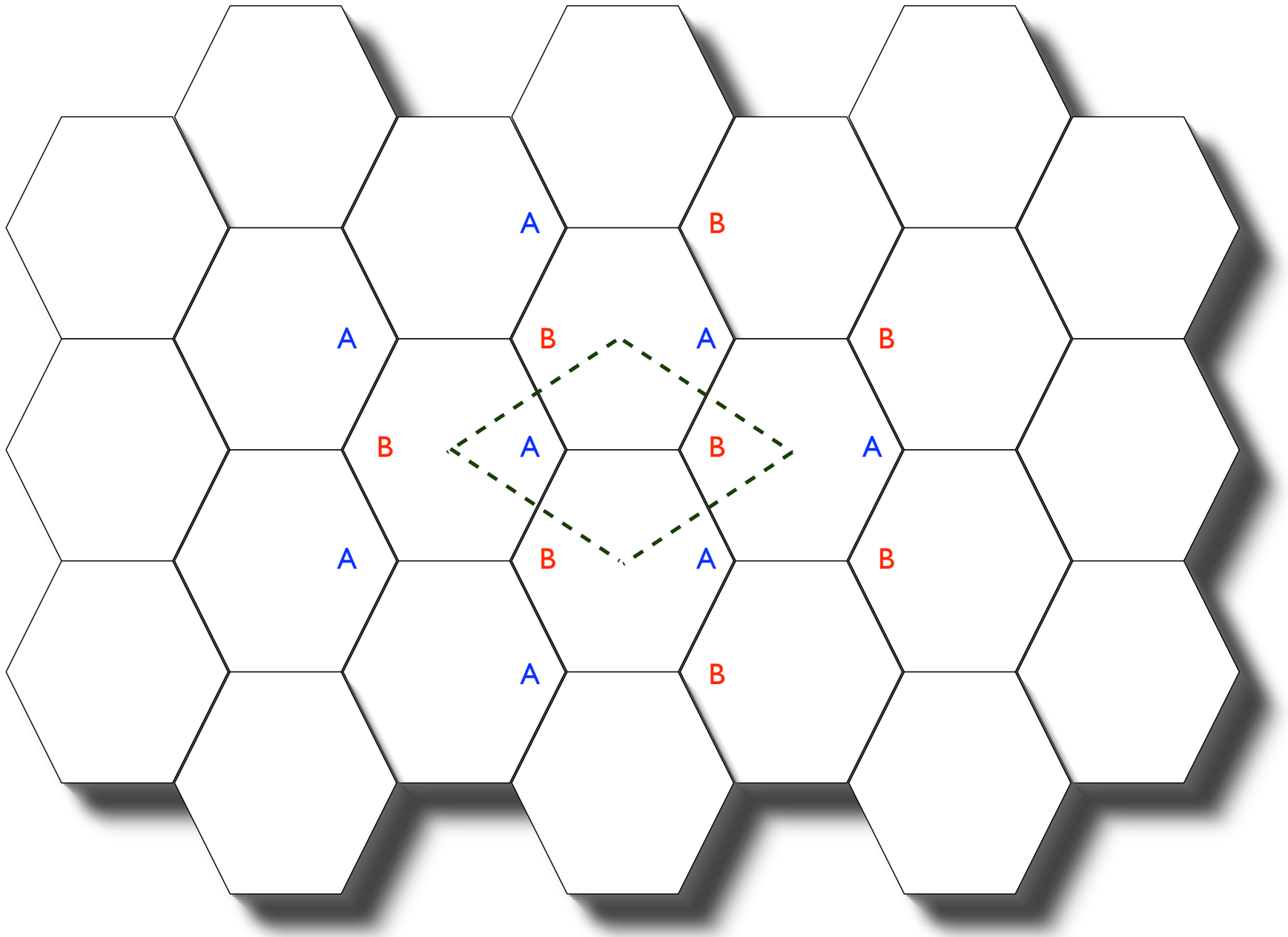
Chen *et al.*,
Nat. Phys. 4, 377 (2008)



Chen *et al.*,
Solid State Comm. 149, 1080 (2009)

Electron-hole coherent effects? Weak localization?

Bipartite lattice gives pseudospin



Graphene band structure

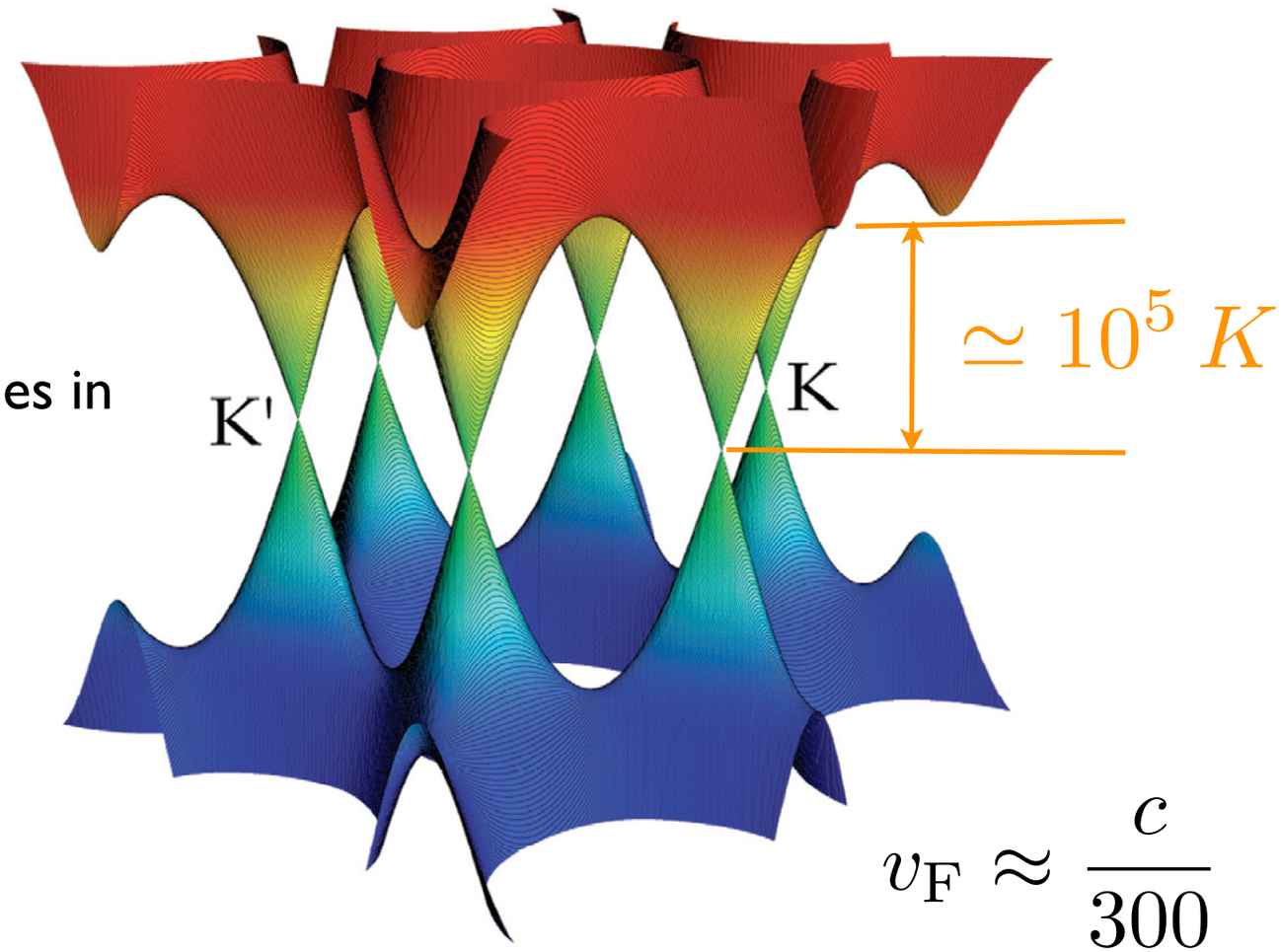
Wallace 1947
Semenoff 1984

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j \quad \overset{p \approx 0}{\Longrightarrow} \quad H_K = v_{\mathrm{F}} \begin{pmatrix} 0 & p_x - i p_y \\ p_x + i p_y & 0 \end{pmatrix}$$

Electrons

$$E_+ = +v_{\mathrm{F}} p$$

Two inequivalent Dirac cones in the first Brillouin zone



Holes

$$E_- = -v_{\mathrm{F}} p$$

$$v_{\mathrm{F}} \approx \frac{c}{300}$$

2x2 matrix index = = pseudospin index= =sublattice index

Multilayer graphene

Single-layer graphene

$$H_K = v_{\rm F} \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v_{\rm F}\, \vec{p} \cdot \vec{\sigma}$$

N-layer graphene, low energy bands

$$H_K \sim \begin{pmatrix} 0 & (p_x - ip_y)^N \\ (p_x + ip_y)^N & 0 \end{pmatrix}$$

Boltzmann equation

$$\partial_t f_{\boldsymbol{k}} + \boldsymbol{v} \cdot \partial_{\boldsymbol{x}} f_{\boldsymbol{k}} + e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \cdot \partial_{\boldsymbol{k}} f_{\boldsymbol{k}} \;=\; \mathcal{J}[f]$$

Collision integral

$$\mathcal{J}[f] \;=\; -\int_{\boldsymbol{k'}} \delta(\epsilon_k - \epsilon_{k'}) W_{\boldsymbol{k}\boldsymbol{k'}} (f_{\boldsymbol{k}} - f_{\boldsymbol{k'}}) \sim -\frac{\delta f}{\tau}$$

Relaxation-time approximation

Drude conductivity

$$\sigma_0 = e^2 n \tau / m$$

Drude conductivity

$$\sigma_0 \propto \tau v_{\mathrm{F}} k_{\mathrm{F}} \sim \frac{v_{\mathrm{F}} k_{\mathrm{F}}}{n_{\mathrm{imp}} |U|^2 D(\epsilon_{\mathrm{F}})}$$

Point-like impurities

$$U = \mathrm{const} \qquad \sigma_0 = \mathrm{const}$$

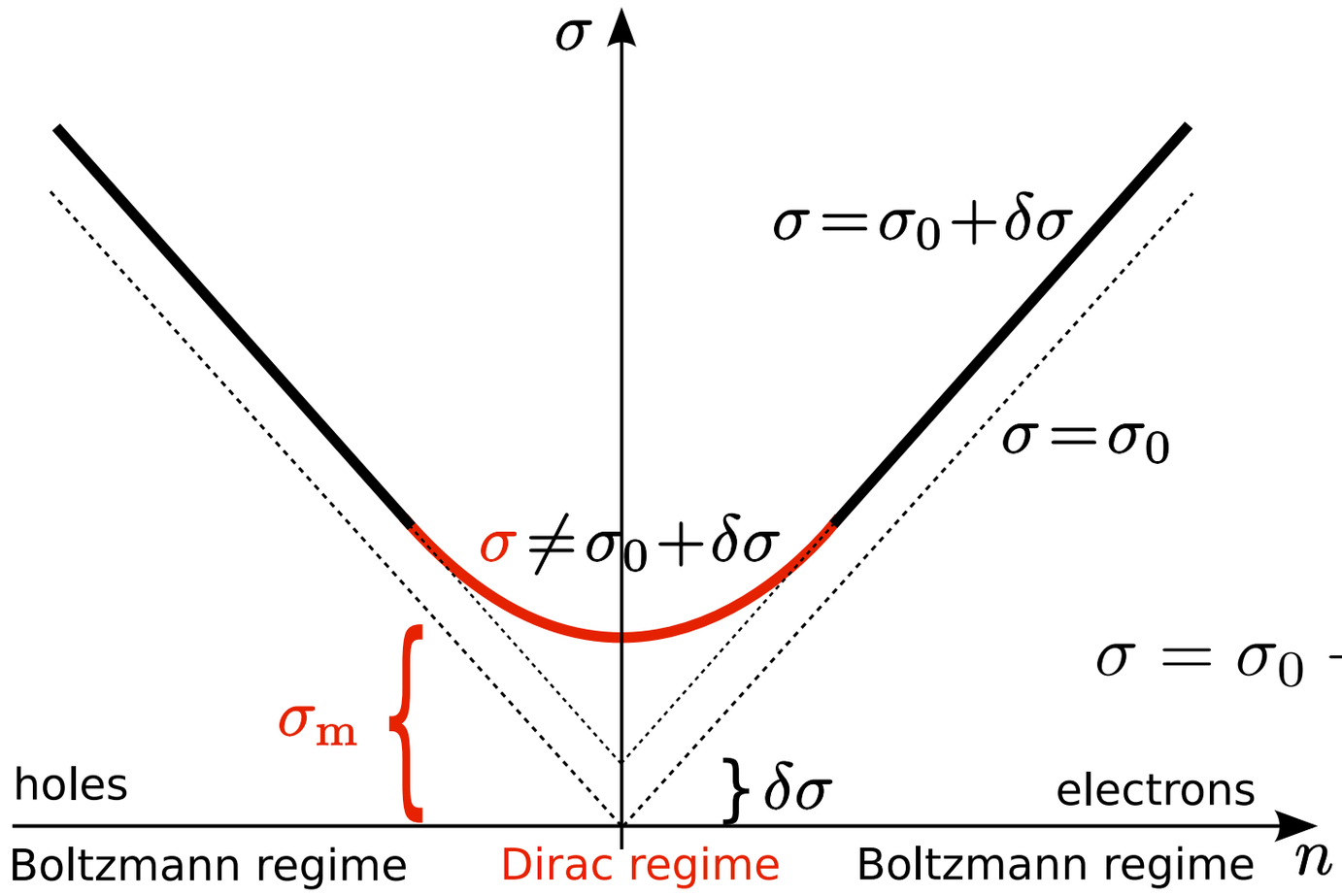
Screened charged impurities (RPA)

$$U_{\boldsymbol{k}\boldsymbol{k}'} = \frac{e^2/\kappa}{|\boldsymbol{k} - \boldsymbol{k}'| + \frac{e^2}{\kappa} D(\epsilon_{\mathrm{F}})} \to \frac{1}{k_{\mathrm{F}}}$$

Thomas-Fermi momentum

$$\sigma_0 \propto n$$

Boltzmann regime



Boltzmann regime

$$\ell k_{\mathrm{F}} = \tau v_{\mathrm{F}} k_{\mathrm{F}} \gg 1$$

Drude conducitivity

$$\sigma_0 = \frac{e^2}{2h} \ell k_{\mathrm{F}}$$

Quantum corrections

$$\sigma = \sigma_0 + c_0 (\ell k_{\mathrm{F}})^0 + c_1 (\ell k_{\mathrm{F}})^{-1} + \dots$$

$\delta\sigma$ σ_m ?

One-band Boltzmann equation

$$\boldsymbol{E} \cdot \partial_{\boldsymbol{k}} f^{\mathrm{eq}}_{\boldsymbol{k}} = -\int_{\boldsymbol{k'}} \delta(\epsilon_k - \epsilon_{k'}) W_{\boldsymbol{k}\boldsymbol{k'}} \cos^2 \frac{\theta_{\boldsymbol{k}} - \theta_{\boldsymbol{k'}}}{2} (f^{(E)}_{\boldsymbol{k}} - f^{(E)}_{\boldsymbol{k'}})$$

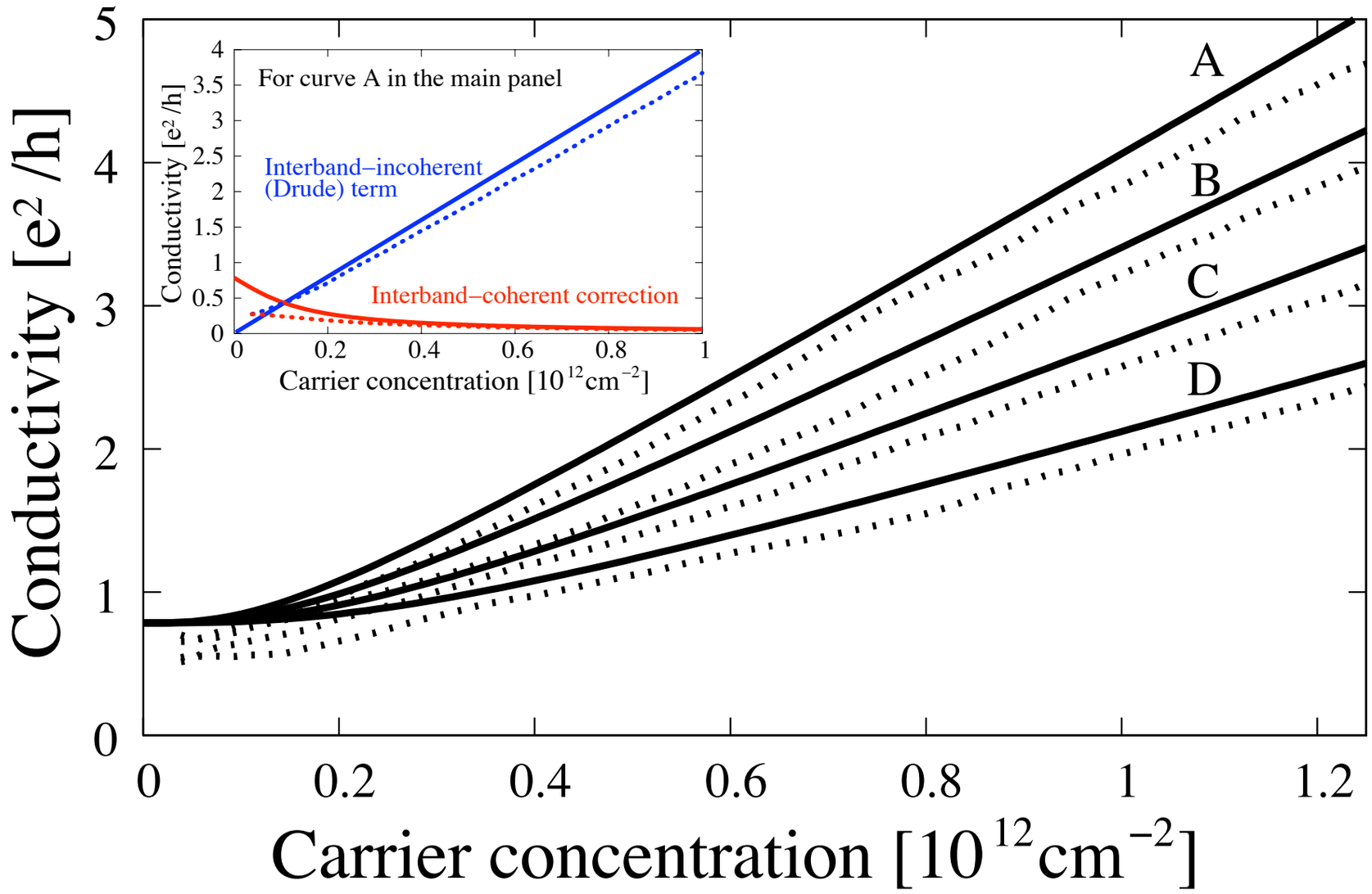
Kubo formula

$$\sigma = -\frac{ie^2}{L^2} \sum_{n,n'} \frac{f^0_{E_n} - f^0_{E_{n'}}}{E_n - E_{n'}} \frac{\langle n|v_x|n'\rangle\langle n'|v_x|n\rangle}{E_n - E_{n'} + i\eta}$$

Applicable also to the Dirac regime.
However, less intuition than with Boltzmann calculations.

Boltzmann vs Kubo in clean bilayer graphene

Clean graphene = no charged impurities. Remaining impurities point-like?



Trushin, Kailasvuori, Schliemann & MacDonald, arxiv:1002.4481

Principal value terms vanish for point-like impurities in bilayers.
Quantum corrections then easier to sum up to all orders.

Residual conductivity

- Weak anti-localization (incoherent bands)?
- Electron-hole coherence originated quantum correction? Only for monolayer graphene! Due to principal value terms! Approach sensitive!

For point-like impurities			$\delta\sigma / \frac{2e^2}{\pi h}$
	G1	GKBA	$-\log\frac{k_\Lambda}{k_\mathrm{F}} - \frac{\pi^2}{8}$
QL &	G1	AA	$-\log\frac{k_\Lambda}{k_\mathrm{F}} + \frac{\pi^2}{8}$
	G1	SKBA	$-\log\frac{k_\Lambda}{k_\mathrm{F}}$
	G2	GKBA	$-\frac{\pi^2}{8}$
	G2	AA	$+\frac{\pi^2}{8}$
	G2	SKBA	0

$$\frac{1}{\omega + i\eta - \epsilon} = \frac{\mathcal{P}}{\omega - \epsilon} - i\pi\delta(\omega - \epsilon)$$

Deriving a band-coherent kinetic equation

Iterating the quantum Liouville equation (interaction picture)

$$\partial_t \rho^{\mathrm{I}} = -i[V^{\mathrm{I}}(t), \rho^{\mathrm{I}}(t_0)] - \int_{t_0}^{t} \mathrm{d}t' [V^{\mathrm{I}}(t), [V(t'), \rho^{\mathrm{I}}(t')]]$$

Kinetic equation $\partial_t \rho(t) - i[H_0, \rho(t)] = \mathcal{J}[\rho]$

For Boltzmann eq., gradient expand $i[H_0, \rho(t)]$

Collision integral $\mathcal{J}[\rho] = -\int \frac{\mathrm{d}\omega}{2\pi} [V, [G^{0\mathrm{R}} V G^{0\mathrm{A}}, \rho]],$

Delta function terms and principal value terms

$$\int \frac{\mathrm{d}\omega}{2\pi} G^{0\mathrm{R}}_{\boldsymbol{k}} V_{\boldsymbol{k}\boldsymbol{k}'} G^{0\mathrm{A}}_{\boldsymbol{k}'} = V_{\boldsymbol{k}\boldsymbol{k}'} \sum_{ss'} \frac{1 + s\hat{\boldsymbol{k}}\cdot\boldsymbol{\sigma}}{2} \frac{1 + s'\hat{\boldsymbol{k}}'\cdot\boldsymbol{\sigma}}{2} \left(\delta(\epsilon^s_{\boldsymbol{k}} - \epsilon^{s'}_{\boldsymbol{k}'}) - i\mathcal{P}\left(\frac{1}{\epsilon^s_{\boldsymbol{k}} - \epsilon^{s'}_{\boldsymbol{k}'}} \right) \right)$$

Green's function derivation

Generalized Kadanoff-Baym eq. $G^< = G^{\rm R}\Sigma^< G^{\rm A}$

two alternative kinetic equations

$$[i\partial_t - H_0, G^<] \;=\; \Sigma^{\rm R}G^< - G^<\Sigma^{\rm A} + \Sigma^<G^{\rm A} - G^{\rm R}\Sigma^< \qquad \text{('G1')}$$

$$[i\partial_t - H_0 - \mathrm{Re}\,\Sigma^{\rm R}, G^<] - [\Sigma^<, \mathrm{Re}\,G^{\rm R}] \;=\; i\{\mathrm{Im}\,\Sigma^{\rm R}, G^<\} - i\{\Sigma^<, \mathrm{Im}\,G^{\rm R}\} \qquad \text{('G2')}$$

The problem of Ansatz (from double-time to single-time)

$$G^<(x_1,t_1,x_2,t_2) \longrightarrow G^<|_{t_2=t_1} = \rho(x_1,x_2,t)$$

$$G^<(x,p,t,\omega) \;=\; \rho(x,p,t)A(x,p,t,\omega) \qquad \text{Kadanoff \& Baym (1962)}$$

(GKBA) $G^<(t_1,t_2) = iG^{\rm R}(t_1,t_2)\rho(t_2) - i\rho(t_1)G^{\rm A}(t_1,t_2)$ Lipavsky *et al.* (1986)

('AA') $G^<(t_1,t_2) = i\rho(t_1)G^{\rm R}(t_1,t_2) - iG^{\rm A}(t_1,t_2)\rho(t_2)$ Kailasvuori *et al.* (2009)

('SKBA') $G^<(t_1,t_2) = \frac{1}{2}A(t_1,t_2)\rho(t_2) + \frac{1}{2}\rho(t_1)A(t_1,t_2)$

Collision integrals with different structure

$$\mathcal{J}[\rho] = -\int \frac{\mathrm{d}\omega}{2\pi}(\ldots)$$

	G1	GKBA	$[V, G^{0\mathrm{R}}[V,\rho]G^{0\mathrm{A}}]$
QL &	G1	AA	$[V, [G^{0\mathrm{R}} V G^{0\mathrm{A}}, \rho]]$
	G1	SKBA	$\frac{1}{2}[V, G^{0\mathrm{R}}[V,\rho]G^{0\mathrm{A}}] + \frac{1}{2}[V, [G^{0\mathrm{R}} V G^{0\mathrm{A}}, \rho]]$
	G2	GKBA	$\frac{1}{2}[V, G^{0\mathrm{R}}[V,\rho]G^{0\mathrm{A}}] + \frac{1}{2}[V, [G^{0\mathrm{A}} V G^{0\mathrm{R}}, \rho]]$
	G2	AA	$\frac{1}{2}[V, G^{0\mathrm{A}}[V,\rho]G^{0\mathrm{R}}] + \frac{1}{2}[V, [G^{0\mathrm{R}} V G^{0\mathrm{A}}, \rho]]$
	G2	SKBA	$\frac{1}{2}(\mathrm{G2GKBA} + \mathrm{G2AA})$

Results

- Semiclassical kinetic approach with coherent bands.
- Role of principal value terms. One mechanism for a residual conductivity.
- Sensitivity to choice of approach. Related density matrix and Green's function approaches.

  Kailasvuori & Lüffe, JSTAT P06024 (2010)
  Kailasvuori, JSTAT P08004 (2009)

Related work: Auslender & Katsnelson, PRB76, 235425 (2007)
Trushin & Schliemann, PRL99, 216602 (2007) +...
Culcer & Winkler, PRB78, 235417 (2007) +...

- Input to the conductivity minimum problem.

  Trushin, Kailasvuori, Schliemann & MacDonald, arxiv:1002.4481