Conductivity of Chiral Particles

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Hamiltonian

We investigate the conductivity of chiral carriers with the winding number N_c and dispersion $E_k = \gamma k^{N_d}$ starting from the Hamiltonian

$$H_{\text{tot}} = H_0 + V_{\text{disorder}}, \qquad H_0 = \gamma k^{N_d} \begin{pmatrix} 0 & \exp(-iN_c\theta) \\ \exp(iN_c\theta) & 0 \end{pmatrix}, \tag{1}$$

where k is the absolute value of the particle wave vector, $\theta = \arctan(k_y/k_x)$, γ is a constant determined by the band parameters, and V_{disorder} represents the randomized δ-shaped impurity potential.

In the special case of $N_d = N_c$ the Hamiltonian describes the low energy behavior of carriers in chirally stacked multilayer graphene [1], but the general choice of $N_c \neq N_d$ makes it possible to distinguish the true pseudospin coherent conductivity contribution from the effects related to the change of the density of states.

The questions addressed

- What are the roles of the winding number N_c and the power of dispersion N_d in the conductivity behavior of chiral particles?
- What is the correct treatment for the collision integral in the Boltzmann equation for chiral particles?
- To which extent the Boltzmann equation together with the Born approximation are applicable to the pseudospin coherent conductivity description?

Methods

- The kinetic equation can be obtained from the Liouville-like equation for the density matrix ρ:

$$\frac{1}{\hbar}\left\{ e\mathbf{E}\frac{\partial \rho}{\partial \mathbf{k}} + i\,[H_0, \rho] \right\} = \mathrm{I}[\rho], \tag{2}$$

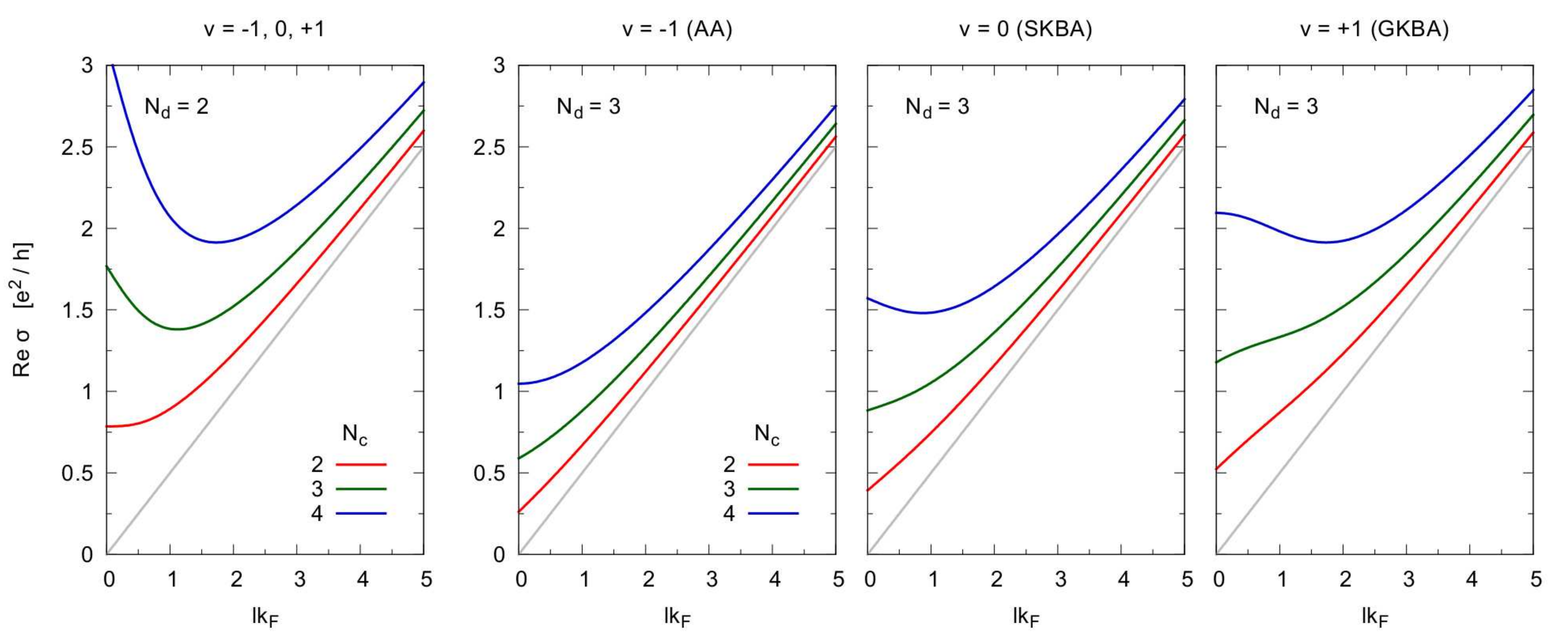
where $\mathrm{I}[\rho]$ is the collision integral whose form depends on the Ansatz involved [4]. It depends, in particular, on whether the Markov approximation is done in the interaction picture [2,3] $\mathrm{I}[\rho] = -\int_0^\infty d\tau [V_{\text{disorder}}, [\mathrm{e}^{-\frac{i}{\hbar}H_0\tau} V_{\text{disorder}} \mathrm{e}^{\frac{i}{\hbar}H_0\tau}, \rho]]$, or in the Schrödinger picture [5] $\mathrm{I}[\rho] = -\int_0^\infty d\tau [V_{\text{disorder}}, \mathrm{e}^{-\frac{i}{\hbar}H_0\tau}[V_{\text{disorder}}, \rho]\mathrm{e}^{\frac{i}{\hbar}H_0\tau}]$. This does not make a difference in the principle values of $\mathrm{I}[\rho]$ for the particles with the parabolic dispersion but does so in the case of $N_d \neq 2$.

- The finite-size Kubo formula [6] is utilized to prove the analytical outcomes

$$\sigma = -\frac{i\hbar e^2}{L^2} \sum_{n,n'} \frac{f^0_{E_n} - f^0_{E_{n'}}}{E_n - E_{n'}} \frac{\langle n|v_x|n'\rangle\langle n'|v_x|n\rangle}{E_n - E_{n'} + i\eta}, \tag{3}$$

where L^2 is the finite-size system area, η is the coupling to source and drain reservoirs, $\mathbf{v}$ is the velocity operator, $f^0_{E_n}$ is the Fermi-Dirac distribution function, and $|n\rangle$ denotes an exact eigenstate of the numerically solved Schrödinger equation $H_{\text{tot}}\psi_n = E_n\psi_n$. The zero-temperature conductivity curves are smoothed by averaging over several hundreds of disorder potential realizations.

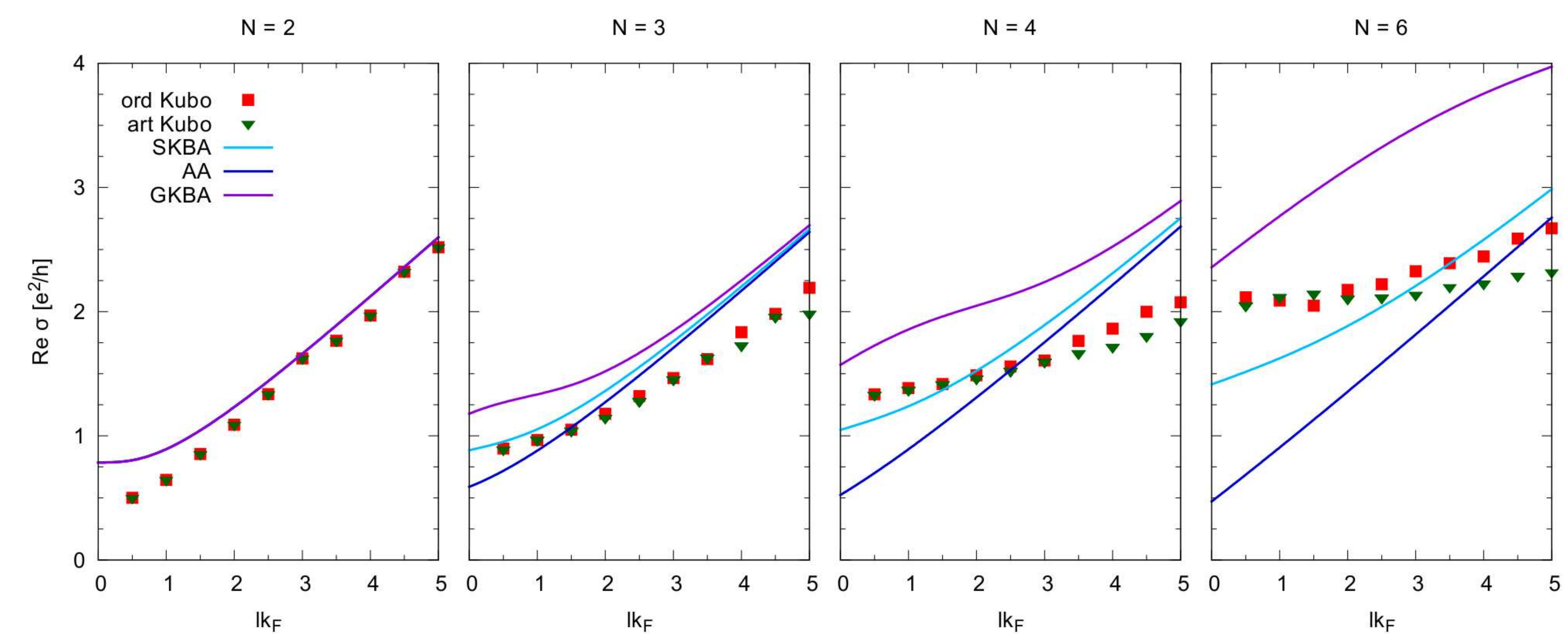
Analytical results



$$\sigma = \frac{e^2}{h}\left(\frac{k_F l}{2} + \frac{N_c^2}{8(N_d - 1)}\left[\frac{\pi}{2} - \operatorname{atan}\left(\frac{2k_F l}{N_d} - \nu\cot\frac{\pi}{N_d} \right) \right] \right), \quad N_d > 1, \tag{4}$$

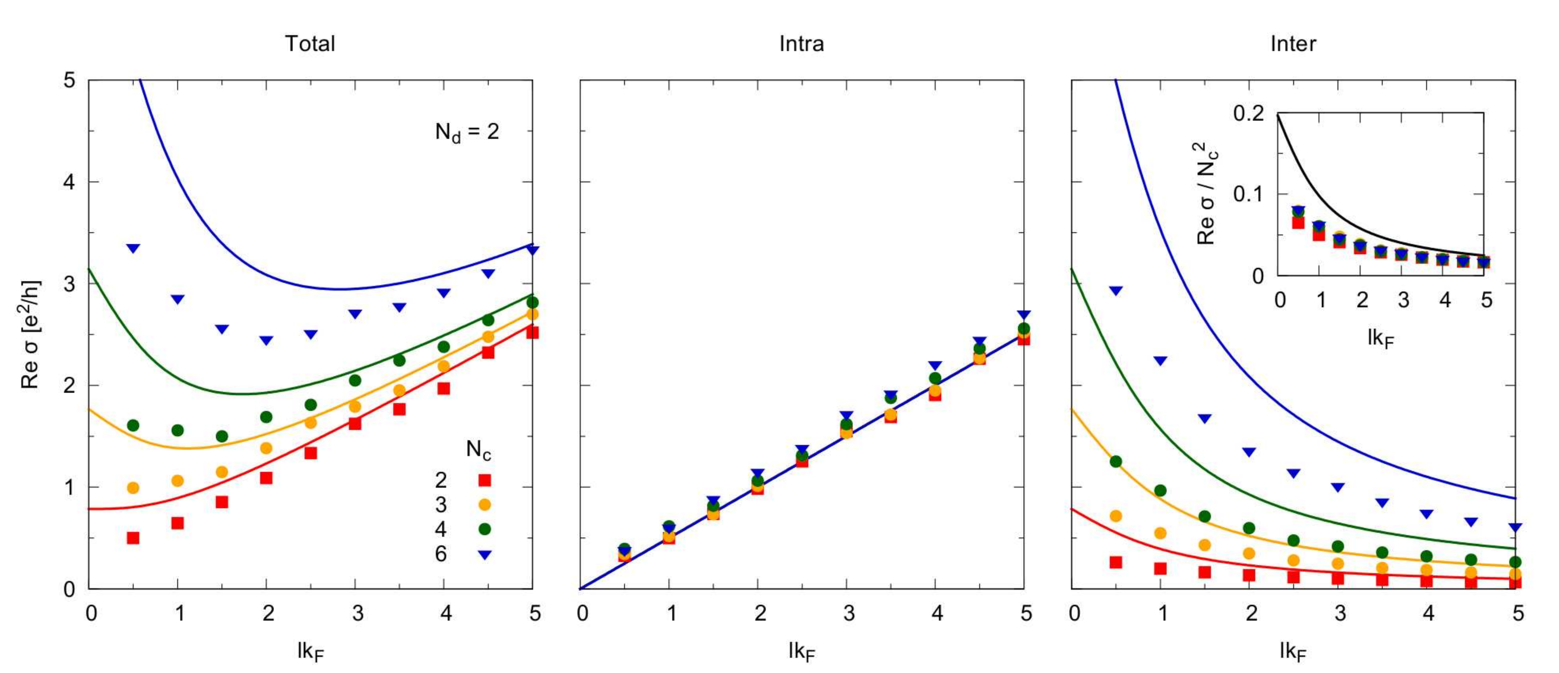
where k_F is the Fermi wave vector, l is the mean free path, and ν may acquire the values ± 1, 0 and characterizes the way how the intrinsically inelastic principle value terms in the collision integral are treated. The gray line represents the pseudospin incoherent Drude conductivity $\frac{e^2}{h}\frac{k_F l}{2}$.

Numerical vs. analytical conductivity curves, $N_c = N_d = N$



The numerical *dc* conductivity can be obtained from Eq. (3) by extracting the limit in which the system size first approaches ∞, and then η approaches zero maintaining a value larger than the typical level spacing δE. The finite value of η can be understood as representing energy uncertainty due to the finite lifetime of electrons in a system coupled to source and drain reservoirs. The scattering potential is chosen to be weak enough to make the Born approximation valid. The analytical curve in the middle is closest to the numerically predicted one and corresponds to the case of $\nu = 0$ in Eq. (4) when the principle value collision integral terms are absent.

Intraband and interband conductivities for $N_d = 2$



To quantify the role of the pseudospin coherence we separate both velocity operators in Eq. (3) into intra-band and inter-band contributions and express the conductivity as the sum of intra-band ($\propto \mathbf{v}_{\pm\pm}\mathbf{v}_{\pm\pm}$), inter-band ($\propto \mathbf{v}_{\pm\mp}\mathbf{v}_{\mp\pm}$), and interference ($\propto \mathbf{v}_{\pm\pm}\mathbf{v}_{\pm\mp}$) terms. We find that the interference terms average to negligible values. The intra-band contribution does not depend on N_c and dominates in the higher carrier density Boltzmann transport regime, as expected. The inter-band contribution, in contrast, depends on N_c strongly and increases substantially near the neutrality point. The solid curves represent the corresponding analytical results (4) which all agree for $N_d = 2$.

Summary

- The increase of the chiral winding number N_c pushes up the pseudospin-coherent conductivity near the neutrality point, whereas the increase of the dispersion power N_d makes the conductivity lower. If $N_c = N_d = N$ (the case of chirally stacked multilayer graphene), then the conductivity increases with N.
- The principle value terms in the collision integral seem not to be a part of the correct derivation of the pseudospin-coherent Boltzmann equation. In an approach where they are present one does best in neglecting them.
- The pseudospin coherent Boltzmann approach together with the Born approximation work surprisingly well for the conductivity description of chiral particles at $N_d = 2$. At $N_d > 2$ the agreement between approximated and exact solutions is not that convincing. The case $N_d = 1$ is special, where the Born approximation seems to be unsuitable at all.

References

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