Quantum Fluid Models for Electron Transport in Graphene

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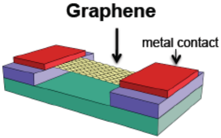
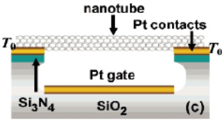
Graphene: the new frontier of nanoelectronics

Graphene is a new semiconductor material created in the first decade of this century by Geim and Novoselov. It has remarkable electronic properties which make it a candidate for the construction of new electronic devices with strongly increased performances with respect to the usual silicon semiconductors.



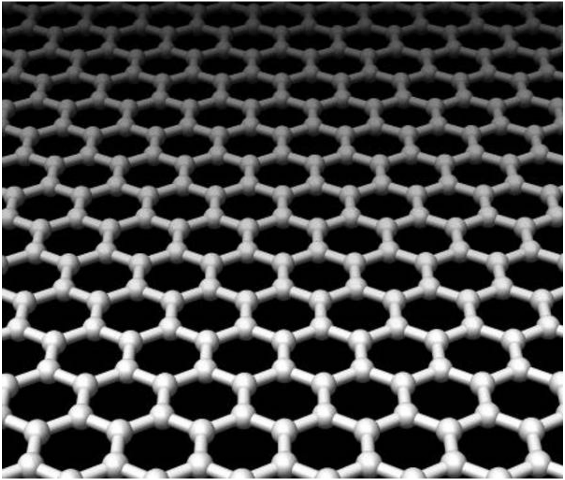
M. Freitag, nature nanotechnology **3**, 455 (2008).



D. Mann, et al.: J. Phys. Chem. B. **110,** 1502 (2005)

Graphene: the new frontier of nanoelectronics

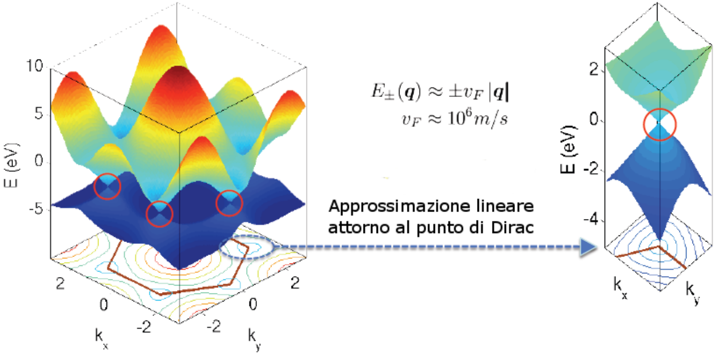
Physically speaking, graphene is a single layer of carbon atoms disposed as an honeycomb lattice, that is, a single sheet of graphite.



Graphene: the new frontier of nanoelectronics

Features of charge carriers in graphene:

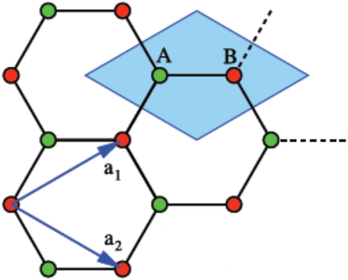
- Graphene is a zero-gap semiconductor, that is, the valence band of the energy spectrum intersects the conduction band in some isolated points, named *Dirac points*;
- around such points the energy of electrons is approximately proportional to the modulus of momentum: $E = \pm v_F |p|$.
  $\rightarrow$ **Relativistic massless** quasiparticles!



Graphene: the new frontier of nanoelectronics

Graphene cristal lattice is split into two nonequivalent sublattices.

- Charge carriers have a discrete degree of freedom, called pseudospin.
- Different from electron spin!



Graphene: the new frontier of nanoelectronics

Hamiltonian (low-energy approximation, zero potential):

$$H_0 = \mathrm{Op}_\hbar[v_F(p_1\sigma_1 + p_2\sigma_2)] = -i\hbar v_F \left(\sigma_1 \frac{\partial}{\partial x_1} + \sigma_2 \frac{\partial}{\partial x_2} \right);$$

- $v_F \approx 10^6 \, \mathrm{m/s}$ is the Fermi speed;
- $\hbar$ denotes the reduced Planck constant;
- σ_1, σ_2 are Pauli matrices:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

- $\mathrm{Op}_\hbar$ is the Weyl quantization: given a symbol $\gamma = \gamma(x, p)$,

$$(\mathrm{Op}_\hbar(\gamma)\psi)(x) = (2\pi\hbar)^{-2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \gamma\left(\frac{x+y}{2}, p \right) \psi(y) e^{i(x-y)\cdot p/\hbar} \, dydp\,,$$

for all $\psi \in L^2(\mathbb{R}^2, \mathbb{C})$.

A kinetic model for graphene

Goal: Derive and study several fluid models for quantum transport of electrons in graphene.

Fluid models derived from kinetic models $\equiv$ Wigner equations.

$w = w(x, p, t)$ system Wigner function.

Spinorial system $\Rightarrow$ w is **not** a scalar function!

$w(x, p, t)$ is, for all (x, p, t), a complex hermitian 2×2 matrix.

Serious computational difficulties!

However, we can write it in the Pauli basis: $w = \sum_{s=0}^{3} w_s \sigma_s$, with $w_s(x, p, t)$ suitable *real* scalar functions.

Collisionless Wigner equations for graphene

Wigner equations for quantum transport in graphene, derivated from the Von Neumann equation with the one-particle Hamiltonian $H_0 + V$:[1]

$$\begin{aligned} \partial_t w_0 + v_F \vec{\nabla} \cdot \vec{w} + \Theta_\hbar(V) w_0 &= 0\,, \\ \partial_t \vec{w} + v_F \left[\vec{\nabla} w_0 + \frac{2}{\hbar} \vec{w} \wedge \vec{p} \right] + \Theta_\hbar(V) \vec{w} &= 0\,, \end{aligned} \qquad \text{(W0)}$$

where $\vec{w} \equiv (w_1, w_2, w_3)$ and:

$$(\Theta_\hbar(V) w)(x,p) =$$
$$\frac{i}{\hbar}(2\pi)^{-2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \left[V\left(x + \frac{\hbar}{2}\xi \right) - V\left(x - \frac{\hbar}{2}\xi \right) \right] w(x,p') e^{-i(p-p')\cdot\xi} d\xi dp'\,.$$

[1] For the derivation of (W0) see:
N. Zamponi and L. Barletti, *Quantum electronic transport in graphene: A kinetic and fluid-dynamic approach*;
N. Zamponi, *Some fluid-dynamic models for quantum electron transport in graphene via entropy minimization*.

Non-statistical closure: the pure state case

A first fluid-dynamic model can be derived from the Wigner equations under the hypothesis of pure state:

$$\rho_{ij}(x,y) = \psi_i(x)\overline{\psi_j(y)} \qquad (i,j = 1,2)\,,$$

where ρ is the system density matrix, while ψ is the wavefunction.

Non-statistical closure: the pure state case

Let us consider the following moments, for $k = 1,2$, $s = 1,2,3$:

$$n_0 = \int w_0\, dp \qquad \text{charge density,}$$

$$n_s = \int w_s\, dp \qquad \text{pseudospin density,}$$

$$J_k = \int p_k w_0\, dp \qquad \text{pseudomomentum current,}$$

$$t_{sk} = \int p_k w_s\, dp \qquad \text{pseudospin currents.}$$

By taking moments of the Wigner equations it is easy to find the following system of not-closed fluid equations:

$$\partial_t n_0 + v_F \partial_j n_j = 0\,,$$

$$\partial_t n_s + v_F \partial_s n_0 + \frac{2v_F}{\hbar}\eta_{sij} t_{ij} = 0 \qquad (s = 1,2,3)\,,$$

$$\partial_t J_k + v_F \partial_s t_{sk} + n_0 \partial_k V = 0 \qquad (k = 1,2)\,.$$

Non-statistical closure: the pure state case

From the pure state hypothesis it follows:

$$\begin{aligned} n_0 t_{sk} &= n_s J_k - \frac{\hbar}{2}\eta_{s\alpha\beta} n_\alpha \partial_k n_\beta \qquad (k = 1, 2,\ s = 1, 2, 3)\,, \\ n_0 &= |\vec{n}| = \sqrt{n_1^2 + n_2^2 + n_3^2}\,. \end{aligned}$$

So we found the following pure-state fluid model ($\sim$ Madelung equations for a quantum particle described by the Hamiltonian H_0):

$$\begin{aligned} &\partial_t n_0 + v_F \vec{\nabla} \cdot \vec{n} = 0\,, \\ &\partial_t \vec{n} + v_F \vec{\nabla} n_0 + \frac{2v_F}{\hbar}\frac{\vec{n}\wedge\vec{J}}{n_0} + \frac{v_F}{n_0}(\vec{\nabla}\cdot\vec{n} - \vec{n}\cdot\vec{\nabla})\vec{n} = 0\,, \\ &\partial_t \vec{J} + v_F \vec{\nabla}\cdot\left(\frac{\vec{J}\otimes\vec{n}}{n_0}\right) - \frac{v_F\hbar}{2}\partial_s\left(\frac{1}{n_0}\eta_{sij} n_i \vec{\nabla} n_j\right) + n_0\vec{\nabla} V = 0\,. \end{aligned}$$

$\rightarrow$ The first equation in redundant!

Beyond the pure state assumption

Goal: Derive several models not based on the pure state hypothesis.

Statistical closure: close the fluid equations by means of an equilibrium distribution obtained as a minimizer of a suitable quantum entropy functional.

Problem: Which statistics should we choose?

Since the energy spectrum of H_0 is not bounded from below, Fermi-Dirac statistics would be more adequate to describe quantum electron transport in this material, rather than Maxwell-Boltzmann's one; neverthless, we used in our work the Maxwell-Boltzmann statistics, for the sake of simplicity and to obtain explicit models, at the price of a modification of the hamiltonian operator H_0:

$$H = \mathrm{Op}_\hbar\left[v_F(p_1\sigma_1 + p_2\sigma_2) + \frac{|p|^2}{2m}\sigma_0\right] = H_0 - \sigma_0\frac{\hbar^2}{2m}\Delta\,,$$

with $m > 0$ parameter (with the dimensions of a mass).

Collisional Wigner equations

Wigner equations for quantum transport in graphene, derivated from the Von Neumann equation with the one-particle Hamiltonian $H + V$, with a collisional term of BGK type:

$$\begin{aligned} \partial_t w_0 + \left[\frac{\vec{p}}{m} \cdot \vec{\nabla}\right] w_0 + v_F \vec{\nabla} \cdot \vec{w} + \Theta_\hbar(V) w_0 &= \frac{g_0 - w_0}{\tau_c} \,, \\ \partial_t \vec{w} + \left[\frac{\vec{p}}{m} \cdot \vec{\nabla}\right] \vec{w} + v_F \left[\vec{\nabla} w_0 + \frac{2}{\hbar} \vec{w} \wedge \vec{p}\right] + \Theta_\hbar(V) \vec{w} &= \frac{\vec{g} - \vec{w}}{\tau_c} \,. \end{aligned} \tag{W}$$

Here:

- g is the thermal equilibrium distribution;
- τ_c is the relaxation time.

Different scalings of the Wigner equations

Isothermal system: thermal equilibrium with phonon bath at constant temperature T.

Two different scalings of the collisional Wigner equations (W):

- a diffusive scaling;
- an hydrodynamic scaling.

Diffusive scaling of the Wigner equations

Diffusive scaling:

$$x \mapsto \hat{x}x\,, \quad t \mapsto \hat{t}t\,, \quad p \mapsto \hat{p}p\,, \quad V \mapsto \hat{V}V\,,$$

with $\hat{x}$, $\hat{t}$, $\hat{p}$, $\hat{V}$ satisfying:

$$\frac{2v_F\hat{p}}{\hbar} = \frac{\hat{V}}{\hat{x}\hat{p}}\,, \quad \frac{2\hat{p}v_F\tau_c}{\hbar} = \frac{\hbar}{2\hat{p}v_F\hat{t}}\,, \quad \hat{p} = \sqrt{mk_BT}\,;$$

we define the *semiclassical parameter* ϵ, the *diffusive parameter* τ and the *scaled Fermi speed* c as:

$$\epsilon = \frac{\hbar}{\hat{x}\hat{p}}\,, \quad \tau = \frac{2\hat{p}v_F\tau_c}{\hbar}\,, \quad c = \sqrt{\frac{mv_F^2}{k_BT}}\,.$$

Finally let $\gamma = c/\epsilon$.

Different scalings of the Wigner equations

Collisional Wigner equations under diffusive scaling:

$$\tau \partial_t w_0 + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{w} + \Theta_\epsilon[V] w_0 = \frac{g_0 - w_0}{\tau}\,,$$

$$\tau \partial_t \vec{w} + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} \vec{w} + \frac{\epsilon}{2}\vec{\nabla} w_0 + \Theta_\epsilon[V]\vec{w} + \vec{w}\wedge\vec{p} = \frac{\vec{g} - \vec{w}}{\tau}\,, \qquad \text{(WD)}$$

where:

$$(\Theta_\epsilon(V)w)(x,p) = \frac{i}{\epsilon}(2\pi)^{-2}\int_{\mathbb{R}^2\times\mathbb{R}^2} \delta\tilde{V}(x,\xi) w(x,p') e^{-i(p-p')\cdot\xi} d\xi dp'\,,$$

$$\delta\tilde{V}(x,\xi) = V\left(x + \frac{\epsilon}{2}\xi\right) - V\left(x - \frac{\epsilon}{2}\xi\right).$$

Hydrodynamic scaling of the Wigner equations

Hydrodynamic scaling:

$$x \mapsto \hat{x}x\,, \quad t \mapsto \hat{t}t\,, \quad p \mapsto \hat{p}p\,, \quad V \mapsto \hat{V}V\,,$$

with $\hat{x}$, $\hat{t}$, $\hat{p}$, $\hat{V}$ satisfying:

$$\frac{1}{\hat{t}} = \frac{2v_F\hat{p}}{\hbar} = \frac{\hat{V}}{\hat{x}\hat{p}}\,, \quad \hat{p} = \sqrt{mk_BT}\,;$$

we define the *semiclassical parameter* ϵ, the *hydrodynamic parameter* τ and the *scaled Fermi speed* as:

$$\epsilon = \frac{\hbar}{\hat{x}\hat{p}}\,, \quad \tau = \frac{\tau_c}{\hat{t}}\,, \quad c = \sqrt{\frac{mv_F^2}{k_BT}}\,.$$

Again let $\gamma = c/\epsilon$.

Hydrodynamic scaling of the Wigner equations

Collisional Wigner equations under hydrodynamic scaling:

$$\begin{aligned} \partial_t w_0 + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{w} + \Theta_\epsilon[V]w_0 &= \frac{g_0 - w_0}{\tau}\,, \\ \partial_t \vec{w} + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{w} + \frac{\epsilon}{2}\vec{\nabla} w_0 + \vec{w}\wedge\vec{p} + \Theta_\epsilon[V]\vec{w} &= \frac{\vec{g}-\vec{w}}{\tau}\,. \end{aligned} \tag{WH}$$

where (again):

$$\begin{aligned} (\Theta_\epsilon(V)w)(x,p) &= \frac{i}{\epsilon}(2\pi)^{-2}\int_{\mathbb{R}^2\times\mathbb{R}^2} \delta\tilde{V}(x,\xi)w(x,p')e^{-i(p-p')\cdot\xi}d\xi dp'\,, \\ \delta\tilde{V}(x,\xi) &= V\left(x+\frac{\epsilon}{2}\xi\right) - V\left(x-\frac{\epsilon}{2}\xi\right). \end{aligned}$$

Different scalings of the Wigner equations

Two main assumptions:

1. The *semiclassical hypothesis*:

$$\epsilon \ll 1\,;$$

2. The *Low Scaled Fermi Speed* (LSFS):

$$c \sim \epsilon\,.$$

As a consequence: $\gamma = c/\epsilon \sim 1$.

Equilibrium distribution through MEP

Minimum Entropy Principle (MEP):

> Given a quantum system, we define the equilibrium distribution associated to the system as the minimizer of a suitable quantum entropy functional under the constraints of given fluid-dynamic moments.

Quantum Entropy Functional (actually the *free energy*):

$$\mathscr{A}(S) = \mathrm{Tr}[S \log S - S + H/k_B T]\,,$$

defined for $S \in \mathcal{D}(\mathscr{A})$ suitable subset of the set of the density operators associated to the system.

Equilibrium distribution through MEP

Let now:

- $\left\{\mu_0^{(k)}(p)\right\}_{k=1\ldots N}$, $\left\{\mu_s^{(k)}(p)\right\}_{s=1,2,3,\ k=1\ldots N}$ real functions of $p \in \mathbb{R}^2$;
- $\left\{M^{(k)}(x)\right\}_{k=1\ldots N}$ real functions of $x \in \mathbb{R}^2$;
- $\mu^{(k)} \equiv \mu_0^{(k)}(p)\sigma_0 + \mu_s^{(k)}\sigma_s$, for $k = 1 \ldots N$.

We define the *equilibrium distribution at thermal equilibrium* g associated to the moments $\left\{M^{(k)}\right\}_{k=1\ldots N}$ as the Wigner transform $g \equiv \mathcal{W}G$ of the solution of the constrained minimization problem:

$$\mathscr{A}(G) = \min \Big\{ \mathscr{A}(S) \ : \ S = \mathrm{Op}(w) \in \mathcal{D}(\mathscr{A}) \, ,$$

$$\mathrm{tr} \int \mu^{(k)}(p) w(x,p)\, dp = M^{(k)}(x) \, , \quad k = 1 \ldots N \, , \ x \in \mathbb{R}^2 \Big\} .$$

Equilibrium distribution through MEP

This problem can be solved formally by means of Lagrange multipliers.

Solution as a density operator:

$$G = \exp(-H + \mathrm{Op}(\mu^{(k)}(p)\hat{\xi}^{(k)}(x)))\,.$$

Solution as a Wigner function:

$$g = \mathcal{E}\mathrm{xp}(-\hat{h}[\hat{\xi}])\,, \quad \hat{h}[\hat{\xi}] = \mathrm{Op}^{-1}H - \mu^{(k)}(p)\hat{\xi}^{(k)}(x)\,.$$

Here $\mathcal{E}\mathrm{xp}$ is the so-called *quantum exponential*, defined by:

$$\mathcal{E}\mathrm{xp}(w) \equiv \mathrm{Op}^{-1}(\exp(\mathrm{Op}(w)))\,, \qquad \forall w \text{ Wigner function.}$$

Semiclassical expansion of the quantum exponential

Goal: find an explicit approximation of the quantum exponential of an arbitrary classical symbol with linear ϵ-dependence:

$$g_\epsilon(\beta) = \mathcal{E}\mathrm{xp}_\epsilon(\beta(a + \epsilon b)), \qquad \beta \in \mathbb{R},$$

with $a = a_0\sigma_0 + \vec{a} \cdot \vec{\sigma}$, $b = b_0\sigma_0 + \vec{b} \cdot \vec{\sigma}$ arbitrary classical symbols.

Moyal product between arbitrary classical symbols f_1, f_2:

$$f_1 \#_\epsilon f_2 = \mathrm{Op}_\epsilon^{-1}(\mathrm{Op}_\epsilon(f_1)\mathrm{Op}_\epsilon(f_2)).$$

Semiclassical expansion of the quantum exponential

Semiclassical expansion of the Moyal product:

$$\#_\epsilon = \sum_{n=0}^{\infty} \epsilon^n \#^{(n)} ,$$

$$f_1 \#^{(0)} f_2 = f_1 f_2 ,$$

$$f_1 \#^{(1)} f_2 = \frac{i}{2} \left(\partial_{x_s} f_1 \partial_{p_s} f_2 - \partial_{p_s} f_1 \partial_{x_s} f_2 \right) ,$$

$$f_1 \#^{(2)} f_2 = -\frac{1}{8} \left(\partial^2_{x_j x_s} f_1 \partial^2_{p_j p_s} f_2 - 2\partial^2_{x_j p_s} f_1 \partial^2_{p_j x_s} f_2 + \partial^2_{p_j p_s} f_1 \partial^2_{x_j x_s} f_2 \right) ,$$

$$\ldots$$

Semiclassical expansion of the quantum exponential

Let us differentiate with respect to β the function $g_\epsilon(\beta)$:

$$\partial_\beta g_\epsilon(\beta) = \frac{1}{2}((a+\epsilon b)\#_\epsilon g_\epsilon(\beta) + g_\epsilon(\beta)\#_\epsilon(a+\epsilon b)),$$
$$g_\epsilon(0) = \sigma_0 .$$

Expansion in powers of ϵ:

$$\partial_\beta g^{(0)}(\beta) = \frac{1}{2}(g^{(0)}(\beta)a + a g^{(0)}(\beta)),$$
$$g^{(0)}(0) = \sigma_0 ,$$

$$\partial_\beta g^{(1)}(\beta) = \frac{1}{2}(g^{(1)}(\beta)a + a g^{(1)}(\beta)) + \frac{1}{2}(g^{(0)}(\beta)b + b g^{(0)}(\beta))$$
$$+ \frac{1}{2}(g^{(0)}(\beta)\#^{(1)} a + a\#^{(1)} g^{(0)}(\beta)),$$
$$g^{(1)}(0) = 0 .$$

→ Hierarchy of ODE: first solve eq. for $g^{(0)}(\beta)$, then eq. for $g^{(1)}(\beta)$.

Semiclassical expansion of the quantum exponential

$$g_0^{(0)}(\beta) = e^{\beta a_0} \cosh(\beta|\vec{a}|)\,, \qquad \vec{g}^{(0)}(\beta) = e^{\beta a_0} \sinh(\beta|\vec{a}|)\frac{\vec{a}}{|\vec{a}|}\,,$$

$$g_0^{(1)}(\beta) = \beta e^{\beta a_0} \left(\cosh(\beta|\vec{a}|) b_0 + \sinh\left(\beta|\vec{a}|\right) \frac{\vec{a}\cdot\vec{b}}{|\vec{a}|} \right) + \beta e^{\beta a_0} \frac{\sinh(\beta|\vec{a}|) - \beta|\vec{a}|\cosh(\beta|\vec{a}|)}{4\beta|\vec{a}|^3} \eta_{jks}\{a_j, a_k\} a_s\,,$$

$$\vec{g}^{(1)}(\beta) = \beta e^{\beta a_0} \left[\sinh(\beta|\vec{a}|) \left(b_0 - \frac{\eta_{jks}\{a_j, a_k\}a_s}{4|\vec{a}|^2} \right) + \cosh\left(\beta|\vec{a}|\right) \frac{\vec{a}\cdot\vec{b}}{|\vec{a}|} \right] \frac{\vec{a}}{|\vec{a}|} + \beta e^{\beta a_0} \frac{\sinh(\beta|\vec{a}|)}{\beta|\vec{a}|} \left(\frac{\vec{a}\wedge\vec{b}}{|\vec{a}|} \right) \wedge \frac{\vec{a}}{|\vec{a}|} + + \beta e^{\beta a_0} \frac{\sinh(\beta|\vec{a}|)}{2|\vec{a}|^2} a_j\{a_j, \vec{a}\} \wedge \frac{\vec{a}}{|\vec{a}|} + \beta e^{\beta a_0} \frac{\beta|\vec{a}|\cosh(\beta|\vec{a}|) - \sinh(\beta|\vec{a}|)}{2\beta|\vec{a}|^2} \{a_0, \vec{a}\} \wedge \frac{\vec{a}}{|\vec{a}|}\,.$$

Fluid models

Fluid models for quantum electron transport in graphene:

- **two-band models**:
  - first order two-band hydrodynamic model;
  - first order two-band diffusive model;
  - second order two-band diffusive model;
- **spinorial models**:
  - first order spinorial hydrodynamic model;
  - second order spinorial hydrodynamic model;
  - first order spinorial diffusive model;
  - first order spinorial diffusive model with pseudo-magnetic field.

Two-band models

We will consider moments of this type:

$$m_k = \int \mu_k(p) \left(w_0(r,p) \pm \frac{\vec{p}}{|\vec{p}|} \cdot \vec{w}(r,p) \right) dp \qquad k = 1 \dots n\,,$$

with $\{\mu_k \,: \mathbb{R}^2 \to \mathbb{R} \mid k = 1 \dots n\}$ suitable functions of p, and $n \in \mathbb{N}$ given.

The functions:

$$w_\pm(r,p) \equiv w_0(r,p) \pm \frac{\vec{p}}{|\vec{p}|} \cdot \vec{w}(r,p)$$

are the distribution functions of the two bands (w_+ is related to the conduction band, w_- is related to the valence band).

Two-band hydrodynamic model

Now we present a hydrodynamic model for quantum transport of electrons in graphene with two-band structure. This model will be obtained by computing moments of the Wigner equations (WH) and making a semiclassical expansion of the equilibrium distribution g appearing in Eqs. (WD).

Moments:

$$n_\pm(x) = \int w_\pm(x,p)\,dp\,, \qquad J^k_\pm(x) = \int p^k w_\pm(x,p)\,dp \quad (k = 1, 2)\,.$$

- The moments $n_\pm$ are the so-called *band densities*, and measure the contribution of each band to the charge density $n_0 = (n_+ + n_-)/2$.
- The moments $J^1_\pm$, $J^2_\pm$ are the cartesian components of the *band currents*: they measure the contribution of each band to the current $J = (J^1_+ + J^1_-, J^2_+ + J^2_-)$.

Two-band hydrodynamic model

The (scaled) equilibrium distribution has the following form:

$$g[n_+, n_-, J_+, J_-] = \mathcal{E}\mathrm{xp}(-h_\xi)\,,$$

$$h_\xi = \left(\frac{|p|^2}{2} + A_0 + A_1 p_1 + A_2 p_2\right)\sigma_0 + (c|p| + B_0 + B_1 p_1 + B_2 p_2)\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,,$$

where $A_j = A_j(x)$, $B_j = B_j(x)$ $(j = 0, 1, 2)$ have to be determined in such a way that:

$$\int g_\pm[n_+, n_-, J_+, J_-](x, p)\,dp = n_\pm(x) \qquad x \in \mathbb{R}^2\,,$$

$$\int p^k g_\pm[n_+, n_-, J_+, J_-](x, p)\,dp = J^k_\pm(x) \qquad x \in \mathbb{R}^2\,,\ k = 1, 2\,.$$

Fully quantum two-band hydrodynamic model.

The following proposition holds:

Proposition

Let $n^{\tau}_{\pm}$, $\vec{J}^{\tau}_{\pm}$ the moments of a solution w^{τ} of Eqs. (WH), and let $g = g[n^{\tau}_{+}, n^{\tau}_{-}, J^{\tau}_{+}, J^{\tau}_{-}]$. If $n^{\tau}_{\pm} \to n_{\pm}$, $\vec{J}^{\tau}_{\pm} \to \vec{J}_{\pm}$ as $\tau \to 0$ for suitable functions $n_{\pm}$, $\vec{J}_{\pm}$, then the limit moments $n_{\pm}$, $\vec{J}_{\pm}$ satisfy:

$$\partial_t n_{\pm} + \partial_k \left\{ \frac{1}{2\gamma} J^k_{\pm} + \frac{\epsilon}{2} \int g_k \pm \frac{p_k}{|\vec{p}|} g_0 \, dp \right\} \pm \int \frac{p_k}{|\vec{p}|} \Theta_{\epsilon} g_k \, dp = 0 \, ,$$

$$\partial_t J^i_{\pm} + \partial_k \left\{ \frac{1}{2\gamma} \int p_i p_k g_{\pm} \, dp + \frac{\epsilon}{2} \int p_i \left(g_k \pm \frac{p_k}{|\vec{p}|} g_0 \right) dp \right\}$$

$$+ n_0 \partial_i V \pm \int \frac{p_i p_k}{|\vec{p}|} \Theta_{\epsilon} g_k \, dp = 0 \, , \qquad (i = 1, 2) \, .$$

Semiclassical expansion of the equilibrium

In order to obtain an explicit model, we make first-order approximation of the previous fluid equations with respect to the semiclassical parameter ϵ. So we perform a *semiclassical expansion* of the equilibrium distribution g through this strategy:

1. we compute a first order expansion of the quantum exponential in the *spinorial* case: $g = g^{(0)} + \epsilon g^{(1)}$;
2. we impose that the approximation we found satisfies the contraints:

$$\int (g_\pm^{(0)} + \epsilon g_\pm^{(1)})\, dp = n_\pm + O(\epsilon^2)\,, \quad \int p_i (g_\pm^{(0)} + \epsilon g_\pm^{(1)})\, dp = J_\pm^i + O(\epsilon^2)\,.$$

Semiclassical expansion of the equilibrium

$$g_\pm = \frac{n_\pm}{2\pi}\left[1 \pm \epsilon\left(F(u_\pm) - |p| + (p^k - u^k_\pm)\frac{\partial F}{\partial u_k}(u_\pm)\right)\right] e^{-|p-u_\pm|^2/2} + O(\epsilon^2)\,,$$

$$F(u) \equiv \int |p| e^{-|p-u|^2/2}\frac{dp}{2\pi} \qquad \forall u \in \mathbb{R}^2\,, \qquad u^k_\pm \equiv J^k_\pm / n_\pm \quad (k=1,2)\,;$$

$$\vec{g}^\perp \equiv \vec{g} - |p|^{-2}(\vec{g}\cdot\vec{p})\vec{p} = \epsilon|\vec{p}\,|^{-2}\,\vec{\Lambda}\wedge\vec{p} + O(\epsilon^2)\,,$$

$$\vec{\Lambda}(x,p) \equiv \frac{\sqrt{n_+ n_-}}{2\pi}\exp\left[-\frac{1}{2}\left(\left|\frac{\vec{u}_+ - \vec{u}_-}{2}\right|^2 + \left|p - \frac{u_+ + u_-}{2}\right|^2\right)\right]\vec{\Psi}(x,p)\,,$$

$$\vec{\Psi}(x,p) \equiv \left[\sinh\Phi + \frac{1-\cosh\Phi}{\Phi}\right]\vec{\nabla}_x\Phi + \left[\frac{\sinh\Phi}{\Phi} - \cosh\Phi\right]\vec{\nabla}_x\Xi\,,$$

$$\Xi(x,p) \equiv \frac{|\vec{u}_+|^2 + |\vec{u}_-|^2}{4} - \frac{1}{2}\log\left(\frac{n_+ n_-}{4\pi^2}\right) - \frac{\vec{u}_+ + \vec{u}_-}{2}\cdot\vec{p}\,,$$

$$\Phi(x,p) \equiv \frac{|\vec{u}_+|^2 - |\vec{u}_-|^2}{4} - \frac{1}{2}\log\left(\frac{n_+}{n_-}\right) - \frac{\vec{u}_+ - \vec{u}_-}{2}\cdot\vec{p}\,.$$

First-order two-band hydrodynamic model:

$$\partial_t n_\pm + \frac{1}{2\gamma}\partial_k J^k_\pm \pm \frac{\epsilon}{2}\partial_k \left(n_\pm \frac{\partial F}{\partial u_k}(u_\pm) \right)$$

$$\pm \epsilon \vec{\nabla}_x V \cdot \int \frac{[\vec{\Lambda}(x,p) - \vec{\Lambda}(x,-p)] \wedge \vec{p}}{2|p|^3}\, dp = 0\,,$$

$$\partial_t J^i_\pm + \frac{1}{2\gamma}\partial_k \Bigg\{ n_\pm (1 \pm \epsilon F(u_\pm))(\delta_{ik} + u^i_\pm u^k_\pm)$$

$$\pm \epsilon n_\pm \Bigg[(\delta_{ik} - u^i_\pm u^k_\pm) F(u_\pm) + u^i_\pm \frac{\partial F}{\partial u^k_\pm}(u_\pm)$$

$$- \frac{\partial^2 F}{\partial u^i_\pm \partial u^k_\pm}(u_\pm) - \delta_{ik} u^s_\pm \frac{\partial F}{\partial u^s_\pm}(u_\pm) \Bigg] \Bigg\}$$

$$\pm \frac{\epsilon}{2}\partial_k \left[n_\pm \left(\frac{\partial^2 F}{\partial u_i \partial u_k}(u_\pm) - u^k_\pm \frac{\partial F}{\partial u_i}(u_\pm) \right) \right]$$

$$+ n_\pm \partial_i V \pm \epsilon \vec{\nabla}_x V \cdot \int p^i \frac{\vec{\Lambda}(x,p) \wedge \vec{p}}{|\vec{p}|^3}\, dp = 0 \qquad (i = 1, 2)\,.$$

Two-band diffusive models

Now we present two diffusive models for quantum transport of electrons in graphene with two-band structure. These two models will be based on a Chapman-Enskog expansion of the Wigner distribution w and a semiclassical expansion of the equilibrium distribution g that appear in Eqs. (WD).

The moments we choose are the *band densities*:

$$n_\pm = \int w_\pm \, dp \,, \qquad w_\pm = w_0 \pm \frac{\vec{p}}{|p|} \cdot \vec{w} \,.$$

Two-band diffusive models

The (scaled) equilibrium distribution has the following form:

$$g[n_+, n_-] = \mathcal{E}\mathrm{xp}_\epsilon(-h_\xi)\,, \quad h_\xi = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + (c|p| + B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,,$$

where $A = A(x)$, $B = B(x)$ have to be determined in such a way that:

$$\int g_\pm[n_+, n_-](x,p)\,dp = n_\pm(x)\,, \qquad x \in \mathbb{R}^2\,.$$

The following (formal) result holds:

Theorem

Let n^τ_+, n^τ_- the moments of a solution $w = w^\tau$ of (WD), and let $g = g[n^\tau_+, n^\tau_-]$. Let us suppose that: $n^\tau_\pm \to n_\pm$ as $\tau \to 0$ for suitable functions n_+, n_-; then the limit moments n_+, n_- satisfy:

$$\partial_t n_\pm = \int (TTg[n_+, n_-])_\pm \, dp \,,$$

where:

$$\begin{aligned} Tw =& \sigma_0 T_0 w + \vec{\sigma} \cdot \vec{T} w \,, \\ T_0 w =& \frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{w} + \Theta_\epsilon[V] w_0 \,, \\ \vec{T} w =& \frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} \vec{w} + \frac{\epsilon}{2} \vec{\nabla} w_0 + \Theta_\epsilon[V] \vec{w} + \vec{w} \wedge \vec{p} \,. \end{aligned}$$

First order semiclassical expansion of equilibrium

First order semiclassical expansion of the equilibrium distribution g:

$$g_0[n_+, n_-] = \frac{e^{-|\vec{p}|^2/2}}{2\pi} \left\{ n_0 + \epsilon\gamma \left(\sqrt{\frac{\pi}{2}} - |\vec{p}| \right) n_\sigma \right\} + O(\epsilon^2) \,,$$

$$\vec{g}[n_+, n_-] = \frac{e^{-|\vec{p}|^2/2}}{2\pi} \left\{ \left[n_\sigma + \epsilon\gamma \left(\sqrt{\frac{\pi}{2}} - |\vec{p}| \right) n_0 \right] \frac{\vec{p}}{|\vec{p}|} + \epsilon \vec{F} \wedge \frac{\vec{p}}{|\vec{p}|^2} \right\} + O(\epsilon^2) \,,$$

with:

$$n_0 \equiv \frac{1}{2}(n_+ + n_-) \qquad \text{charge density,}$$

$$n_\sigma \equiv \frac{1}{2}(n_+ - n_-) \qquad \text{pseudo-spin polarization,}$$

$$\vec{F} \equiv \frac{1}{2}\vec{\nabla}_x n_0 - \frac{n_\sigma \vec{\nabla}_x n_0 + \left[\sqrt{n_0^2 - n_\sigma^2} - n_0 \right] \vec{\nabla}_x n_\sigma}{\left[\log(n_0 + n_\sigma) - \log(n_0 - n_\sigma) \right] \sqrt{n_0^2 - n_\sigma^2}} \,.$$

First order two-band diffusive model

First order two-band diffusive model:

$$
\begin{aligned}
\partial_t n_0 =& \frac{1}{4\gamma^2}\Delta\left(n_0 + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_\sigma\right) + \frac{1}{2\gamma}\vec{\nabla}\cdot\left(n_0\vec{\nabla}V\right) + O(\epsilon^2)\,,\\
\partial_t n_\sigma =& \frac{1}{4\gamma^2}\Delta\left(n_\sigma + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_0\right) + \frac{1}{2\gamma}\vec{\nabla}\cdot\left[\left(n_\sigma + \frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}\,n_0\right)\vec{\nabla}V\right]\\
& - \frac{\epsilon}{2\gamma}\sqrt{\frac{\pi}{2}}\vec{\nabla}V\cdot\left[\vec{\nabla}\wedge\vec{F} + \gamma\vec{F}\right] + \frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\vec{\nabla}n_0\cdot\vec{\nabla}V\\
& + \frac{|\vec{\nabla}V|^2}{2}\left[\left(n_\sigma + \epsilon\gamma\sqrt{\frac{\pi}{2}}n_0\right)\Gamma + \epsilon\gamma\sqrt{\frac{\pi}{2}}n_0\right] + O(\epsilon^2)\,,\\
\Gamma \equiv& \int_0^\infty e^{-\rho^2/2}\rho\log\rho\,d\rho > 0\,.
\end{aligned}
$$

Second order two-band diffusive model: assumptions

We are going to derive another diffusive model for quantum transport in graphene.

- Exploit the Wigner equations in diffusive scaling (WD).
- Same fluid-dynamic moments $n_\pm$ of the Wigner distribution w.
- Same equilibrium distribution.
- ▶ Stronger assumptions than (LSFS): consider also $O(\epsilon^2)-$terms in the fluid equations.

Second order two-band diffusive model: assumptions

Assumptions:

- semiclassical hypothesis $\epsilon \ll 1$;
- *Strongly Mixed State* hypothesis (SMS):

$$c \sim \epsilon\,, \qquad B = O(\epsilon)\,.$$

Remember that:

$$g[n_+, n_-] = \mathcal{E}\mathrm{xp}(-h_\xi)\,, \quad h_\xi = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + (c|p| + B)\frac{\vec{p}}{|p|}\cdot\vec{\sigma}\,,$$

$$\int g_\pm[n_+, n_-](x,p)\,dp = n_\pm(x) \qquad x \in \mathbb{R}^2\,.$$

These further assumptions are necessary to overcome the computational difficulties arising from the spinorial nature of the problem: without these hypothesis, it would be hard to compute the second order expansion of the equilibrium distribution.

Second order two-band diffusive model: assumptions

- Consequence on the choice of moments:

$$\left| \frac{n_+ - n_-}{n_+ + n_-} \right| = \left| \frac{n_\sigma}{n_0} \right| = O(\epsilon)\,.$$

- Decoupling of h_ξ in a scalar part of order 1 and a spinorial perturbation of order ϵ; this fact will be very useful in computations.

Second order two-band diffusive model: semiclassical expansion of equilibrium

Now let us define, for an arbitrary positive scalar function $n(x)$:

$$\mathcal{M}_\epsilon[n] \equiv \frac{n}{2\pi} e^{-|p|^2/2} \left[1 + \frac{\epsilon^2}{24} \vec{\nabla} \cdot \Big((\sigma_0 - \vec{p} \otimes \vec{p}) \vec{\nabla} \log n \Big) \right] \; ;$$

then the equilibrium distribution has this semiclassical expansion:

$$\begin{aligned} g_\epsilon[n_+, n_-] = & \mathcal{M}_\epsilon \left[n_0 - \frac{n_0}{2} \left(\left(2 - \frac{\pi}{2} \right) \epsilon^2 \gamma^2 + \frac{n_\sigma^2}{n_0^2} \right) \right] \sigma_0 \\ & + \frac{n_0}{2\pi} e^{-|p|^2/2} \left[\epsilon\gamma \left(\sqrt{\frac{\pi}{2}} - |p| \right) + \frac{n_\sigma}{n_0} \right] \frac{\vec{p}}{|p|} \cdot \vec{\sigma} \\ & + \frac{n_0}{4\pi} e^{-|p|^2/2} \left[\epsilon\gamma \left(\sqrt{\frac{\pi}{2}} - |p| \right) + \frac{n_\sigma}{n_0} \right]^2 \sigma_0 + O(\epsilon^3) \, . \end{aligned}$$

Exploiting this expansion and the fully quantum two-band diffusive equations, we obtain:

Second order two-band diffusive model:

$$
\begin{aligned}
\partial_t n_0 =& \frac{\Delta}{4\gamma^2}\left[\left(1+\epsilon^2\gamma^2\frac{\pi}{4}\right)n_0+\frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_\sigma\right]+\frac{\vec{\nabla}}{2\gamma}\cdot\left(n_0\vec{\nabla}(V+V_B)\right)+O(\epsilon^3)\,,\\
\partial_t n_\sigma =& \frac{\Delta}{4\gamma^2}\left[\frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}n_0+n_\sigma\right]+\frac{\vec{\nabla}}{2\gamma}\cdot\left[\left(n_\sigma+\frac{\epsilon\gamma}{2}\sqrt{\frac{\pi}{2}}\,n_0\right)\vec{\nabla}V\right]\\
&+\frac{\epsilon}{4}\sqrt{\frac{\pi}{2}}\,\vec{\nabla}n_0\cdot\vec{\nabla}V+\frac{|\nabla V|^2}{2}\left\{\epsilon\gamma\sqrt{\frac{\pi}{2}}(1+\Gamma)n_0+\Gamma n_\sigma\right\}+O(\epsilon^3)\,.
\end{aligned}
$$

where V_B is (up to a constant) the so-called *Bohm potential*:

$$
V_B = -\frac{1}{2\gamma}\frac{\epsilon^2}{6}\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\,.
$$

Spinorial models

Now we will derive two spinorial hydrodynamic models and two spinorial diffusive models for quantum electron transport in graphene following a strategy similar to that one employed in the derivation of the previous diffusive models.

Spinorial models: the Pauli components of the Wigner matrix are considered *separately* from each other, not through a linear combination.

Spinorial hydrodynamic models

Moments:

$$n_s = \int w_s \, dp \quad (s = 0, 1, 2, 3), \qquad J_k = \int p_k w_0 \, dp \quad (k = 1, 2).$$

- n_0 is the *charge density*;
- $\vec{n} = (n_1, n_2, n_3)$ is the *spin vector*;
- $\vec{J} = (J_1, J_2, 0)$ is the *current vector*.

Note that the current vector has only two components because graphene's cristal lattice is a two-dimensional object.

Spinorial hydrodynamic models

The equilibrium distribution has the following form:

$$g[n_0, \vec{n}, \vec{J}] = \mathcal{E}\mathrm{xp}(-h_\xi)\,,$$
$$h_\xi = \left(\frac{|p|^2}{2} + p_k \Xi_k + \xi_0\right)\sigma_0 + (\xi_s + c p_s)\sigma_s\,,$$

with $\xi_0(x)$, $(\xi_s(x))_{s=1,2,3}$, $(\Xi_k(x))_{k=1,2}$ Lagrange multipliers to be determined in such a way that:

$$\langle g_0[n_0, \vec{n}, \vec{J}]\rangle(x) = n_0(x)\,,\ \langle \vec{g}[n_0, \vec{n}, \vec{J}]\rangle(x) = \vec{n}(x)\,,\ \langle \vec{p} g_0[n_0, \vec{n}, \vec{J}]\rangle(x) = \vec{J}(x)\,,$$

for $x \in \mathbb{R}^2$.

Spinorial hydrodynamic models, fully quantum system

The following theorem holds:

Theorem

Let n_0^τ, $\vec{n}^\tau$, $\vec{J}^\tau$ the moments of a solution w^τ of Eqs. (WH), and let $g = g[n_0^\tau, \vec{n}^\tau, \vec{J}^\tau]$. If $n_0^\tau \to n_0$, $\vec{n}^\tau \to \vec{n}$, $\vec{J}^\tau \to \vec{J}$ as $\tau \to 0$, then the limit moments n_0, $\vec{n}$, $\vec{J}$ satisfy:

$$
\begin{aligned}
\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot \vec{J} + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{n} &= 0 \\
\partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot \int \vec{g} \otimes \vec{p} \, dp + \frac{\epsilon}{2} \vec{\nabla} n_0 + \int \vec{g} \wedge \vec{p} \, dp &= 0 \\
\partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\frac{\vec{J} \otimes \vec{J}}{n_0} + \mathscr{P} \right) + \frac{\epsilon}{2} \vec{\nabla} \cdot \int \vec{p} \otimes \vec{g} \, dp + n_0 \vec{\nabla} V &= 0
\end{aligned}
$$

where $\mathscr{P}$ is the so-called quantum stress tensor:

$$
\mathscr{P} = \int (\vec{p} - \vec{J}/n_0) \otimes (\vec{p} - \vec{J}/n_0) g_0 \, dp
$$

First-order semiclassical expansion of the equilibrium distribution

First-order semiclassical expansion of the equilibrium distribution:

$$g_0[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} + O(\epsilon^2)\,,$$
$$\vec{g}[n_0, \vec{n}, \vec{J}] = \frac{n_0}{2\pi} e^{-|\vec{p}-\vec{u}|^2/2} \left(\frac{\vec{n}}{n_0} - \epsilon\gamma\mathcal{Z}(\vec{p}-\vec{u}) \right) + O(\epsilon^2)\,,$$

$$\mathcal{Z}_{ij} \equiv \frac{n_i n_j}{|\vec{n}|^2} + \omega \left(\delta_{ij} - \frac{n_i n_j}{|\vec{n}|^2} \right) + \frac{1-\omega}{2\gamma} \eta_{iks} \frac{n_k}{|\vec{n}|} \partial_j \left(\frac{n_s}{|\vec{n}|} \right) \quad (i,j = 1,2,3)\,,$$
$$\omega \equiv \frac{|\vec{n}|/n_0}{\log \sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}}\,.$$

Exploiting this expansion and the fully quantum hydrodynamic spinorial equations, we obtain:

First-order spinorial hydrodynamic model:

$$\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\vec{J} + \epsilon\gamma\vec{n} \right) = 0 \,,$$

$$\partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot (\vec{n} \otimes \vec{u} - \epsilon\gamma n_0 \mathcal{Z} + \epsilon\gamma n_0\, I) + \vec{n} \wedge \vec{u}$$
$$+ \frac{\epsilon}{2} n_0 (1-\omega)[\vec{\nabla} \cdot \vec{s} - \vec{s} \cdot \vec{\nabla}\,]\vec{s} = 0 \,,$$

$$\partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left[n_0 (I + \vec{u} \otimes \vec{u}) + \epsilon\gamma \left(\vec{u} \otimes \vec{n} - \epsilon\gamma n_0 \mathcal{Z}^T \right) \right] + n_0 \vec{\nabla} V = 0 \,,$$

where:

$$\vec{s} \equiv \frac{\vec{n}}{|\vec{n}|} \,.$$

Second order spinorial hydrodynamic model: assumption

We are going to derive another hydrodynamic model for quantum transport in graphene.

- Exploit the Wigner equations in hydrodynamic scaling (WH).
- Same fluid-dynamic moments n_0, $\vec{n}$, $\vec{J}$ of the Wigner distribution w.
- Same equilibrium distribution.
- Stronger assumptions than (LSFS): consider also $O(\epsilon^2)-$terms in the fluid equations.

Second order spinorial hydrodynamic model: assumptions

Assumptions:

- semiclassical hypothesis $\epsilon \ll 1$;
- *Strongly Mixed State* hypothesis (SMS):

$$c \sim \epsilon \,, \qquad \left[\sum_{s=1}^{3} (\xi_s)^2 \right]^{1/2} = O(\epsilon) \,.$$

Remember that:

$$g[n_0, \vec{n}, \vec{J}] = \mathcal{E}\text{xp}(-h_\xi) \,, \quad h_\xi = \left(\frac{|p|^2}{2} + p_k \Xi_k + \xi_0 \right) \sigma_0 + (\xi_s + c p_s) \sigma_s \,,$$

$$\int g_s[n_0, \vec{n}, \vec{J}](x,p)\, dp = n_s(x) \qquad (s = 0,1,2,3) \,, \quad x \in \mathbb{R}^2 \,,$$

$$\int p_k g_0[n_0, \vec{n}, \vec{J}](x,p)\, dp = J_k(x) \qquad (k = 1,2) \,, \quad x \in \mathbb{R}^2 \,.$$

These further assumptions are necessary to overcome the computational difficulties arising from the spinorial nature of the problem: without these hypothesis, it would be hard to compute the second order expansion of the equilibrium distribution.

Second order spinorial hydrodynamic model: assumptions

- Consequence on the choice of moments:

$$\left|\frac{\vec{n}}{n_0}\right| = O(\epsilon)\,.$$

- Decoupling of h_ξ in a scalar part of order 1 and a spinorial perturbation of order ϵ; this fact will be very useful in computations.

Second order spinorial hydrodynamic model: semiclassical expansion of equilibrium

Let us define, for an arbitrary positive function $\mathcal{N}(x)$ and an arbitrary vector function $\vec{\mathcal{J}}(x) = (\mathcal{J}_1(x), \mathcal{J}_2(x), 0)$:

$$\mathcal{M}_\epsilon[\mathcal{N}, \vec{\mathcal{J}}] = \frac{\mathcal{N}}{2\pi} e^{-|\vec{p}-\vec{\mathcal{U}}|^2/2} \left[1 - \frac{\epsilon^2}{24} \left(2\Delta \log \mathcal{N} + \frac{|\nabla \mathcal{N}|^2}{\mathcal{N}^2} - \mathcal{Q}(\mathcal{N}, \vec{\mathcal{J}}) \right) \right],$$

where:

$$\begin{aligned} \mathcal{Q}(\mathcal{N}, \vec{\mathcal{J}}) =& 3(\Delta \mathcal{A} + p_k \Delta \mathcal{U}_k + \partial_i \mathcal{U}_j \, \partial_j \mathcal{U}_i) - 2\partial_i \mathcal{U}_j (p_i - \mathcal{U}_i)(\partial_j \mathcal{A} + p_k \partial_j \mathcal{U}_k) \\ & - (\partial^2_{ij} \mathcal{A} + p_k \partial^2_{ij} \mathcal{U}_k)(p_i - \mathcal{U}_i)(p_j - \mathcal{U}_j) + |\nabla(\mathcal{A} + p_k \mathcal{U}_k)|^2, \\ \vec{\mathcal{U}} =& \vec{\mathcal{J}}/\mathcal{N}, \qquad \mathcal{A} = \log\left(\frac{\mathcal{N}}{2\pi}\right) - \frac{|\vec{\mathcal{U}}|^2}{2}. \end{aligned}$$

Second order spinorial hydrodynamic model: semiclassical expansion of equilibrium

Second-order semiclassical expansion of the equilibrium distribution:

$$g_0[n_0,\vec{n},\vec{J}] = \mathcal{M}_\epsilon\left[n_0 - n_0\left(\frac{|\vec{n}|^2}{2n_0^2}+\epsilon^2\gamma^2\right), \vec{J}+\epsilon\gamma\vec{n}-\left(\frac{|\vec{n}|^2}{2n_0^2}+\epsilon^2\gamma^2\right)\vec{J}\right]$$
$$+\frac{n_0}{4\pi}e^{-|\vec{p}-\vec{J}/n_0|^2/2}\left|\frac{\vec{n}}{n_0}-\epsilon\gamma\left(\vec{p}-\frac{\vec{J}}{n_0}\right)\right|^2+O(\epsilon^3),$$
$$\vec{g}[n_0,\vec{n},\vec{J}] = \frac{n_0}{2\pi}e^{-|\vec{p}-\vec{J}/n_0|^2/2}\left(\frac{\vec{n}}{n_0}-\epsilon\gamma\left(\vec{p}-\frac{\vec{J}}{n_0}\right)\right)+O(\epsilon^3).$$

Exploiting this expansion and the fully quantum hydrodynamic spinorial equations, we obtain:

Second order spinorial hydrodynamic model:

$$\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot (\vec{J} + \epsilon\gamma\vec{n}) = O(\epsilon^3)\,,$$

$$\partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\frac{\vec{n} \otimes \vec{J}}{n_0} \right) + \frac{\vec{n} \wedge \vec{J}}{n_0} = O(\epsilon^3)\,,$$

$$\partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left(\frac{\vec{J} \otimes (\vec{J} + \epsilon\gamma\vec{n})}{n_0} \right) + \frac{\vec{\nabla} n_0}{2\gamma} + n_0 \vec{\nabla}(V + V_B) = O(\epsilon^3)\,,$$

where V_B is again (up to a constant) the so-called *Bohm potential*:

$$V_B = -\frac{1}{2\gamma}\frac{\epsilon^2}{6}\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\,.$$

Spinorial diffusive models

Now we will present two spinorial drift-diffusion model for quantum transport of electrons in graphene.

- Both first-order model: second order too much computationally demanding!
- Difference: a theoretical "Pseudo-Magnetic" external field which is supposed to interact with the charge carriers pseudo-spin and which will provide a strong coupling between the second model equations.

Spinorial diffusive models

Moments:

$$n_0(x,t) = \int w_0(x,p,t)\,dp \qquad \text{charge density,}$$
$$\vec{n}(x,t) = \int \vec{w}(x,p,t)\,dp \qquad \text{spin vector.}$$

The (scaled) equilibrium distribution can be written as:

$$g[n_0,\vec{n}] = \mathcal{E}\mathrm{xp}(-h_{A,\vec{B}})\,, \qquad h_{A,\vec{B}} = \left(\frac{|p|^2}{2} + A\right)\sigma_0 + (c\vec{p} + \vec{B})\cdot\vec{\sigma}\,,$$

where $A(x,t)$, $\vec{B}(x,t) = (B_1(x,t), B_2(x,t), B_3(x,t))$ are Lagrange multipliers to be determined in such a way that:

$$\int g_0[n_0,\vec{n}](x,p,t)\,dp = n_0(x,t)\,, \quad \int \vec{g}[n_0,\vec{n}](x,p,t)\,dp = \vec{n}(x,t)\,,$$

for $(x,t) \in \mathbb{R}^2 \times \mathbb{R}$.

Spinorial diffusive models: assumptions

We assume that the semiclassical parameter ϵ and the diffusive parameter τ are of the same order and small, so we will perform a limit $\tau \to 0$ in the Wigner equations:

$$c \sim \epsilon \sim \tau \,.$$

Moreover we define:

$$\lambda \equiv \frac{c}{\tau} \sim 1 \,.$$

Spinorial diffusive models: semiclassical expansion of equilibrium

First order semiclassical expansion of equilibrium distribution:

$$
\begin{aligned}
g[n_0,\vec{n}] =& g^{(0)}[n_0,\vec{n}] + \epsilon g^{(1)}[n_0,\vec{n}] + O(\epsilon^2)\,, \\
g_0^{(0)}[n_0,\vec{n}] =& \frac{e^{-|p|^2/2}}{2\pi} n_0\,, \qquad \vec{g}^{(0)}[n_0,\vec{n}] = \frac{e^{-|p|^2/2}}{2\pi}\vec{n}\,, \\
g_0^{(1)}[n_0,\vec{n}] =& -\gamma\frac{e^{-|p|^2/2}}{2\pi}\vec{n}\cdot\vec{p}\,, \\
\vec{g}^{(1)}[n_0,\vec{n}] =& -\gamma\frac{e^{-|p|^2/2}}{2\pi} n_0\left[\left((1-\omega)\frac{\vec{n}\otimes\vec{n}}{|\vec{n}|^2} + \omega\, I\right)\vec{p}\right. \\
& \left. - (1-\omega)\frac{[(\vec{p}\cdot\vec{\nabla}_x)\vec{n}]\wedge\vec{n}}{2\gamma|\vec{n}|^2}\right],
\end{aligned}
$$

with:

$$
\omega \equiv \frac{|\vec{n}|}{n_0}\left\{\log\sqrt{\frac{n_0+|\vec{n}|}{n_0-|\vec{n}|}}\right\}^{-1}.
$$

First order spinorial drift-diffusion model: derivation

- From eqs. (WD) make a Chapman-Enskog expansion of the Wigner function w.
- Take moments of eqs. (WD).
- Exploit the semiclassical expansion of the equilibrium.

We obtain:

First order spinorial drift-diffusion model.

First order spinorial drift-diffusion model $\equiv$
Quantum Spin Diffusion Equations 1 (QSDE1):

$$\partial_t n_0 = \Delta n_0 + \mathrm{div}(n_0 \nabla V)\,,$$

$$\partial_t n_j = \partial_s A_{js} + F_j\,, \qquad (j = 1,2,3)$$

$$A_{js} = \left(\delta_{jl} + b_k\left[\frac{\vec{n}}{n_0}\right]\eta_{jkl}\right)\partial_s n_l + n_j \partial_s V$$

$$- 2\eta_{jsl} n_l + b_k\left[\frac{\vec{n}}{n_0}\right](\delta_{jk} n_s - \delta_{js} n_k)\,, \qquad (j,s = 1,2,3)$$

$$F_j = \eta_{jkl} n_k \partial_l V - 2n_j + b_s\left[\frac{\vec{n}}{n_0}\right]\partial_s n_j - b_j\left[\frac{\vec{n}}{n_0}\right]\partial_s n_s\,, \qquad (j = 1,2,3)$$

where we defined, for all $\vec{v} \in \mathbb{R}^3$, $0 < |v| < 1$:

$$\vec{b}[\vec{v}] = \lambda \frac{\vec{v}}{|\vec{v}|^2}\left[1 - \frac{2|\vec{v}|}{\log(1+|\vec{v}|) - \log(1-|\vec{v}|)}\right]\,.$$

First order spinorial drift-diffusion model with pseudo-magnetic field

In the model QSDE1 the charge density n_0 evolves independently from the spin vector $\vec{n}$: we are going to modify the QSDE1 model in order to obtain a fully coupled system by adding a "pseudo-magnetic" field able to interact with the charge carriers pseudospin.

Negulescu and Possanner, in their article[2], consider a semiconductor subject to a magnetic field interacting with the electron spin, and derive a purely semiclassical (without quantum corrections) diffusive model for the charge density n_0 and the spin vector $\vec{n}$ throught a Chapman-Enskog espansion of the Boltzmann distribution. We will follow a similar procedure to obtain our new model.

[2] S. Possanner and C. Negulescu. Diffusion limit of a generalized matrix Boltzmann equation for spin-polarized transport. *Kinetic and Related Models* (2011).

First order spinorial drift-diffusion model with pseudo-magnetic field: derivation

We define two quantities:

$$\begin{aligned} \zeta =& \zeta(x,t) \qquad \text{pseudo-spin polarization of scattering rate;} \\ \vec{\omega} =& \vec{\omega}(x,t) \qquad \text{direction of local pseudo-magnetization.} \end{aligned}$$

$$s_{\uparrow} = \frac{1+|\zeta(x,t)|}{1-|\zeta(x,t)|} s_{\downarrow} \, ,$$

where $s_{\uparrow\downarrow}$ are the scattering rates of electrons in the upper band and in the lower band; it is bounded between 0 and 1. The vector $\vec{\omega}$, being a direction, has modulus equal to 1.

First order spinorial drift-diffusion model with pseudo-magnetic field: derivation

New Wigner equations in diffusive scaling:

$$\begin{aligned} \tau\partial_t w_0 + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2}\vec{\nabla}\cdot\vec{w} + \Theta_\epsilon[V]w_0 &= \frac{Q_0(w)}{\tau}\,, \\ \tau\partial_t \vec{w} + \frac{\vec{p}\cdot\vec{\nabla}}{2\gamma}\vec{w} + \frac{\epsilon}{2}\vec{\nabla} w_0 + \vec{w}\wedge\vec{p} + \Theta_\epsilon[V]\vec{w} + \tau\vec{\omega}\wedge\vec{w} &= \frac{\vec{Q}(w)}{\tau}\,, \end{aligned} \qquad \text{(WD2)}$$

with the collision operator $Q(w)$ defined by:

$$Q(w) = \mathcal{P}^{1/2}(g-w)\mathcal{P}^{1/2}\,, \qquad \mathcal{P} = \sigma_0 + \zeta\vec{\omega}\cdot\vec{\sigma}\,.$$

$\mathcal{P}$ is the so-called *polarization matrix*.

First order spinorial drift-diffusion model with pseudo-magnetic field: derivation

- From eqs. (WD2) make a Chapman-Enskog expansion of the Wigner function w.
- Take moments of eqs. (WD2).
- Exploit the semiclassical expansion of the equilibrium.

We obtain:

First order spinorial drift-diffusion model with pseudo-magnetic field

First-order spinorial drift-diffusion model with pseudo-magnetic field $\equiv$ Quantum Spin Diffusion Equation 2 (QSDE2):

$$
\begin{aligned}
\partial_t n_0 =& \partial_s M_{0s} \,, \\
\partial_t n_j =& \partial_s M_{js} + \eta_{jks}(M_{ks} + n_k \omega_s) \\
& + \partial_s \left\{ b_k \left[\frac{\vec{n}}{n_0} \right] (\eta_{jkl} \partial_s n_l + \delta_{jk} n_s - \delta_{js} n_k) \right\} \\
& + b_s \left[\frac{\vec{n}}{n_0} \right] \partial_s n_j - b_j \left[\frac{\vec{n}}{n_0} \right] \partial_s n_s \qquad (j = 1, 2, 3) \,, \\
M_{0s} =& \phi^{-2} \{ (n_0 + n_0 \partial_s V) - \zeta \omega_k (\partial_s n_k + n_k \partial_s V + \eta_{kls} n_l) \} \,, \\
M_{js} =& \phi^{-2} \{ -\zeta \omega_j (n_0 + n_0 \partial_s V) \\
& + [\omega_j \omega_k + \phi(\delta_{jk} - \omega_j \omega_k)](\partial_s n_k + n_k \partial_s V + \eta_{kls} n_l) \} \,, \\
\phi =& \sqrt{1 - \zeta^2} \,, \quad \vec{b}[\vec{v}] = \lambda \frac{\vec{v}}{|\vec{v}|^2} \left[1 - \frac{2|\vec{v}|}{\log(1 + |\vec{v}|) - \log(1 - |\vec{v}|)} \right] .
\end{aligned}
$$

Analytical results

Now we present some analytical results concerning the model QSDE1.

- Existence and uniqueness of (weak) solutions satisfying suitable L^∞ bounds.
- Entropy inequality.
- Long-time behaviour of the solutions.

Analytical results

We considered model QSDE1 for $(x,t) \in \Omega_T \equiv \Omega \times [0,T]$ with $\Omega \subset \mathbb{R}^2$ bounded domain:

$$\begin{cases} \partial_t n_0 = \mathrm{div}\,(\nabla n_0 + n_0 \nabla V) & x \in \Omega\,,\ t \in [0,T]\,, \\ \partial_t \vec{n} = \mathrm{div}\, J + \vec{F} & x \in \Omega\,,\ t \in [0,T]\,, \\ -\lambda_D^2 \Delta V = n_0 - C(x) & x \in \Omega\,,\ t \in [0,T]\,, \\ n_0(x,t) = n_\Gamma(x,t) & x \in \partial\Omega\,,\ t \in [0,T]\,, \\ \vec{n}(x,t) = 0 & x \in \partial\Omega\,,\ t \in [0,T]\,, \\ V(x,t) = \mathcal{U}(x,t) & x \in \partial\Omega\,,\ t \in [0,T]\,, \\ n_0(x,0) = n_{0I}(x) & x \in \Omega\,, \\ \vec{n}(x,0) = \vec{n}_I(x) & x \in \Omega\,, \end{cases} \qquad \text{(Pb)}$$

$$F_j = \eta_{jk\ell} n_k \partial_\ell V - 2n_j + b_k[\vec{n}/n_0]\partial_k n_j - b_j[\vec{n}/n_0]\vec{\nabla}\cdot\vec{n},$$

$$J_{js} = \big(\delta_{j\ell} + b_k[\vec{n}/n_0]\eta_{jk\ell}\big)\partial_s n_\ell + n_j \partial_s V - 2\eta_{js\ell} n_\ell + b_k[\vec{n}/n_0](\delta_{jk} n_s - \delta_{js} n_k)\,, \qquad (j,s = 1,2,3)\,,$$

$$\vec{b}[\vec{v}] = \lambda \frac{\vec{v}}{|\vec{v}|^2}\left[1 - 2|\vec{v}|\left\{\log\left(\frac{1+|\vec{v}|}{1-|\vec{v}|}\right)\right\}^{-1}\right] \qquad \vec{v} \in \mathbb{R}^3,\ 0 < |\vec{v}| < 1\,.$$

Analytical results

We split problem (Pb) into the following two problems:

$$\begin{cases} \partial_t n_0 = \operatorname{div}(\nabla n_0 + n_0 \nabla V) & x \in \Omega\,, \ \ t \in [0,T]\,, \\ -\lambda_D^2 \Delta V = n_0 - C(x) & x \in \Omega\,, \ \ t \in [0,T]\,, \\ n_0(x,t) = n_\Gamma(x,t) & x \in \partial\Omega\,, \ \ t \in [0,T]\,, \\ V(x,t) = \mathcal{U}(x,t) & x \in \partial\Omega\,, \ \ t \in [0,T]\,, \\ n_0(x,0) = n_{0I}(x) & x \in \Omega\,, \end{cases} \qquad \text{(Pb-n0V)}$$

$$\begin{cases} \partial_t \vec{n} = \operatorname{div} J + \vec{F} & x \in \Omega\,, \quad t \in [0,T]\,, \\ \vec{n}(x,t) = 0 & x \in \partial\Omega\,, \ \ t \in [0,T]\,, \\ \vec{n}(x,0) = \vec{n}_I(x) & x \in \Omega\,, \end{cases} \qquad \text{(Pb-ns)}$$

$$F_j = \eta_{jk\ell} n_k \partial_\ell V - 2n_j + b_k[\vec{n}/n_0]\partial_k n_j - b_j[\vec{n}/n_0]\vec{\nabla}\cdot\vec{n},$$

$$J_{js} = \big(\delta_{j\ell} + b_k[\vec{n}/n_0]\eta_{jk\ell}\big)\partial_s n_\ell + n_j \partial_s V$$
$$\quad - 2\eta_{js\ell} n_\ell + b_k[\vec{n}/n_0](\delta_{jk} n_s - \delta_{js} n_k)\,, \qquad (j,s = 1,2,3)\,,$$

$$\vec{b}[\vec{v}] = \lambda \frac{\vec{v}}{|\vec{v}|^2}\left[1 - 2|\vec{v}|\left\{\log\left(\frac{1+|\vec{v}|}{1-|\vec{v}|}\right)\right\}^{-1}\right] \qquad \vec{v} \in \mathbb{R}^3,\ 0 < |\vec{v}| < 1\,.$$

Analytical results: existence and regularity for first problem

We studied first the existence and regularity of solutions (n_0, V) of pb. (Pb-n0V).

Conditions on the data:

$$n_\Gamma \in H^1(0,T;H^2(\Omega)) \cap H^2(0,T;L^2(\Omega)) \cap L^\infty(0,T;L^\infty(\Omega)),$$
$$n_{0I} \in H^1(\Omega), \quad \inf_\Omega n_{0I} > 0, \quad n_{0I} = n_\Gamma(0) \quad \text{on } \partial\Omega, \quad \inf_{\partial\Omega\times(0,T)} n_\Gamma > 0,$$
$$\mathcal{U} \in L^\infty(0,T;W^{2,p}(\Omega)) \cap H^1(0,T;H^1(\Omega)), \quad C \in L^\infty(\Omega), \; C \geq 0 \text{ in } \Omega,$$

for some $p > 2$.

Analytical results: existence, uniqueness and regularity for first problem

Theorem

Let $T > 0$. *Under the previous assumptions there exists a unique solution* (n_0, V) *to pb. (Pb-n0V) satisfying:*

$$n_0 \in L^\infty([0,T], H^2(\Omega)) \cap H^1([0,T], H^1(\Omega)) \cap H^2([0,T], (H^1(\Omega))'),$$
$$V \in L^\infty([0,T], W^{1,\infty}(\Omega)) \cap H^1([0,T], H^2(\Omega)),$$
$$0 < me^{-\mu t} \le n_0 \le M \quad in\ \Omega,\ t > 0,$$

where $\mu = \lambda_D^{-2}$ *and*

$$M = \max\left\{ \sup_{\partial\Omega\times(0,T)} n_\Gamma,\ \sup_\Omega n_{0I},\ \sup_\Omega C \right\},$$
$$m = \min\left\{ \inf_{\partial\Omega\times(0,T)} n_\Gamma,\ \inf_\Omega n_{0I} \right\} > 0.$$

Analytical results: existence and uniqueness for second problem

Theorem

Let (n_0, V) be the solution to pb. (Pb-n0V) according to the previous theorem and $\vec{n}^0 \in H_0^1(\Omega)$ such that:

$$\sup_{x\in\Omega} \frac{|\vec{n}^0(x)|}{n_{0I}(x)} < 1\,;$$

then pb. (Pb-ns) has a solution $\vec{n}$ such that:

$$\vec{n} \in L^2([0,T], H_0^1(\Omega)) \cap H^1([0,T], H^{-1}(\Omega))\,, \quad \sup_{\Omega_T} \frac{|\vec{n}|}{n_0} < 1\,;$$

furthermore, there exists at most one weak solution with the property stated above and satisfying $\vec{n} \in L^\infty([0,T], W^{1,4}(\Omega))$.

Entropicity of the system

Let $(n_0, \vec{n}, V)$ be a solution to pb. (Pb) according to previously stated existence theorems. We assume that the boundary data is in global equilibrium, i.e.

$$n_\Gamma = e^{-\mathcal{U}}, \quad V = \mathcal{U}, \quad \vec{n} = 0 \quad \text{on } \partial\Omega,$$

where $\mathcal{U} = \mathcal{U}(x)$ is time-independent. Then the macroscopic entropy:

$$\begin{aligned} S(t) = \int_\Omega \Big\{ & \frac{1}{2}(n_0 + |\vec{n}|)\big(\log(n_0 + |\vec{n}|) - 1\big) \\ & + \frac{1}{2}(n_0 - |\vec{n}|)\big(\log(n_0 - |\vec{n}|) - 1\big) \\ & + (n_0 - C(x))V - \frac{\lambda_D^2}{2}|\nabla V|^2 \Big\}\, dx \end{aligned}$$

is nonincreasing in time.

Entropicity of the system

Proposition

The entropy dissipation dS/dt can be written as:

$$\frac{dS}{dt} = -\frac{1}{2}\int (n_0 + |\vec{n}|)\left|\nabla(\log(n_0 + |\vec{n}|) + V)\right|^2 - \frac{1}{2}\int (n_0 - |\vec{n}|)\left|\nabla(\log(n_0 - |\vec{n}|) + V)\right|^2 - \frac{1}{2}\int |\vec{n}| \log\left(\frac{n_0 + |\vec{n}|}{n_0 - |\vec{n}|}\right) \mathscr{G}\left[\frac{\vec{n}}{|\vec{n}|}\right] \leq 0\,,$$

where $\mathscr{G}$ is defined by:

$$\mathscr{G}[\vec{v}] \equiv \sum_{j,k} (\partial_j v_k)^2 + 2\vec{v}\cdot curl\ \vec{v} + 2|\vec{v}|^2 \geq 0 \qquad \forall \vec{v} \in H^1(\Omega)^3\,.$$

Long-time decay of the solutions

Let $(n_0, \vec{n}, V)$ be a solution to pb. (Pb) according to the existence theorems. It is possible to prove that, under suitable assumptions on the electric potential, the spin vector converges to zero as $t \to \infty$.

To prove the stated result we exploited the following:

Lemma

Let $\mathscr{G}$ as in the previous proposition:

$$\mathscr{G}[\vec{v}] = \sum_{j,k} (\partial_j v_k)^2 + 2\vec{v} \cdot curl\ \vec{v} + 2|\vec{v}|^2 \qquad \forall \vec{v} \in H^1(\Omega)^3 .$$

A constant $\mathcal{K}_\Omega > 0$ exists, depending only on Ω, such that:

$$\int \mathscr{G}[\vec{u}] \geq \mathcal{K}_\Omega \int |\vec{u}|^2 , \quad \forall \vec{u} \in H^1(\Omega)^3 .$$

Long-time decay of the solutions

Theorem

Let $\mathcal{K}_\Omega$ *as in the previous Lemma, and let* $2 < p < \infty$ *arbitrary.*

1. *A positive constant* $c = c(p, \Omega)$ *exists such that: if* $\sup_{\Omega_T} |\nabla V| < c$ *then:*

   $$\|\vec{n}\|_{L^p(\Omega)}(t) \leq \|\vec{n}_I\|_{L^p(\Omega)} e^{-kt} \qquad \forall t > 0\,,$$

   for a suitable number $k = k(p, \Omega, \sup_{\Omega_T} |\nabla V|) > 0$.

2. *If* $\sup_{\Omega_T} \Delta V < \mathcal{K}_\Omega$ *then:*

   $$\|\vec{n}\|_{L^2(\Omega)}(t) \leq \|\vec{n}_I\|_{L^2(\Omega)} e^{-k' t} \qquad \forall t > 0\,,$$

   with $k' = 2\mathcal{K}_\Omega - \sup_{\Omega_T} \Delta V > 0$.

3. *If* $\sup_{\Omega_T} \Delta V < 0$ *then:*

   $$\|\vec{n}\|_{L^\infty(\Omega)}(t) \leq \|\vec{n}_I\|_{L^\infty(\Omega)} e^{-k'' t} \qquad \forall t > 0\,,$$

   with $k'' = -\sup_{\Omega_T} \Delta V > 0$.

Numerical simulations

We solved model (QSDE2) and, as a particular case, model (QSDE1), in one space dimension, by means of Crank-Nicholson finite difference scheme. We simulated a ballistic diode to which a certain bias is applied: we chose global equilibrium initial conditions and we observed the evolution of the system towards a new equilibrium due to the applied potential.

Boundary conditions:

$$n_0 = C, \quad \vec{n} = 0, \quad V = U \quad \text{on } \partial\Omega = \{0,1\},\ t > 0,$$

where $U(x) = V_A\, x/L$, $V_A = 1$ v is the applied voltage, and $L = 10^{-7}$ m is the device lenght.

Initial conditions:

$$n_0(x,0) = q\exp(-V_{\mathrm{eq}}(x)), \quad \vec{n}(x,0) = 0,$$

where $q = 1.6 \times 10^{-2}$ C m^{-2}, V_{eq} is the (scaled) equilibrium potential:

$$-\lambda_D^2 \partial_{xx}^2 V_{\mathrm{eq}} = \exp(-V_{\mathrm{eq}}) - C/q \quad \text{in } \Omega, \quad V_{\mathrm{eq}}(0) = V_{\mathrm{eq}}(1) = 0,$$

and $\lambda_D^2 = 10^{-3} L^2$.

The pseudo-spin polarization and the direction of the local magnetization are defined by:

$$\zeta = 0.5, \quad \vec{\omega} = (0,0,1)\,.$$

Numerical simulations

The doping profile corresponding to a ballistic diode:

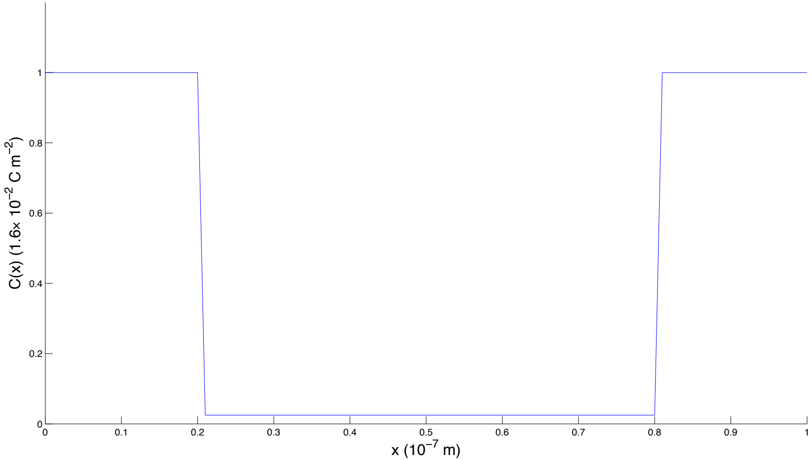


Figure: Doping profile corresponding to a ballistic diode.

Numerical simulations

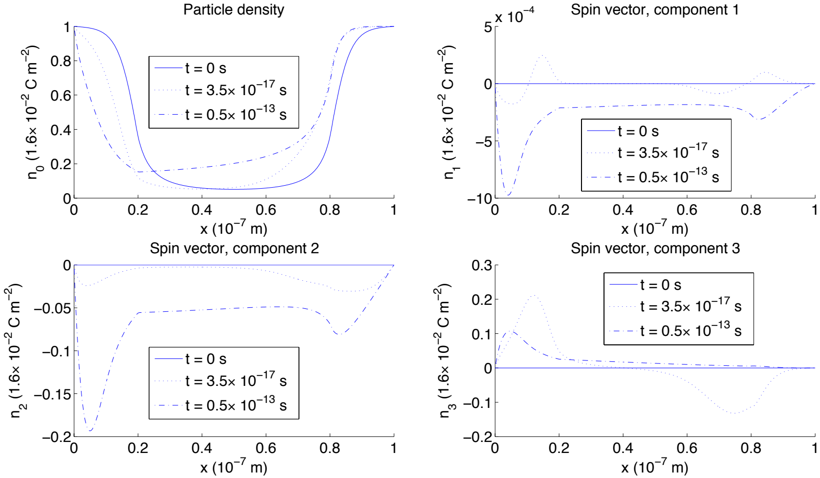


Figure: Model QSDE2: Particle density and components of the spin vector versus position at times $t = 0$ s, $t = 3.5 \times 10^{-17}$ s, and $t = 0.5 \times 10^{-13}$ s.

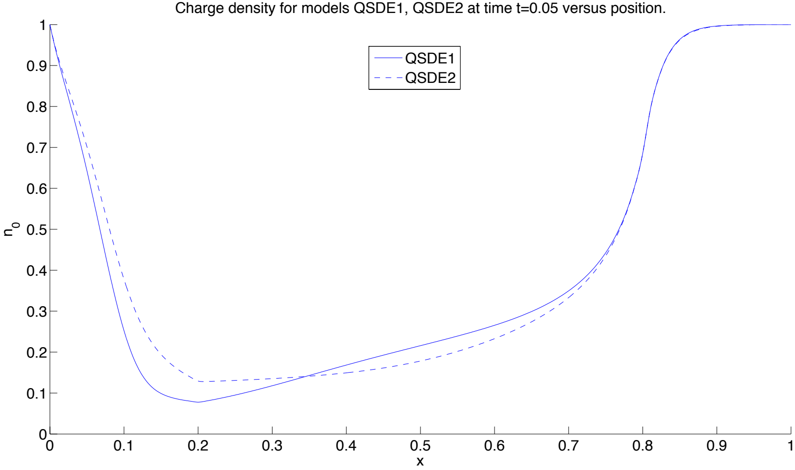


Figure: Charge density for models QSDE1 and QSDE2 versus position at time $t = 2.5 \times 10^{-15}$ s (maximized difference).

Numerical simulations

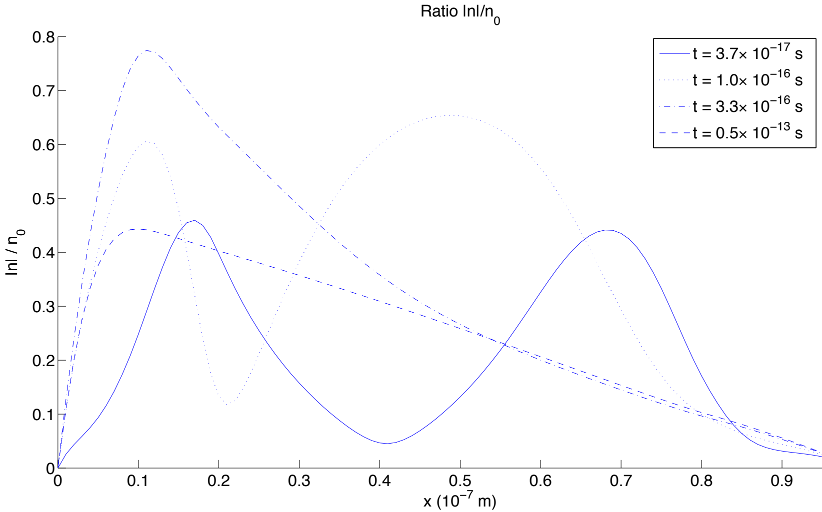


Figure: Model QSDE2: Ratio $|\vec{n}|/n_0$ versus position at several times.

Numerical simulations

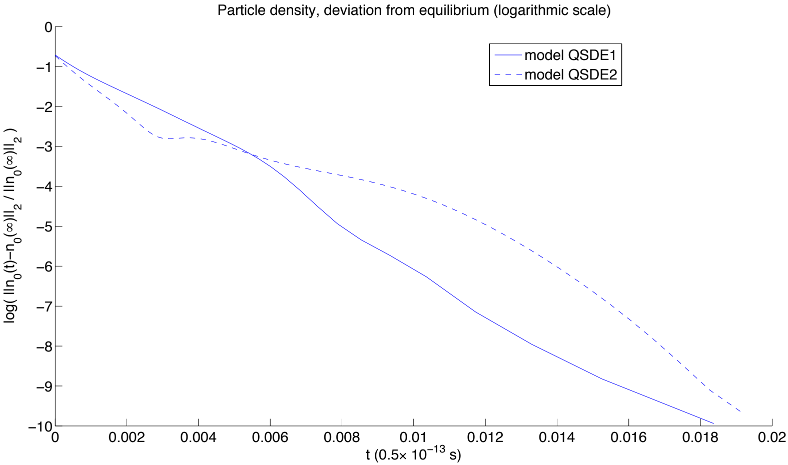


Figure: Relative difference $\|n_0(t) - n_0(\infty)\|/\|n_0(t)\|$ versus time (semilogarithmic plot) for the models QSDE1 (solid line) and QSDE2 (dashed line).

Numerical simulations

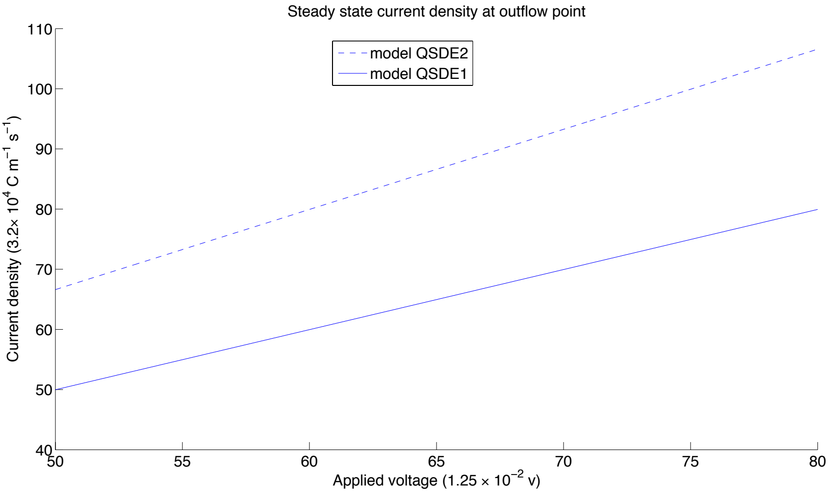


Figure: Static current-voltage characteristics for the models QSDE1 and QSDE2.

Conclusions

The purpose of our work was the description of quantum transport of electrons in graphene by means of fluid models:

- we presented a kinetic model, that is, the Wigner equation, as the starting point of the derivation of fluid models;
- we defined the quantum equilibrium distribution by means of the quantum minimum entropy principle, computing a semiclassical expansion of the quantum exponential in the spinorial case;
- we derived one hydrodynamic and two diffusive two-band models, which means, models for conduction and valence band densities;
- we derived two hydrodynamic and two diffusive spinorial models, including all the components of the spin vector;
- we performed an analysis of the first diffusive spinorial model, proving existence of solutions, uniqueness of the solution under a regularity condition on the moments, entropicity for the model and long-time decay of the spin vector;
- we obtained some numerical simulations for the spinorial diffusive models, showing the temporal evolution of the moments.

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Thank you for your attention!

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