Some fluid-dynamic models for quantum electron transport in graphene

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What is Graphene?

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Graphene electronic properties

Graphene is a zero-gap semiconductor, that is, the valence band of the energy spectrum touches the conduction band in some isolated points, named Dirac points; around such points the energy of electrons is approximately linear with respect to the modulus of momentum.

Hamiltonian (low-energy approximation, zero potential):

\[ H_0 = -i \hbar v_F (\sigma_1 \partial_x + \sigma_2 \partial_y), \]

where \( v_F \approx 10^6 \text{m/s} \), is the Fermi speed and, as usual, \( \hbar \) denotes the reduced Planck constant. We recall the Pauli matrices

\[ \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]

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Two types of models for quantum transport

In the following we will present two types of models for quantum electron transport in graphene:

\[\text{Quantum Diffusion Equations;} \]

\[\text{Quantum Hydrodynamic Equations.} \]

Both classes of models are obtained through this strategy:

\[\text{we consider the Wigner equations for the system and rescale them with diffusive or hydrodynamic scaling;} \]

\[\text{we build from the scaled Wigner system a suitable set of moments equations;} \]

\[\text{we close these latter by choosing the Wigner distribution equal to an equilibrium distribution, defined as a minimizer of a suitable entropy functional, according to the theory of Degond and Ringhofer (MEP, Minimum Entropy Principle).} \]

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Why Fluid-dynamic models?

Fluid-dynamic models are competitive with respect to "basic" methods (Schrödinger, Von Neumann, Wigner equations) for the following reasons:

▶ Physical interpretation: fluid-dynamic models contain already the physically most interesting quantities (particle, momentum, spin densities), while other models contain only "auxiliary" quantities (wavefunctions, density matrices, Wigner functions) which do not have an immediate physical interpretation;

▶ Numerical computation: fluid-dynamic models are sets of PDE in 2 space variables and 1 time variable, while other models have more complicated structures (for example, Wigner equations are sets of PDE with 4 space variables and 1 time variable); so fluid-dynamic models are more easily and fastly solvable via numerical computation than other models.
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Wigner equations

Let $w = \sum_{s=0}^{3} w_s \sigma_s$ the system Wigner function, $w_s$ its Pauli components, $\vec{w} = (w_1, w_2, w_3)$, $\partial_t = \partial / \partial t$, $\vec{\nabla} = (\partial / \partial r_1, \partial / \partial r_2, 0)$, $\vec{p} = (p_1, p_2, 0)$.

The Wigner equations for graphene, associated with the one-particle Hamiltonian $H_0 + V$ ($V$ being the potential) are:

$$
\begin{align*}
\partial_t w_0 + v_F \vec{\nabla} \cdot \vec{w}_0 + \Theta \hbar (V) w_0 &= w_{\text{eq}} - w_0 \tau_c \\
\partial_t \vec{w}_0 + v_F [\vec{\nabla} w_0 + 2 \hbar \vec{w}_0 \wedge \vec{p}] + \Theta \hbar (V) \vec{w}_0 &= \vec{w}_{\text{eq}} - \vec{w}_0 \tau_c
\end{align*}
$$

The terms on the right side are relaxation terms of BGK type, with $w_{\text{eq}}$ the local thermal equilibrium Wigner distribution. 

$$(\Theta \hbar (V) w)(r, p) = i \hbar (2\pi)^{-2} \int R^2 \times R^2 \delta V(r, \xi) w(r, p') e^{-i(p - p') \cdot \xi} d\xi dp'$$

$\delta V(r, \xi) = V(r + \hbar^2 \frac{\xi}{2}) - V(r - \hbar^2 \frac{\xi}{2})$. 

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\begin{cases}
\partial_t w_0 + v_F \vec{\nabla} \cdot \vec{w} + \Theta_h(V) w_0 = \frac{w_0^{eq} - w_0}{\tau_c} \\
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(WE)

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(\Theta_h(V) w)(r, p) = \frac{i}{\hbar} (2\pi)^{-2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \delta V(r, \xi) w(r, p') e^{-i(p-p') \cdot \xi} d\xi dp',
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\delta V(r, \xi) = V\left(r + \frac{\hbar}{2} \xi\right) - V\left(r - \frac{\hbar}{2} \xi\right).
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We perform the following diffusive scaling of the Wigner equations:

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\begin{align*}
    x & \mapsto x_0, \\
    t & \mapsto t_0, \\
    p & \mapsto p_0, \\
    V & \mapsto V_0,
\end{align*}
\]

\[
\begin{align*}
    t_0 &= x_0^2 v^2 F \tau_c, \\
    V_0 &= v F p_0, \\
    \epsilon &= \hbar x_0 p_0, \\
    \tau &= \tau_c v F x_0.
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- \(\epsilon\) is the semiclassical parameter;
- \(\tau\) is the diffusive parameter.
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\begin{align*}
  x & \mapsto x_0 x, & t & \mapsto t_0 t, & p & \mapsto p_0 p, & V & \mapsto V_0 V, \\
  t_0 &= \frac{x_0^2}{v_F^2 \tau_c}, & V_0 &= v_F p_0, \\
  \epsilon &= \frac{\hbar}{x_0 p_0}, & \tau &= \frac{\tau_c v_F}{x_0}.
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- \(\epsilon\) is the **semiclassical parameter**;
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The Wigner equations in diffusive scaling

By performing the scaling (DSCAL), we obtain:

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\begin{align*}
\tau \partial_t w_0 + T_0(w) &= w_{\text{eq}} - w_0 \\
\tau \partial_t w_s + T_s(w) &= w_{\text{eq}} - w_s \tau \\
\end{align*}
\]

(\text{WDIFF})

where:

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\begin{align*}
T_0(w) &= \partial_s w_s + \Theta \epsilon [V] w_0 \\
T_j(w) &= \partial_j w_0 + \Theta \epsilon [V] w_j + 2 \epsilon \eta_{jsp} w_s p_k \\
\end{align*}
\]

and \( \eta_{jsp} \) denotes the only antisymmetric \( 3 \times 3 \) tensor which is invariant for cyclic permutations of indices and such that \( \eta_{123} = 1 \) (in other words, \( \eta_{jsp} a_s b_k = (a \wedge b)_j \)).
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Choice of moments

The moments we choose are the following two:

\[ n^{\pm}(r) = \int \left( w_0(r, p) \mp \nu_s(p) w_s(r, p) \right) dp, \]

where:

\[ \nu_s(p) = \left| p \right|, \quad \nu_3(p) = 0. \]

\( n^{\pm} \) are the so-called band densities, that is, the partial trace (w.r.t. \( p \)) of the quantum operators band projections \( \Pi^{\pm} = \text{Op}(P^{\pm}) \):

\[ \Pi^{\pm} = \text{Op}(P^{\pm})(p) = \sigma_0^{\pm} \sigma_s. \]

\[ n^{\pm}(r) = 1/2 \text{Tr}(\Pi^{\pm} S|_r) = \int 1/2 \text{tr}(P^{\pm}(p) w(r, p)) dp; \]

the matrices \( P^{\pm}(p) \) are the projection operators into the eigenspaces of the classical symbol \( h_0 \) of the quantum Hamiltonian \( H_0 \), that is:

\[ H_0 = \text{Op}(h_0), \quad h_0(p) = E_+^{(p)} P^+(p) + E_-^{(p)} P^-(p), \]

and \( E^{\pm}(p) \) are the eigenvalues of \( h_0 \):

\[ E^{\pm}(p) = \pm \nu_F |p|. \]
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Quantum Entropy

We define the quantum entropy functional with two equivalent formulations.

\[ W(w) := \int \frac{1}{2} \text{tr}(w \log(w) - 1 + h/\theta) \, drdp \]

\[ A(S) := \frac{1}{2} \text{Tr}(S \log(S) - 1 + H/\theta) \]

where \( S = \text{Op}(w) \) is the density operator which represents the state of the system, \( \log(w) := \text{Op}^{-1} \log \text{Op}(w) \) is the so-called quantum logarithm of \( w \), \( \theta = k_B T \), \( k_B \) is the Boltzmann constant, and \( T > 0 \) is the system temperature (which we assume constant) and \( H = \text{Op}(h) \) is the Hamiltonian.
Quantum Entropy

We define the *quantum entropy functional* with two equivalent formulations.

▶ Wigner function formulation:

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A(w) := \int \frac{1}{2} \text{tr}(w(\log(w) - 1 + \frac{h}{\theta})) \, dp \, dq
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▶ Density operators formulation:

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Hamiltonian

Notice an important fact:

\[ H = \text{Op} \left( \frac{|\mathbf{p}|^2}{2m} \sigma_0 + v \mathbf{F} \cdot \mathbf{p} \right) = H_0 + \text{Op} \left( \frac{|\mathbf{p}|^2}{2m} \sigma_0 \right); \tag{H} \]

so \( H \neq H_0 \) defined in \( (H_0) \), but we added a quadratic term in \( |\mathbf{p}| \). This choice is justified by two reasons:

▶ both the \( (H_0) \) and the \( (H) \) are approximations of the exact hamiltonian valid for \( |\mathbf{p}| \) small, but \( (H) \) is a more precise approximation than the \( (H_0) \) to describe equilibrium;

▶ if we choose \( (H_0) \) as the system hamiltonian, we would obtain a not summable equilibrium distribution, while the choice \( (H) \) assure that we obtain a summable equilibrium distribution with convergent moments.
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H = \text{Op} (|p|^2/m) + v_F \vec{\sigma} \cdot \vec{p} = H_0 + \text{Op} (|p|^2/m) ; \tag{H}
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- if we choose (H0) as the system hamiltonian, we would obtain a not summable equilibrium distribution, while the choice (H) assure that we obtain a summable equilibrium distribution with convergent moments.
Equilibrium distribution

Let $W$ be the set of all Wigner functions $w : \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow \mathbb{C}^2 \times \mathbb{C}^2$. For all $w \in W$ we set:

$$w \pm v_s(p) = w_0 \pm v_s.$$  

Moreover, let $\langle f \rangle = \int f(p) dp$ for all function $f(p)$ defined in $\mathbb{R}^2$. Finally, let $n = (n_+ , n_-)$ a couple of fluid-dynamic moments. We define the Wigner distribution at local thermal equilibrium related to moments $n$ the solution $w_{eq} = g[n]$ of the problem:

$$A(w_{eq}) = \min \{ A(w) : w \in W, \langle w \pm v_s \rangle = n \pm n_s \}$$ (CEM-D)
Equilibrium distribution

Let $\mathcal{W}$ the set of all Wigner functions $w : \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow \mathbb{C}^{2 \times 2}$.
For all $w \in \mathcal{W}$ we set:

$$w_\pm := w_0 \pm v_s(p)w_s.$$ 

Moreover, let $\langle f \rangle := \int f \, dp$ for all function $f(p)$ defined in $\mathbb{R}^2$. 

Finally, let $n = (n_+, n_-)$ a couple of fluid-dynamic moments.

We define the Wigner distribution at local thermal equilibrium related to moments the solution $w_{eq} = g[n]$ of the problem:

$$A(w_{eq}) = \min \left\{ A(w) : w \in \mathcal{W}, \langle w \pm \rangle = n \pm \right\}$$
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(CEM-D)
Equilibrium distribution

Let us define the lagrangian functional:

\[ \mathcal{L}(w, \xi_+, \xi_-) = A(w) + \int \left[ \xi_+ (n_+ - \langle w_+ \rangle) + \xi_- (n_- - \langle w_- \rangle) \right] dx , \]

for \( w \in \mathcal{W} \), \( \xi_\pm (r) \) real functions.
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for \( w \in \mathcal{W} \), \( \xi_\pm(r) \) real functions.

The Lagrange multipliers theory tells us that a necessary condition for the \( w^{eq} \) to solve the problem (CEM-D) is that the Gateau derivative of \( \mathcal{L} \) w.r.t. \( S = \text{Op}(w) \) must vanish at \( w = w^{eq}, \xi_+ = \xi_+^*, \xi_- = \xi_-^* \), for a suitable choice of \( \xi_+^*(r), \xi_-^*(r) \) (Lagrange multipliers):

\[ \frac{\delta \mathcal{L}}{\delta S}(w^{eq}, \xi_+^*, \xi_-^*) = 0 \]
Equilibrium distribution

By making some calculations we can deduce that the equilibrium distribution has the following form:

\[ g[n] = \exp(-h\xi) \equiv \exp(-1)(\exp(h\xi)) \]

\[ h\xi = (|p|^2 + A)\sigma_0 + Q(|p|) \cdot |p| \cdot \vec{\sigma}, \]

\[ Q(|p|) = c|p| + B, \]

where \( A = A(r), \) \( B = B(r) \) depends on the Lagrange multipliers \( \xi^* \pm (r), \) and have to be determined in such a way that \( \langle g[n] \rangle = n \pm . \) Notice that we perform the scaling (DSCAL) choosing:

\[ p_0 = \sqrt{m\theta}, \]

and we defined:

\[ c = \frac{v_F p_0}{\theta} = \frac{v_F}{\sqrt{m k_B T}} \text{Scaled Fermi Speed}. \]
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\[
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\end{cases}
\]

where \( A = A(r) , B = B(r) \) depends on the Lagrange multipliers \( \xi^*_\pm(r) \), and have to be determined in such a way that \( \langle g_\pm[n] \rangle = n_\pm \). Notice that we perform the scaling (DSCAL) choosing:

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QDE model, formal closure

Let \( n_\tau := (n_\tau^+, n_\tau^-) \) the couple of moments of the solution \( w_\tau \) of \((\text{WDIFF})\). The following result holds:

Theorem

Let us suppose that:

\[
(n_\tau^- + n_\tau^-, n_\tau^- - n_\tau^-) \to (n_\tau^+, n_\tau^-) \quad \text{as} \quad \tau \to 0,
\]

and:

\[
\langle (Tg[n_\tau^-])^\pm \rangle = 0 \quad \forall \tau > 0.
\]

Then \( n_\tau^+, n_\tau^- \) satisfy:

\[
\partial_t n_\tau^\pm = \langle (TTg[n_\tau^-])^\pm \rangle.
\]

(QDE-FORM)
QDE model, formal closure

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**Theorem**

*Let us suppose that:*

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\end{align*}
\]

*Then \( n_+ \), \( n_- \) satisfy:*

\[
\partial_t n_{\pm} = \langle (TTg[n])_{\pm} \rangle. \quad \text{(QDE-FORM)}
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The system (QDE-FORM) is formally closed, but very implicit. In order to write (QDE-FORM) in an explicit way, we make the \textit{semiclassical approximation}:
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We will expand the equilibrium distribution $g[n]$ at the first order in $\epsilon$, neglecting $O(\epsilon^2)$ terms.
The system (QDE-FORM) is formally closed, but very implicit. In order to write (QDE-FORM) in an explicit way, we make the *semiclassical approximation*:

\[ \epsilon \ll 1 \]

We will expand the equilibrium distribution \( g[n] \) at the first order in \( \epsilon \), neglecting \( O(\epsilon^2) \) terms. We start by approximating the quantum exponential.
Quantum exponential semiclassical expansion, general strategy

We present here a general strategy for expanding the quantum exponential of a complex hermitian matrix-valued classical symbol $a(r, p)$. Let us consider the following function of the real positive variable $\beta$:

$$f_{\epsilon}(\beta) := \exp(\epsilon (\beta a)) = \exp(\epsilon (\beta (a(0) + \epsilon a(1))))$$

We are interested in approximating it up to an arbitrary order w.r.t. $\epsilon$. To do so, we formally derive $f_{\epsilon}(\beta)$ w.r.t. $\beta$ and notice that $f_{\epsilon}(0) = I$. 


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$$a = a_\epsilon = a^{(0)} + \epsilon a^{(1)},$$

with $a^{(0)}(r, p), a^{(1)}(r, p)$ independent of $\epsilon$. 

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Quantum exponential semiclassical expansion, general strategy

\[
\begin{aligned}
\partial_\beta f_\epsilon(\beta) &= \frac{1}{2}(a_\epsilon \#_\epsilon f_\epsilon(\beta) + f_\epsilon(\beta) \#_\epsilon a_\epsilon), \\
f_\epsilon(0) &= I,
\end{aligned}
\]  

(FBETA)

where \( \#_\epsilon \) is the so-called Moyal product, defined as:

\[
a\#_\epsilon b = \text{Op}_\epsilon^{-1}(\text{Op}_\epsilon(a) \text{Op}_\epsilon(b)),
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for all \( a(r, p), b(r, p) \) classical symbols.
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It is known in literature that, for all \( a(r, p), b(r, p) \) classical symbols:

\[
a_\epsilon \#_\epsilon b = \sum_{k=0}^{\infty} \epsilon^k \sum_{|\alpha_1| + |\alpha_2| = k} \left( \frac{i}{2} \right)^k \frac{(-1)^{|\alpha_2|}}{\alpha_1 \alpha_2} \partial_r^{\alpha_1} \partial_p^{\alpha_2} a \partial_r^{\alpha_2} \partial_p^{\alpha_1} b;
\]
Quantum exponential semiclassical expansion, general strategy

\[
\begin{aligned}
\left\{ \begin{array}{l}
\partial_{\beta} f_\epsilon(\beta) = \frac{1}{2} (a_\epsilon \#_\epsilon f_\epsilon(\beta) + f_\epsilon(\beta) \#_\epsilon a_\epsilon), \\
f_\epsilon(0) = I,
\end{array} \right.
\end{aligned}
\]

where \(\#_\epsilon\) is the so-called Moyal product, defined as:

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\]

so we write: \(\#_\epsilon = \sum_{k=0}^{\infty} \epsilon^k \#^{(k)}\), \(f(\beta) = \sum_{k=0}^{\infty} \epsilon^k f^{(k)}(\beta)\), we substitute these two expansions inside the (FBETA) and matching the terms with equal power of \(\epsilon\) we find the following hierarchy:
Quantum exponential semiclassical expansion, general strategy

\[
\begin{aligned}
\partial_\beta f^{(0)}(\beta) &= \frac{1}{2} (a^{(0)} f^{(0)}(\beta) + f^{(0)}(\beta) a^{(0)}) \\
f^{(0)}(0) &= I \\
\partial_\beta f^{(1)}(\beta) &= \frac{1}{2} (a^{(0)} f^{(1)}(\beta) + f^{(1)}(\beta) a^{(0)} a^{(1)} f^{(0)}(\beta) + f^{(0)}(\beta) a^{(1)} + a^{(0)} \#^{(1)} f^{(0)}(\beta) + f^{(0)}(\beta) \#^{(1)} a^{(0)}) \\
f^{(1)}(0) &= 0 \\
\partial_\beta f^{(2)}(\beta) &= \frac{1}{2} (a^{(0)} f^{(2)}(\beta) + f^{(2)}(\beta) a^{(0)} a^{(1)} f^{(1)}(\beta) + f^{(1)}(\beta) a^{(1)} + a^{(1)} \#^{(1)} f^{(0)}(\beta) + f^{(0)}(\beta) \#^{(1)} a^{(1)} + a^{(0)} \#^{(2)} f^{(0)}(\beta) + f^{(0)}(\beta) \#^{(2)} a^{(0)}) \\
f^{(2)}(0) &= 0
\end{aligned}
\]
Quantum exponential semiclassical expansion, general strategy

for each $n \geq 1$, the $n^{\text{th}}$ system of the previous hierarchy is a Cauchy problem for a first-order linear ODE with constant coefficients and forcing terms (equal to zero for the first system) containing only:

$$f^{(0)}(\beta) \ldots f^{(n-2)}(\beta);$$

by solving the first $n$ systems of the hierarchy we find an approximation of $f_\epsilon(\beta)$ up to an order $O(\epsilon^n)$. 
Quantum exponential semiclassical expansion, first order

We apply this strategy to compute the $O(\epsilon^2)$—approximation of $\exp(a)$ when the classical symbol $a$ is independent of $\epsilon$. Let:

$$\{f, g\} = \hat{\nabla}_r f \cdot \hat{\nabla}_p g - \hat{\nabla}_p f \cdot \hat{\nabla}_r g,$$

for all $f(r, p), g(r, p)$ scalar smooth functions.
For all $a = a_0 \sigma_0 + \bar{a} \cdot \bar{\sigma}$ the following holds:
Quantum exponential semiclassical expansion, first order

\[ \mathcal{E}x p(a) = \mathcal{E}x p(a)^{(0)} + \epsilon \mathcal{E}x p(a)^{(1)} + O(\epsilon^2) \quad (\epsilon \to 0), \]

\[ \mathcal{E}x p(a)^{(0)} = e^{a_0} \left( \cosh |\vec{a}| + \frac{\sinh |\vec{a}|}{|\vec{a}|} \vec{a} \cdot \vec{\sigma} \right), \]

\[ \mathcal{E}x p(a)^{(1)} = -\frac{e^{a_0}}{2} \left\{ \frac{1}{2|\vec{a}|^2} \left[ \cosh |\vec{a}| - \frac{\sinh |\vec{a}|}{|\vec{a}|} \right] \eta_{rsj} a_r \{ a_s, a_j \} \sigma_0 + \eta_{rsj} \left[ \frac{1}{4} \left( \frac{\sinh |\vec{a}|}{|\vec{a}|} + \frac{|\vec{a}| \cosh |\vec{a}| - \sinh |\vec{a}|}{|\vec{a}|^3} \right) a_s \{ a_0, a_j \} + \right. \]

\[ + \left( \frac{1}{2} \left( \delta_{sk} - \frac{a_s a_k}{|\vec{a}|^2} \right) \right) \frac{\sinh |\vec{a}|}{|\vec{a}|} + \]

\[ + \frac{a_s a_k}{4|\vec{a}|^2} \left( \cosh |\vec{a}| + \frac{\sinh |\vec{a}|}{|\vec{a}|} \right) \right\} \{ a_k, a_j \} \sigma_r \right\}. \]
By substituting $a = -\hbar \xi$ modified hamiltonian with diffusive scaling in the previous expansion and making some straightforward computations, we obtain:

$$
g[n] = e^{-\left(\frac{|p|^2}{2} + A\right)} \left\{ \cosh(Q\sigma_0) - \sinh(Q\sigma_0) |p| (p_1\sigma_1 + p_2\sigma_2) \right\} + \epsilon^2 |p|^2 \left[ (Q^4 \cosh(Q) + 3) \right] \left( p_1 \partial_r^2 - p_2 \partial_r^1 \right) B + 1 - Q^2 \sinh(Q) \left( p_1 \partial_r^2 - p_2 \partial_r^1 \right) \sigma_3 \right\} + O(\epsilon^2).
$$

By imposing the constraints:

$$
\langle g[n] \rangle = n \pm \epsilon
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By substituting \( a = -h_\xi \) modified Hamiltonian with diffusive scaling in the previous expansion and making some straightforward computations, we obtain:

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g[n] = e^{-(|p|^2/2 + A)} \left\{ \cosh(Q)\sigma_0 - \frac{\sinh(Q)}{|p|}(p^1\sigma_1 + p^2\sigma_2) + \epsilon \frac{2}{|p|^2} \left[ \left( \frac{Q}{4} \cosh(Q) + \frac{3}{4} \sinh(Q) \right)(p^1\partial_{r_2} - p^2\partial_{r_1})B + \frac{1 - Q^2}{4Q} \sinh(Q)(p^1\partial_{r_2} - p^2\partial_{r_1})A \right] \sigma_3 \right\} + O(\epsilon^2)
\]
Equilibrium distribution semiclassical expansion

By substituting $a = -\hbar \xi$ modified hamiltonian with diffusive scaling in the previous expansion and making some straightforward computations, we obtain:

$$
\begin{align*}
g[n] &= e^{-(|p|^2/2+A)} \left\{ \cosh(Q)\sigma_0 - \frac{\sinh(Q)}{|p|}(p^1\sigma_1 + p^2\sigma_2) + \\
&+ \frac{\epsilon}{2|p|^2} \left[ \left( \frac{Q}{4} \cosh(Q) + \frac{3}{4} \sinh(Q) \right)(p^1\partial_{r_2} - p^2\partial_{r_1})B + \\
&\frac{1 - Q^2}{4Q} \sinh(Q)(p^1\partial_{r_2} - p^2\partial_{r_1})A \right] \sigma_3 \right\} + O(\epsilon^2).
\end{align*}
$$

By imposing the constraints: $\langle g_\pm[n] \rangle = n_\pm$ we find:
Equilibrium distribution semiclassical expansion

\[ A = \frac{1}{2} \log \left( \frac{4\pi^2 \Gamma_+ \Gamma_-}{n_+ n_-} \right), \quad B = \frac{1}{2} \log \left( \frac{\Gamma_+ n_-}{\Gamma_- n_+} \right), \]

up to \( O(\epsilon^2) \) terms, with:

\[ \Gamma_\pm = \Phi(\pm c), \quad \Phi(z) = 1 - ze^{z^2/2} \int_z^\infty e^{-\rho^2/2} \, d\rho \quad \forall z \in \mathbb{R}. \]
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At this point, after some computations we finally obtain the following diffusive model, which we name QDE:
QDE model

\[ \partial_t n_\pm = \Delta \left( \frac{n_+ + n_-}{2} \right) + \text{div}(\sigma_+ \vec{\nabla} n_+ + \sigma_- \vec{\nabla} n_-) \]
\[ \pm \left[ \Delta \left( \frac{n_+ - n_-}{4} \right) + Q_+ + Q_- \right] + O(\epsilon), \]  

where we defined the following functions of \( n_\pm \):

\[ Q_\pm = \zeta_\pm \vec{\nabla} V \cdot \vec{\nabla} n_\pm + (A_\pm \Delta V + \lambda_\pm |\vec{\nabla} V|^2) n_\pm, \]
\[ \sigma_\pm = -\frac{1}{16\pi n_\pm} \sqrt{\frac{n_+ n_-}{\Gamma_+ \Gamma_-}} \int e^{-|p|^2/2} \left[ \frac{1 \pm 3Q - Q^2}{Q} \sinh(Q) \pm \cosh(Q) \right] dp, \]
\[ \zeta_\pm = 2A_\pm - \frac{1}{16\pi n_\pm} \sqrt{\frac{n_+ n_-}{\Gamma_+ \Gamma_-}} \int e^{-|p|^2/2} \left[ \frac{1 \pm 3Q - Q^2}{Q} \sinh(Q) \pm \cosh(Q) \right] \frac{dp}{|p|}, \]
\[ Q = c |p| + \frac{1}{2} \log \left( \frac{n_- \Gamma_+}{n_+ \Gamma_-} \right), \]

and \( A_\pm, \lambda_\pm \) are (known) constants.
QDE model: remarks

- Second order w.r.t. space derivatives;
- Neglected $O(\epsilon)$ terms (very low accuracy);
- Necessary to evaluate 2 integrals at each step during numerical resolution.

→ Not a very nice model.

In the following, we will build another diffusive model, which will rely on further hypothesis but will be simpler and more expressive than the (QDE).
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Wigner equations: refinement

The Wigner system (WE) is built from the one particle hamiltonian ($H_0$), which describes the electronic motion near a Dirac point: it can be seen as a first order approximation w.r.t. the (crystal) momentum $p$. The hamiltonian ($H$) is a more precise approximation of the correct system hamiltonian, so we will build a new set of Wigner equations by using ($H$).

The "refined" Wigner equations for graphene are:

$$\begin{align*}
\partial_t w_0 + [\vec{p}_m \cdot \vec{\nabla}] w_0 + v_F \vec{\nabla} \cdot \vec{w}_0 + \Theta \hbar (V) w_0 &= w_{eq} - w_0 \\
\partial_t \vec{w} + [\vec{p}_m \cdot \vec{\nabla}] \vec{w} + v_F [\vec{\nabla} w_0 + 2 \hbar \vec{w} \wedge \vec{p}] + \Theta \hbar (V) \vec{w} &= \vec{w}_{eq} - \vec{w}_0
\end{align*}$$

(WE2)

The (WE2) are identical to the (WE) except for the presence of the drift terms: $[\vec{p}_m \cdot \vec{\nabla}] w_0$, $[\vec{p}_m \cdot \vec{\nabla}] \vec{w}$. 
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    \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{w_0^\text{eq} - 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{w}^\text{eq} - \vec{w}}{\tau_c}
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\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_h(V) \vec{w} &= \frac{\vec{w}^{eq} - \vec{w}}{\tau_c}
\end{align*}$$

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The (WE2) are identical to the (WE) except for the presence of the drift terms:

$$\left[ \frac{\vec{p}}{m} \cdot \vec{\nabla} \right] w_0, \quad \left[ \frac{\vec{p}}{m} \cdot \vec{\nabla} \right] \vec{w}.$$
Further approximations

Remember the quantum maxwellian we found:

\[ g[n] = \exp(-\hbar \xi) \]

\[ \hbar \xi = (|p|^2 \sigma_0 + c|p| + B \vec{p} |p| \cdot \vec{\sigma}) \]

Recall also that:

\[ c = v_F \sqrt{m k_B T} \]

We perform two further approximations, which we call SMS (Strongly Mixed State):

\[ c = O(\epsilon) \]

\[ B = O(\epsilon) \]
Further approximations

Remember the quantum maxwellian we found:

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\[ h_\xi = \left( \frac{|p|^2}{2} + A \right) \sigma_0 + (c |p| + B) \frac{\vec{p}}{|p|} \cdot \vec{\sigma}; \]

recall also that:

\[ c = v_F \sqrt{\frac{m}{k_B T}}. \]

We perform two further approximations, which we call SMS (Strongly Mixed State):
Further approximations

Remember the quantum maxwellian we found:

\[ g[n] = \exp(-h_\xi), \]

\[ h_\xi = \left( \frac{|p|^2}{2} + A \right) \sigma_0 + (c |p| + B) \frac{\hat{p}}{|p|} \cdot \vec{\sigma}; \]

recall also that:

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We perform two further approximations, which we call SMS (Strongly Mixed State):

\[ c = O(\epsilon), \quad B = O(\epsilon). \]
Further approximations

We will see that the two approximations will result in the fact:

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

where:

\[
n_0 = \frac{1}{2} (n_+ + n_-) \quad \text{particle density},
\]

\[
n_\sigma = \frac{1}{2} (n_+ - n_-) \quad \text{band gap density}.
\]

This means that the charge carriers have more or less the same probability of being found in the conduction band or in the valence band of the energy spectrum, or equivalently, there is little difference (w.r.t. the total charge density) between the electron density and the hole density.
We perform the following diffusive scaling of the Wigner equations (WE2):

\[
\begin{align*}
\mathbf{x} & \mapsto x_0 \mathbf{x}, \\
\mathbf{t} & \mapsto t_0 \mathbf{t}, \\
\mathbf{p} & \mapsto p_0 \mathbf{p}, \\
\mathbf{V} & \mapsto V_0 \mathbf{V},
\end{align*}
\]

\[
\frac{2}{\hbar} v_F p_0^2 = V_0 x_0 p_0, \\
\frac{2}{\hbar} p_0^2 v_F \tau_c = \hbar \tau c v_F x_0, \\
p_0 = \sqrt{m k_B T},
\]

\(\epsilon\) is the semiclassical parameter; \(\tau\) is the diffusive parameter.
Wigner equations, diffusive scaling

We perform the following diffusive scaling of the Wigner equations \((\text{WE2})\):

\[
\begin{cases}
x \mapsto x_0 x, & t \mapsto t_0 t, & p \mapsto p_0 p, & V \mapsto V_0 V, \\
\frac{2v_F p_0}{\hbar} = \frac{V_0}{x_0 p_0}, & \frac{2p_0 v_F \tau_c}{\hbar} = \frac{\hbar}{2p_0 v_F t_0}, & p_0 = \sqrt{mk_B T}, & (\text{DSCAL2})
\end{cases}
\]

\[\epsilon := \frac{\hbar}{x_0 p_0}, \quad \tau := \frac{\tau_c v_F}{x_0}.\]
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We perform the following diffusive scaling of the Wigner equations (WE2):

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\epsilon &:= \frac{\hbar}{x_0 p_0}, \quad \tau := \frac{\tau_c v_F}{x_0}.
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$\epsilon$ is the \textit{semiclassical parameter};
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\]

(DSCAL2)

- \( \epsilon \) is the *semiclassical parameter*;
- \( \tau \) is the *diffusive parameter*.
Wigner system in diffusive scaling

We obtain the following scaled Wigner system:

\[
\begin{align*}
\tau \partial_t w_0 + \tilde{T}_0(w) &= \frac{w_0^{eq} - w_0}{\tau} \\
\tau \partial_t w_s + \tilde{T}_s(w) &= \frac{w_s^{eq} - w_s}{\tau} \quad s = 1, 2, 3
\end{align*}
\]  
(WDIFF2)

where:

\[
\begin{align*}
\tilde{T}_0(w) &= \frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2} \partial^s w_s + \Theta \epsilon [V] w_0 , \\
\tilde{T}_j(w) &= \frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} \hat{w} + \frac{\epsilon}{2} \partial^j w_0 + \Theta \epsilon [V] w_j + \eta_{jsk} w_s p^k ,
\end{align*}
\]

and:

\[
\gamma = \frac{c}{\epsilon} = \mathcal{O}(1) \quad (\epsilon \to 0).
\]
QDE model, formal closure

Let \( n_\tau := (n_\tau +, n_\tau -) \) the couple of moments of the solution \( w = w_\tau \) of \((\text{WDIFF2})\). The following result holds:

Theorem

Let us suppose that:

\( n_\tau \to (n_\tau +, n_\tau -) \) as \( \tau \to 0 \),

and:

\[ \langle (\tilde{T} g[n_\tau])^\pm \rangle = 0 \quad \forall \tau > 0. \]

Then \( n_\tau +, n_\tau - \) satisfy:

\[ \partial_t n_\tau^\pm = \langle (\tilde{T} \tilde{T} g[n_\tau])^\pm \rangle. \]

\((\text{QDE2-FORM})\)
QDE model, formal closure

Let \( n^\tau := (n^\tau_+, n^\tau_-) \) the couple of moments of the solution \( w = w^\tau \) of (WDIFF2). The following result holds:

**Theorem**

Let us suppose that:

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n^\tau &\to n = (n_+, n_-) \quad \text{as } \tau \to 0, \\
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\end{align*}
\]

Then \( n_+, n_- \) satisfy:

\[
\partial_t n_\pm = \langle (\tilde{T} \tilde{T} g[n])_\pm \rangle. \quad \text{(QDE2-FORM)}
\]
For the sake of simplicity let us redefine $B \rightarrow \epsilon B$ and consider $B = O(1)$.

Under our hypothesis, the classical symbol of the modified hamiltonian becomes:

$$h_{\xi} = h_0\xi + \epsilon h_1\xi,$$

where $h_0\xi = |p|^2 + A$, and $h_1\xi = (\gamma |p| + B) \vec{p} |p| \cdot \vec{\sigma}$; that is, the modified hamiltonian decouples in a scalar part of order $O(1)$ and a spinorial part of order $O(\epsilon)$.

This fact leads to remarkable simplifications in computations.
Modified hamiltonian

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Equilibrium distribution, semiclassical approximation
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Thanks to the approximations we have done, the quantum maxwellian $g[n] = \exp(-h_\xi)$ reduces to:

$$\begin{cases} 
    g_0[n] = \exp \left( -\frac{|p|^2}{2} - A \right) + O(\epsilon^3), \\
    \bar{g}[n] = -\epsilon e^{-|p|^2/2 - A} (B + \gamma |p|) \frac{\bar{p}}{|p|} + O(\epsilon^3); 
\end{cases}$$
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\vec{g}[n] &= -\epsilon e^{-|p|^2/2-A} (B + \gamma |p|) \frac{\vec{p}}{|p|} + O(\epsilon^3);
\end{align*}
\]

recall the constraints on \( g[n] \):

\[
\langle g_0[n] \rangle = n_0, \quad \langle g_\sigma[n] \rangle \equiv \langle \vec{g}[n] \cdot \vec{p}/|p| \rangle = n_\sigma;
\]
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Thanks to the approximations we have done, the quantum maxwellian $g[n] = \mathcal{E}\exp(-h\xi)$ reduces to:

$$
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\begin{array}{l}
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\end{array}
\right.
\end{align*}
$$

recall the constraints on $g[n]$:

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\langle g_0[n] \rangle = n_0, \quad \langle g_\sigma[n] \rangle \equiv \langle \bar{g}[n] \cdot \vec{p}/|p| \rangle = n_\sigma;
$$

because of $g_0[n]$ contains only $A(r)$ and not $B(r)$, the first equation can be solved independendly from the second; moreover, the specific form of $g_0[n]$ and of the constraint on it tell us that $g_0[n]$ is the $O(\epsilon^3)$-approximation of the quantum maxwellian of the scalar case related to the moment $n_0$, which is well know in literature.
Equilibrium distribution, semiclassical approximation

By solving the constraints on $g[n]$ we are able to write $A(r), B(r)$ as functions of $n_0, n_σ$, and we obtain the following form for $g[n]$:

$$
\begin{cases}
  g_0[n] = \frac{n_0}{2\pi} e^{-|p|^2/2} \left[ 1 + \frac{\epsilon^2}{24} \left( \nabla \cdot (I - \vec{p} \otimes \vec{p}) \nabla \log n_0 \right) \right] + O(\epsilon^3), \\
  \bar{g}[n] = \epsilon \frac{n_0}{2\pi} e^{-|p|^2/2} \left[ \frac{n_σ}{\epsilon n_0} + \gamma \left( \sqrt{\frac{\pi}{2}} - |p| \right) \right] + O(\epsilon^3).
\end{cases}
$$

We point out that, during the computations, we find:

$$
\epsilon n_0 \left( B + \gamma \sqrt{\frac{\pi}{2}} \right) = -n_σ + O(\epsilon^3),
$$

so we have $n_σ/n_0 = O(\epsilon)$ as anticipated.
Equilibrium distribution, semiclassical approximation

By solving the constraints on \( g[n] \) we are able to write \( A(r) \), \( B(r) \) as functions of \( n_0 \), \( n_{\sigma} \), and we obtain the following form for \( g[n] \):

\[
\begin{align*}
g_0[n] &= \frac{n_0}{2\pi} e^{-|p|^2/2} \left[ 1 + \frac{\epsilon^2}{24} \left( \nabla \cdot (I - \overrightarrow{p} \otimes \overrightarrow{p}) \nabla \log n_0 \right) \right] + O(\epsilon^3), \\
g[n] &= \epsilon \frac{n_0}{2\pi} e^{-|p|^2/2} \left[ \frac{n_{\sigma}}{\epsilon n_0} + \gamma \left( \sqrt{\frac{\pi}{2}} - |p| \right) \right] + O(\epsilon^3).
\end{align*}
\]

We point out that, during the computations, we find:

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\epsilon n_0 \left( B + \gamma \sqrt{\frac{\pi}{2}} \right) = -n_{\sigma} + O(\epsilon^3),
\]

so we have \( n_{\sigma}/n_0 = O(\epsilon) \) as anticipated. Finally, by making all the straightforward computations needed, we obtain the second quantum diffusive model we were looking for:
QDE2 model

\[
\begin{aligned}
\partial_t n_0 &= D_{00} \Delta n_0 + D_{0\sigma} \Delta n_\sigma + \frac{\vec{\nabla}}{2\gamma} \cdot [n_0 \vec{\nabla}(V + V_B)] + O(\epsilon^3), \\
\partial n_\sigma &= D_{\sigma 0} \Delta n_0 + D_{\sigma \sigma} \Delta n_\sigma - \frac{\vec{\nabla}}{2\gamma} \cdot \left[ \left( n_\sigma + \epsilon\gamma \sqrt{\frac{\pi}{2}} n_0 \right) \vec{\nabla} V \right] \\
&+ \frac{1}{2} |\vec{\nabla} V|^2 \left[ -\Gamma n_\sigma + \epsilon\gamma \sqrt{\frac{\pi}{2}} (2 - \Gamma) n_0 \right] \\
&+ \frac{1}{4\gamma} \Delta V \left[ n_\sigma + \epsilon\gamma \sqrt{\frac{\pi}{2}} n_0 \right] + O(\epsilon^3),
\end{aligned}
\]

(QDE2)

where we defined the Böhm potential:

\[ V_B = -\frac{\epsilon^2}{6} \frac{\Delta \sqrt{n_0}}{\sqrt{n_0}} , \]

and the following constants:

\[ D_{00} = \frac{1}{4\gamma^2} + \frac{\epsilon^2}{4} (1 - \gamma(4 - \pi)), \quad D_{0\sigma} = \frac{\epsilon}{4\gamma} \sqrt{\frac{\pi}{2}}, \quad D_{\sigma 0} = \frac{\epsilon}{8\gamma} \sqrt{\frac{\pi}{2}}, \quad D_{\sigma \sigma} = \frac{1}{4\gamma^2} \quad \Gamma = \frac{1}{2\pi} \int_0^\infty e^{-\rho^2/2} \rho \log \rho \, d\rho \approx 0.92256 \times 10^{-2}. \]
QDE2 model: remarks

Fourth order w.r.t. space derivatives (higher order model than the (QDE) model);

- neglected $O(\epsilon^3)$ terms (improved accuracy w.r.t. (QDE) model);

- presence of the Bohm potential in the equation for $n_0$ like in the scalar case, but also presence of a spinorial term, $\Delta n_\sigma$.

- $n_\sigma / n_0$ must be $O(\epsilon)$ for consistency with the hypothesis made; but the equation for $n_\sigma$ is a linear PDE with forcing term $O(\epsilon)$, so we expect that, for a suitable choice of the initial data and the potential, $n_\sigma / n_0 = O(\epsilon)$. 

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Now we are going to build an hydrodynamic model for graphene. We start by using a “rough” approach similar to that one which we employed to build the (QDE) model. Let us reconsider the first set of Wigner equations (WE) and do the following hydrodynamic scaling:

\[
\begin{align*}
&x \mapsto x_0, \\
&t \mapsto t_0, \\
&p \mapsto p_0, \\
&V \mapsto V_0,
\end{align*}
\]

\[
\begin{align*}
&t_0 = 2v_F p_0 \hbar = V_0 x_0 p_0, \\
&p_0 = \sqrt{mk_B T}, \\
&\epsilon := \hbar x_0 p_0, \\
&\tau := \tau_c t_0.
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(HSCAL) ▶ \(\epsilon\) is the semiclassical parameter; ▶ \(\tau\) is the hydrodynamic parameter.
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\begin{cases}
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  \frac{1}{t_0} = \frac{2v_F p_0}{\hbar} = \frac{V_0}{x_0 p_0} , & p_0 = \sqrt{mk_B T} , \\
  \epsilon := \frac{\hbar}{x_0 p_0} , & \tau := \frac{\tau_c}{t_0} .
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\]

\[
p_0 = \sqrt{mk_B T},
\]

\[
\epsilon := \frac{\hbar}{x_0 p_0}, \quad \tau := \frac{\tau_c}{t_0}.
\]

\[
\text{(HSCAL)}
\]

- $\epsilon$ is the \textit{semiclassical parameter};
- $\tau$ is the \textit{hydrodynamic parameter}.
The Wigner equations in hydrodynamic scaling

We obtain the following scaled Wigner system:

\[
\begin{align*}
\partial_t w_0 + \frac{\epsilon}{2} \grad \cdot \vec{w} + \Theta_\epsilon [V] w_0 &= \frac{w_0^{\text{eq}} - w_0}{\tau}, \\
\partial_t \vec{w} + \frac{\epsilon}{2} \grad w_0 + \vec{w} \wedge \vec{p} + \Theta_\epsilon [V] \vec{w} &= \frac{\vec{w}^{\text{eq}} - \vec{w}}{\tau}.
\end{align*}
\]  

(WHYDRO)
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\end{align*}
\]

(\text{WHYDRO})

$w^{\text{eq}}$ is the quantum thermal equilibrium Wigner distribution, which will be, however, different from the diffusive case, because we are going to choose a different set of moments.
Choice of moments

The moments we choose are the following six:
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\[ n_s = \int w_s \, dp \quad s = 0, 1, 2, 3, \]
\[ J^k = \int p^k w_0 \, dp \quad k = 1, 2. \]
Choice of moments

The moments we choose are the following six:

\[ n_s = \int w_s \, dp \quad s = 0, 1, 2, 3, \]
\[ J^k = \int p^k w_0 \, dp \quad k = 1, 2. \]

\( n_0 \) is the particle density, \( \vec{n} = (n_1, n_2, n_3) \) is the spin vector, \( \vec{J} = (J^1, J^2, 0) \) is the flow vector.
We choose the same quantum entropy of the diffusive case, and we define the equilibrium distribution $w_{eq}$ again through the MEP. Let $M = (n_0, \vec{n}, \vec{J})$ a set of given moments. We define the Wigner distribution at local thermal equilibrium related to moments $M$ the solution $w_{eq} = g[M]$ of the problem:

$$A(w_{eq}) = \min \left\{ A(w) : w \in C, \langle w \rangle_0 = n_0, \langle \vec{w} \rangle = \vec{n}, \langle \vec{p}w \rangle = \vec{J} \right\}$$
Equilibrium distribution, hydrodynamic model

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Equilibrium distribution, hydrodynamic model

We choose the same quantum entropy of the diffusive case, and we define the equilibrium distribution \( w^{eq} \) again through the MEP. Let \( M = (n_0, \vec{n}, \vec{J}) \) a set of given moments. We define the Wigner distribution at local thermal equilibrium related to moments \( M \) the solution \( w^{eq} = g[M] \) of the problem:

\[
\mathcal{A}(w^{eq}) = \min \{ \mathcal{A}(w) : w \in \mathcal{C}, \langle w_0 \rangle = n_0, \langle \vec{w} \rangle = \vec{n}, \langle \vec{p}w_0 \rangle = \vec{J} \}
\]
Equilibrium distribution, hydrodynamic model

If we apply the Lagrange multipliers method we find:

$$g[M] = \exp(-h\xi),$$

$$h\xi = (\frac{|p|^2}{2} + p_k\xi_k + \xi_0\sigma_0 + (\xi_0 s + cp_s)\sigma_s),$$

with $$\xi_0(r), (\xi_0 s) = 1, 2, 3, (\xi_k) = 1, 2.$$ Lagrange multipliers, and

c: scaled Fermi speed (the same expression of the diffusive model):

$$c := v_F p_0\theta = v_F \sqrt{m k_B T}.$$
Equilibrium distribution, hydrodynamic model

If we apply the Lagrange multipliers method we find:

\[ g[M] = \exp(-h_\xi), \]

\[ h_\xi = \left( \frac{|p|^2}{2} + p^k \xi^k_0 + \xi^0_0 \right) \sigma_0 + \left( \xi^0_s + cp^s \right) \sigma_s, \]

with \( \xi^0_0(r), (\xi^0_s(r))_{s=1,2,3}, (\xi^k_s(r))_{k=1,2} \) Lagrange multipliers, and \( c \) scaled Fermi speed (the same expression of the diffusive model):

\[ c := \frac{v_F p_0}{\theta} = v_F \sqrt{\frac{m}{k_B T}}. \]
The following theorem holds:

**Theorem**

Let $n_0^\tau, \vec{n}^\tau, \vec{J}^\tau$ hydrodynamic moments of a solution $w^\tau$ of the (WHYDRO). 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:

\[
\begin{align*}
\partial_t n_0 + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{n} &= 0 \\
\partial_t \vec{n} + \frac{\epsilon}{2} \vec{\nabla} n_0 + \langle \vec{g} \wedge \vec{p} \rangle &= 0 \\
\partial_t \vec{J} + \frac{\epsilon}{2} \vec{\nabla} \cdot \langle \vec{p} \otimes \vec{g} \rangle + n_0 \vec{\nabla} V &= 0
\end{align*}
\]  

(QHE-FORM)

where $g = g[n_0, \vec{n}, \vec{J}]$ is the local thermal equilibrium distribution.
Approximations for hydrodynamic model

We perform the semiclassical approximation \( \epsilon \ll 1 \) like in the diffusive case, but we make also another hypothesis, which we call LSFS (Low Scaled Fermi Speed) approximation:

\[
\mathcal{C} = O(\epsilon),
\]
so we write

\[
\mathcal{C} = \epsilon \gamma
\]
with \( \gamma = O(1) \).

This is a necessary hypothesis in order to obtain an explicit model; without this approximation it is not possible to express the equilibrium distribution as an explicit function of the moments \( M \).

By performing these approximations and imposing the constraints:

\[
\langle w_0 \rangle = n_0,
\]
\[
\langle \vec{w} \rangle = \vec{n},
\]
\[
\langle \vec{p} w_0 \rangle = \vec{J},
\]

after not short but straightforward calculations we find:
Approximations for hydrodynamic model

We perform the semiclassical approximation $\epsilon \ll 1$ like in the diffusive case, but we make also another hypothesis, which we call LSFS (Low Scaled Fermi Speed) approximation:

$$c = O(\epsilon),$$

so we write $c := \epsilon \gamma$ with $\gamma = O(1)$.

This is a necessary hypothesis in order to obtain an explicit model; without this approximation it is not possible to express the equilibrium distribution as an explicit function of the moments $M$.

By performing these approximations and imposing the constraints:

$$\langle w_0 \rangle = n_0,$$
$$\langle \vec{w} \rangle = \vec{n},$$
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after not short but straightforward calculations we find:
Equilibrium distribution for hydrodynamic model

\[ g[M] = \frac{n_0}{2\pi} e^{-\frac{1}{2} |\vec{p} - \vec{u}|^2} \left[ \sigma_0 + \vec{v} \cdot \vec{\sigma} + \epsilon \Lambda (\vec{p} - \vec{u}) \cdot \vec{\sigma} \right] + O(\epsilon^2), \]

\[ \Lambda(\vec{z}) := \frac{1}{8} \left[ (\zeta - \zeta^{-1}) |\vec{\nu}| + 1 \right] \frac{\vec{v}}{|\vec{v}|} \wedge (\vec{z} \cdot \vec{\nu}) \frac{\vec{v}}{|\vec{v}|} \]

\[ - c \left[ \frac{|\vec{v}|}{\zeta} \vec{z} + (1 - (1 + \zeta) |\vec{v}|) \frac{\vec{z} \cdot \vec{v}}{|\vec{v}|^2} \vec{v} \right] \quad \forall \vec{z} \in \mathbb{R}^3, \quad \text{(EQDH)} \]

\[ \zeta := \frac{1}{2} \log \left( \frac{1 + |\vec{\nu}|}{1 - |\vec{\nu}|} \right), \]

\[ \vec{v} := \frac{\vec{n}}{n_0}, \quad \vec{u} := \frac{\vec{j}}{n_0}. \]
QHE model

If we use the (EQDH) to explicitly compute the terms in (QHE-FORM) we find the following hydrodynamic equations:

\[
\begin{align*}
\partial_t n_0 + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{n} &= O(\epsilon^2) \\
\partial_t \vec{n} + \frac{\vec{n} \wedge \vec{J}}{n_0} + \frac{\epsilon}{2} \left[ \vec{\nabla} n_0 + F(n_0, |\vec{n}|)(\vec{n} \cdot \vec{\nabla} - \vec{\nabla} \cdot \vec{n}) \vec{n} \right] &= O(\epsilon^2) \\
\partial_t \vec{J} + \frac{\epsilon}{2} \vec{\nabla} \cdot \left( \frac{\vec{J} \otimes \vec{n}}{n_0} \right) + n_0 \vec{\nabla} V &= O(\epsilon^2)
\end{align*}
\]

(QHE)

where we defined, for \( a, b \in \mathbb{R}, 0 < b < a: \)

\[
F(a, b) := \frac{1}{4b^2} \left[ a + b \left( \log \sqrt{\frac{a+b}{a-b}} - \log^{-1} \sqrt{\frac{a+b}{a-b}} \right) \right].
\]
QHE model, remarks

First order w.r.t. space derivatives (low order model, which cannot account for diffusive effects); neglected $O(\epsilon^2)$ terms (more accurate than the (QDE) but less accurate than the (QDE2)).

We are going to improve the (QHE) model through a strategy similar to that one employed for the construction of the (QDE2) model.
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We are going to improve the (QHE) model through a strategy similar to that one employed for the construction of the (QDE2) model.
Further approximations

Remember the quantum maxwellian we found:

\[ g[n_0, \vec{n}, \vec{J}] = \exp(-\hbar \xi) , \]

\[ \hbar \xi = \left( \frac{|p|^2}{2} + p_{k} \xi_{k} + \xi_{0} \right) \sigma_0 + (\xi_{0} s + cp_{s}) \sigma_s . \]

We make the SMS approximation, that is we suppose (recall that we already made the hypothesis \( c = O(\epsilon) \)):

\[ |\vec{\xi}_0| = O(\epsilon) , \]

where \( \vec{\xi}_0 := (\xi_{0,1}, \xi_{0,2}, \xi_{0,3}) \).
Further approximations

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where \( \vec{\xi}^0 := (\xi_1^0, \xi_2^0, \xi_3^0) \).
Wigner equations in hydrodynamic scaling

We perform on the (WE2) the hydrodynamic scaling (HSCAL), obtaining:

\[
\begin{aligned}
\partial_t w_0 + \frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} w_0 + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{w} + \Theta_\epsilon [V] w_0 &= \frac{w_0^{eq} - w_0}{\tau}, \\
\partial_t \vec{w} + \frac{\vec{p} \cdot \vec{\nabla}}{2\gamma} \vec{w} + \frac{\epsilon}{2} \vec{\nabla} w_0 + \vec{w} \wedge \vec{p} + \Theta_\epsilon [V] \vec{w} &= \frac{\vec{w}^{eq} - \vec{w}}{\tau}.
\end{aligned}
\] (WHYDRO2)
QHE2 model, formal closure

Theorem

Let $n^\tau_0, \vec{n}^\tau, \vec{J}^\tau$ hydrodynamic moments of a solution $w^\tau$ of the (WHYDRO2). If $n^\tau_0 \to n_0, \vec{n}^\tau \to \vec{n}, \vec{J}^\tau \to \vec{J}$ as $\tau \to 0$, then the limit moments $n_0, \vec{n}, \vec{J}$ satisfy:

\[
\begin{align*}
\partial_t n_0 + \frac{\vec{\nabla}}{2\gamma} \cdot \vec{J} + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{n} &= 0 \\
\partial_t \vec{n} + \frac{\vec{\nabla}}{2\gamma} \cdot \langle \vec{p} \otimes \vec{g} \rangle + \frac{\epsilon}{2} \vec{\nabla} n_0 + \langle \vec{g} \wedge \vec{p} \rangle &= 0 \\
\partial_t \vec{J} + \frac{\vec{\nabla}}{2\gamma} \cdot \left( \frac{\vec{J} \otimes \vec{J}}{n_0} + \mathcal{P} \right) + \frac{\epsilon}{2} \vec{\nabla} \cdot \langle \vec{p} \otimes \vec{g} \rangle + n_0 \vec{\nabla} V &= 0
\end{align*}
\]

(QHE2-FORM)

where:

\[
\mathcal{P} = \langle (\vec{p} - \vec{u}) \otimes (\vec{p} - \vec{u})g_0 \rangle
\]

is the so-called quantum stress tensor, and $g = g[n_0, \vec{n}, \vec{J}]$ is the local thermal equilibrium distribution.
Modified hamiltonian

For the sake of simplicity, let us redefine:\n\[ \vec{\xi}_0 \mapsto \epsilon \vec{\xi}_0 \]\nand consider:\n\[ |\vec{\xi}_0| = O(1). \]

Under our hypothesis, the classical symbol of the modified hamiltonian becomes:\n\[ h_{\xi} = h_{0\xi} + \epsilon h_{1\xi}, \]
\[ h_{0\xi} = |p|^2 + \xi k_0 p k_0 + \xi_0 0, \]
\[ h_{1\xi} = (\gamma p s + \xi_0 s) \sigma s; \]
that is, the modified hamiltonian decouples in a scalar part of order \( O(1) \) and a spinorial part of order \( O(\epsilon) \).

This fact leads to remarkable simplifications in computations.
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$$h_\xi^0 = \frac{|p|^2}{2} + \xi_0^k p^k + \xi_0^0,$$
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Equilibrium distribution, semiclassical approximation

Thanks to the approximations we have done, the quantum maxwellian
\[ g[n_0, \vec{n}, J] = \exp(-\hbar \xi) \]
reduces to:
\[ \begin{align*}
  g[n_0, \vec{n}, J] &= \exp(-|p|^2/2 - \xi k_0 p - \xi_0) + O(\epsilon^3), \\
  \vec{g}[n_0, \vec{n}, J] &= -\epsilon e^{-|p|^2/2 - \xi k_0 p - \xi_0}(\vec{\xi}_0 + \gamma \vec{p}) + O(\epsilon^3);
\end{align*} \]

recall the constraints on \[ g[n_0, \vec{n}, J] \]:
\[ \langle g_0[n_0, \vec{n}, J] \rangle = n_0, \]
\[ \langle \vec{p} g_0[n_0, \vec{n}, J] \rangle = \vec{J}, \]
\[ \langle \vec{g}[n_0, \vec{n}, J] \rangle = \vec{n}; \]

because of \[ g_0[n_0, \vec{n}, J] \] contains only \( \xi_0 \), \( \xi_k \) \( k = 1, 2 \) and not \( \xi_s \) \( s = 1, 2, 3 \), the first two equations can be solved independently from the third; moreover, the specific form of \[ g_0[n_0, \vec{n}, J] \] and of the constraint on it tell us that \[ g_0[n_0, \vec{n}, J] \] is the \( O(\epsilon^3) \)-approximation of the quantum maxwellian of the scalar case related to the moments \( n_0, \vec{J} \), which is well known in literature.
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Thanks to the approximations we have done, the quantum maxwellian 
\( g[n_0, \vec{n}, \vec{J}] = \exp(-h\xi) \) reduces to:

\[
\begin{align*}
    g_0[n_0, \vec{n}, \vec{J}] &= \exp\left(-\frac{|p|^2}{2} - \xi_0^k p^k - \xi_0^0\right) + O(\epsilon^3), \\
    \bar{g}[n_0, \vec{n}, \vec{J}] &= -\epsilon e^{-|p|^2/2-\xi_0^k p^k-\xi_0^0(\vec{n}^0 + \gamma \vec{p})} + O(\epsilon^3);
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Thanks to the approximations we have done, the quantum maxwellian\n$g[n_0, \vec{n}, \vec{J}] = \exp(-h\xi)$ reduces to:

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g_0[n_0, \vec{n}, \vec{J}] = \exp \left( -\frac{|p|^2}{2} - \xi^k_0 p^k - \xi^0_0 \right) + O(\epsilon^3), \\
\bar{g}[n_0, \vec{n}, \vec{J}] = -\epsilon e^{-|p|^2/2-\xi^k_0 p^k-\xi^0_0} (\vec{\xi}^0 + \gamma \vec{p}) + O(\epsilon^3);
\end{cases}$$

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$$\langle g_0[n_0, \vec{n}, \vec{J}] \rangle = n_0, \quad \langle \vec{p}g_0[n_0, \vec{n}, \vec{J}] \rangle = \vec{J}, \quad \langle \bar{g}[n_0, \vec{n}, \vec{J}] \rangle = \vec{n};$$
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\end{align*}
$$

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$$
\langle g_0[n_0, \vec{n}, \vec{J}] \rangle = n_0, \quad \langle \tilde{p} g_0[n_0, \vec{n}, \vec{J}] \rangle = \vec{J}, \quad \langle \tilde{g}[n_0, \vec{n}, \vec{J}] \rangle = \vec{n};
$$

because of $g_0[n_0, \vec{n}, \vec{J}]$ contains only $\xi_0^0(r), (\xi_0^k(r))_{k=1,2}$ and not $(\xi_s^0(r))_{s=1,2,3}$, the first two equations can be solved independently from the third; moreover, the specific form of $g_0[n_0, \vec{n}, \vec{J}]$ and of the constraint on it tell us that $g_0[n_0, \vec{n}, \vec{J}]$ is the $O(\epsilon^3)$-approximation of the quantum maxwellian of the scalar case related to the moments $n_0, \vec{J}$, which is well known in literature.
So, by solving the constraint for \( g[n_0, \vec{n}, \vec{J}] \) we are able to write \( g[n_0, \vec{n}, \vec{J}] \) as a function of the moments \( n_0, \vec{n}, \vec{J} \); during the computation we find that from the SMS approximation follows:

\[
\frac{|\vec{n}|}{n_0} = \frac{\sqrt{n_1^2 + n_2^2 + n_3^2}}{n_0} = O(\epsilon),
\]

which is analogue to what we find in the diffusive case.
Equilibrium distribution, semiclassical approximation

So, by solving the constraint for $g[n_0, \vec{n}, \vec{J}]$ we are able to write $g[n_0, \vec{n}, \vec{J}]$ as a function of the moments $n_0, \vec{n}, \vec{J}$; during the computation we find that from the SMS approximation follows:

$$\frac{|\vec{n}|}{n_0} = \frac{\sqrt{n_1^2 + n_2^2 + n_3^2}}{n_0} = O(\epsilon),$$

which is analogue to what we find in the diffusive case. By using the $O(\epsilon^3)$-expansion of $g[n_0, \vec{n}, \vec{J}]$ to explicitly calculate the terms inside the (QHE2-FORM) we find the following hydrodynamic model, which we call (QHE2):
The QHE2 model

\[
\begin{align*}
\partial_t n_0 + \frac{\vec{\nabla} \cdot \vec{J}}{2\gamma} + \frac{\epsilon}{2} \vec{\nabla} \cdot \vec{n} &= O(\epsilon^3), \\
\partial_t \vec{n} + \frac{1}{2\gamma} \vec{\nabla} \cdot \left( \frac{\vec{J} \otimes \vec{n}}{n_0} \right) + \frac{\vec{n} \otimes \vec{J}}{n_0} &= O(\epsilon^3), \\
\partial_t \vec{J} + \frac{1}{2\gamma} \left[ \vec{\nabla} \cdot \left( \frac{\vec{J} \otimes \vec{J}}{n_0} \right) + \vec{\nabla} n_0 \right] + \frac{\epsilon}{2} \vec{\nabla} \cdot \left( \frac{\vec{J} \otimes \vec{n}}{n_0} \right) \\
&- \frac{\gamma \epsilon^2}{2} \vec{n}_0 + n_0 \vec{\nabla} (V + V_B) &= O(\epsilon^3),
\end{align*}
\]  

(QHE2)

where \( V_B \) is the Bôhm potential:

\[
V_B = -\frac{\epsilon^2}{6} \frac{\Delta \sqrt{n_0}}{\sqrt{n_0}}.
\]
QHE2 model, remarks

- Third order model (higher order than the QHE model); neglected $O(\epsilon^3)$ terms (more accurate than the (QHE) model);
- Presence of the Böhm potential in the equation for $\vec{J}$ like in the scalar case, but also presence of spinorial terms;
- $|\vec{n}|/n_0$ must be $O(\epsilon)$ for consistency with the hypothesis SMS made; but the equation for $\vec{n}$ is a linear homogeneous PDE, so we expect that, for a suitable choice of the initial data and the potential, $|\vec{n}|/n_0 = O(\epsilon)$. 
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Intentions for the future

- Numerical simulations with the (QDE2) and (QHE2) models, attempting to reproduce the features of charge transport in graphene, with particular attention to the so-called "Klein paradox" (unimpeded penetration of electrons through arbitrary high potential barriers).
- Study of the well-posedness of the (QDE2) and (QHE2) models.
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Thank you for your consideration!