Quantum hydrodynamical models arising from the Wigner equation in high-field regime

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Introduction

- Many devices work at **high-field** regimes. Huge literature about models "corrected" by quantum terms (F. Poupaud, P. Degond, N. Ben Abdallah, I.M. Gamba, A. Jüngel, V. Romano, and many others).

  Common point: semi-classical approach, i.e. Boltzmann equation for semiconductors.

- Advance in semiconductor technology requires to consider **quantum effects** at quasi-ballistic regimes

  \[ \Rightarrow \text{quantum macroscopic models.} \]

- **Quantum Wigner** kinetic description.

- **Wigner**-derived macroscopic models are analytically and numerically challenging.

- **Goal**: present a rigorous (still in progress) study of the accuracy of a **quantum** macroscopic model derived from the Wigner model via a Chapman-Enskog type procedure in high-field conditions.
Wigner-BGK equation

\[ w = w(x, v, t), \ (x, v) \in \mathbb{R}^6, \ t \geq 0 \] quasi-distribution function for an electron ensemble.

\[ \theta = \frac{1}{\kappa \beta} \] environment temperature, \( V \) applied potential (also self-consistent).

\[
\frac{\partial w}{\partial t} + v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w^{eq}), \quad t > 0,
\]

with \( \nu \) inverse relaxation-time, \( m \) effective mass, and \( \mathcal{F} = \mathcal{F}_{v \to \eta} \) Fourier transform.

\[
\Theta[V]w(x, v) := i \mathcal{F}^{-1}_v \left( \frac{1}{\hbar} V x + \frac{\hbar \eta}{2m} - V x - \frac{\hbar \eta}{2m} \right)
\]

since, by Taylor expansion around \( x \),

\[
\frac{i}{\hbar} V x + \frac{\hbar \eta}{2m} - V x - \frac{\hbar \eta}{2m} = \frac{i \eta}{m} \cdot \nabla V(x) + \frac{i \eta^2 \hbar^2}{24m^3} \eta \cdot \Delta \nabla V(x)
\]

then

\[
\Theta[V]w(x, v) = -\frac{1}{m} \nabla V(x) \cdot \nabla_v w(x, v) + \frac{\hbar^2}{24m^3} \nabla \Delta V(x) \cdot \nabla_v \Delta V(x)
\]
Wigner equation: semiclassical limit

From the Taylor expansion of the pseudo-differential term with respect to $\eta$ around $x$:

$$\Theta[V]w \xrightarrow{\hbar \to 0} - \frac{1}{m} \nabla_x V(x) \cdot \nabla_v w$$  \hspace{1cm} \text{Vlasov operator.}$$

$$\Theta[V]w = \frac{1}{m} \nabla_x V(x) \cdot \nabla_v w + \mathcal{O}(\hbar^2).$$

Fact:

$$\Rightarrow \quad \int v^k \Theta[V]w(x,v) \, dv = -(1/m) \int v^k \nabla V(x) \cdot \nabla_v w(x,v) \, dv$$

$$\Rightarrow \quad \text{quantum corrections due to } \Theta[V] \text{ appear for } k \geq 3.$$  

the $v$-moments of $\Theta[V]$ and of $-(1/m) \nabla_x V(x) \cdot \nabla_v$ coincide up to 2nd-order moments.

Instead:

$$\int v^3 \Theta[V]w \, dv = -\frac{1}{m} \int v^3 \nabla_x V(x) \cdot \nabla_v w \, dv + \frac{\hbar^2}{4m^3} n.$$
The thermal equilibrium state

\[ w^{eq}(x, v, t) = n(x, t) C e^{-\beta mv^2/2} \left\{ 1 + \hbar^2 \left[ -\frac{\beta^2 \Delta V(x)}{24m} + \frac{\beta^3}{24} \right] \right\} \]

\[ w^{eq}(x, v, t), \mathcal{O}(\hbar^2)\)-accurate local thermal equilibrium distribution function.

\[ \int w^{eq}(x, v, t) \, dv = n(x, t) := \int w(x, v, t) \, dv, \quad \text{electron position density.} \]

\[ \int v \, w^{eq}(x, v, t) \, dv = 0, \]

\[ \int v^2 \, w^{eq}(x, v, t) \, dv = \frac{3 \kappa \theta}{m} + \frac{\hbar^2}{12m^2 \kappa \theta} \Delta V(x) \]

with \( \theta = 1/(\kappa \beta) \) environment temperature. \( \beta, V(x) \) are given!

Quantum corrections due to \( w^{eq} \), which is \( \mathcal{O}(\hbar^2) \)-accurate, appear already.
The Macroscopic Quantities

Let us define the first and second order unknown macroscopic quantities, i.e. the fluid velocity and the energy density

\[ u = u(x, t) := \frac{1}{n} \int v w(x, v, t) \, dv \]

\[ \mathcal{W} = \mathcal{W}(x, t) := \int \frac{v^2}{2} w(x, v, t) \, dv \]

Moreover, we recall that we can split \( \mathcal{W} \) as

\[ \mathcal{W}(x, t) = \int \frac{(v - u)^2}{2} w(x, v, t) \, dv + n \frac{u^2}{2} =: \mathcal{W}_i(x, t) + \mathcal{K}(x, t) \]

- \( \mathcal{W}_i \) and \( \mathcal{K} \) indicate internal and kinetic velocity, respectively.
- In case of thermodynamical equilibrium with the bath individuated by \( w^{eq} \) for the moments of \( w^{eq} \) we deduce

\[ \Longrightarrow \text{ the fluid velocity is zero, i.e. } u^{eq}(x, t) \equiv 0 \]
**High-field Wigner-BGK equation**

\[ \epsilon w_t + \epsilon v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w^{eq}), \quad t > 0, \]

is the equation in the high-field scaling, where

\[ \epsilon \approx \frac{t_V}{t_0} \approx \frac{t_C}{t_0} \]

with \( t_V, t_C, t_0 \) characteristic times. 

**External potential and interaction with the environment** are the dominant mechanisms in the evolution and balance each other. 

At the leading order, \( \epsilon = 0 \), the solution of \( (\nu - \Theta[V])w = \nu w^{eq} \) is

\[ w^{(0)} := (\nu I - \Theta[V])^{-1} \nu w^{eq} = \nu \mathcal{F}^{-1} \frac{\mathcal{F}w^{eq}}{\nu - i \delta V} \]

The inverse operator \( (\nu - \Theta[V])^{-1} \) is defined in the Fourier space as the factor \( \nu(\nu - i \delta V(x, \eta))^{-1} \), which exists and is bounded for all \( V \) since \( \nu \).
Moments at the Leading Order

$$\epsilon = 0 \Rightarrow \Theta[V]w^{(0)} = \nu(w^{(0)} - w^{eq})$$

Then the moments of $w^{(0)}$ are

$$\int w^{(0)} dv = n$$
$$\int v w^{(0)} dv = -\frac{\nabla x V}{\nu m} n$$
$$\int v \otimes v w^{(0)} dv = \frac{\kappa \theta}{m} I + 2 \frac{\nabla x V}{\nu m} \otimes \frac{\nabla x V}{\nu m} + \frac{\hbar^2}{12 m^2 \kappa \theta} \nabla x \otimes$$
$$\int \frac{v^2}{2} w^{(0)} dv = -\frac{\nabla x V}{\nu m} \left( \int \frac{v^2}{2} w^{(0)} dv + \Pi^{(0)} \right) + \frac{\hbar^2}{8 m^3 \nu} \nabla$$

We remark that, at the leading order, $u^{(0)} = -\frac{\nabla x V}{\nu m}(x)$ is a nonzero-fluid velocity field is constant: in the high-field regime the fluid velocity reaches
The kinetic energy is $\mathcal{K}^{(0)} = \frac{n}{2}(x, t)\frac{\left|\nabla_x V\right|^2}{(\nu m)^2}(x)$, as a consequence

$$\mathcal{W}^{(0)} = \mathcal{W}_i^{(0)} + \mathcal{K}^{(0)} = \frac{n}{2} \frac{3\kappa\theta}{m} + \frac{\left|\nabla_x V\right|^2}{(\nu m)^2} + \frac{\hbar^2}{12m^2\kappa\theta} \Delta_x V$$

In the internal energy it appears a contribute due the external field, with a high-field assumption:

$$\frac{n\left|\nabla_x V\right|^2}{2(\nu m)^2}.$$ 

Instead, in case of a nonzero-fluid velocity equilibrium function $w^{eq}(x, v - w, t)$, the related energy density $\mathcal{W}^{eq}_w$ is

$$\mathcal{W}^{eq}_w = \mathcal{W}^{eq}_{w,i} + \mathcal{K}^{eq}_w = \frac{n}{2} \frac{3\kappa\theta}{m} + \frac{\hbar^2}{12m^2\kappa\theta} \Delta_x V$$

A field contributes in modifying the internal energy $\mathcal{W}_i^{(0)}$ if it has the same order of magnitude as the interaction with the environment.
From high-field Wigner-BGK equation we can obtain evolution equations for $n$ and $W^{(0)}$ by considering $w \simeq w^{(0)}$ and taking $v$-moments.

Then the energy density $W^{(0)}$ can change on time only because of transport.

$$\frac{\partial n}{\partial t} - \nabla_x \cdot n \nabla_x V = 0,$$

$$\frac{\partial W^{(0)}}{\partial t} - \nabla_x \cdot W^{(0)} \frac{\nabla_x V}{\nu m} - \nabla_x \cdot \Pi^{(0)} \frac{\nabla_x V}{\nu m} + \nabla_x \cdot \frac{\hbar^2}{8 m^3 \nu} \nabla_x \Delta V = 0.$$

Let us repeat that the equations above describe only transport, since the electrons are in a regime of drift-collision balance.

On the contrary of low-field case, diffusive term and heat-flux term will appear respectively only as $O(\epsilon)$ corrections via the Chapman-Enskog procedure.
Redistributing the energy density as

\[
\mathcal{W}^{(0)} = \int \frac{|v - u^{(0)}|^2}{2} w^{(0)} \, dv + \frac{n|u^{(0)}|^2}{2} = \mathcal{W}^{(0)}_i + \frac{n|u^{(0)}|^2}{2}
\]

with

\[
\mathcal{W}^{(0)}_i = \frac{n(x, t)}{2} \frac{3\kappa \theta}{m} + \frac{\nabla_x V^2(x)}{(\nu m)^2} + \frac{\hbar^2}{12m^2\kappa \theta} \Delta_x V(x)
\]

and defining

\[
\mathcal{P}^{(0)}(x, t) := \int (v - u^{(0)}) \otimes (v - u^{(0)}) \, w^{(0)}(x, t) \, dv
\]

Consequently, the equations read as follows:

\[
\frac{\partial n}{\partial t} - \nabla_x \cdot \mathcal{W}^{(0)}_i = 0
\]

\[
\frac{\partial \mathcal{W}^{(0)}_i}{\partial t} - \nabla_x \cdot \mathcal{W}^{(0)}_i \frac{\nabla_x V}{\nu m} - \nabla_x \cdot \mathcal{P}^{(0)} \frac{\nabla_x V}{\nu m} + \nabla_x \cdot \frac{\hbar^2}{8m^3\nu} \Delta_x V
\]

**Next steps:** Derive via a Chapman-Enskog procedure corrections of \(O(\epsilon)\) for the previous equations.
The Chapman-Enskog procedure

The procedure consists of two assumptions:

**First**, we assume that the microscopic unknown $w$ depends on time only through the macroscopic quantities. Since among the unknown $n$ and $\mathcal{W}^{(0)}$, the only $t$-dependent function is $n(\mathcal{W}(0))$, we express

$$\frac{\partial w}{\partial t} = \frac{\partial w}{\partial n} \frac{\partial n}{\partial t}.$$  

**Secondly**, we assume that the macroscopic unknown $n$ is an $O(1)$ quantity, while we use instead the following expansion

$$w = \sum_{k=1}^{\infty} \epsilon^k w^k \sim w^{(0)} + \epsilon w^{(1)}.$$  

to compute the other $v$-moments.

Let us compute the 0th-order moment of the high-field Wigner-BGK equation, the continuity equation for $n$

$$\frac{\partial}{\partial t} \int w dv + \nabla_x \cdot \int v w dv = 0.$$
This allows us to express $\frac{\partial w}{\partial t}$ in (2) as

$$\frac{\partial w}{\partial t} = \frac{\partial w}{\partial n} - \nabla_x \cdot \int vwdv .$$

By substituting this expression in the Wigner equation, we obtain

$$\epsilon \frac{\partial w}{\partial n} - \nabla_x \cdot \int vwdv \right) + \epsilon v \cdot \nabla_x w = \Theta[V]w - \nu(w - w_{eq}) .$$

Then we expand the unknown $w \sim w^{(0)} + \epsilon w^{(1)}$.

At the 0-th order in $\epsilon$, we obtain

$$\Theta[V]w^{(0)} - \nu(w^{(0)} - w_{eq}) = 0 ,$$
whose solution is given formally by

\[ w^{(0)} = (\nu - \Theta[V])^{-1} \nu w_{eq} \]

\[ = \mathcal{F}^{-1} \frac{\nu \mathcal{F}w_{eq}}{\nu - i\delta V(x, \eta)} \]

\[ (x, v, t) = n(x, t)M(x, v) \]

where

\[ M(x, v) := \mathcal{F}^{-1} \frac{\nu \mathcal{F}(F + \hbar^2 F^h)}{\nu - i\delta V(x, \eta)} \]

\[ (x, v) \]

At the first order in \( \epsilon \)

\[ \frac{\partial w^{(0)}}{\partial n} - \nabla_x \cdot \int vw^{(0)} dv + v \cdot \nabla_x w^{(0)} = \Theta[V] - \]

Taking into account \( \frac{\partial w^{(0)}}{\partial n} = M \), we obtain

\[ M \nabla_x \cdot n \frac{\nabla_x V}{\nu m} + v \cdot \nabla_x w^{(0)} = \Theta[V] - \nu \]

Then we have
Thus, we can rewrite the continuity equation with unknown $n$ by using the expressions for $w^{(0)}$ and $w^{(1)}$. We get a correction of order $O(\epsilon)$ for the continuity equation.

\[
\frac{\partial n}{\partial t} + \nabla_x \cdot \int v w^{(0)} dv + \epsilon \nabla_x \cdot \int v w^{(1)} dv = 0
\]

In order to write Eq. (3) in a more explicit form, we need the moments of $w^{(1)}$:

\[
\int w^{(1)} dv = 0
\]

\[
\int v w^{(1)} dv = -\frac{1}{\nu} \nabla_x \cdot \Pi^{(0)} + \frac{1}{\nu} \nabla_x \cdot n u^{(0)} u^{(0)}
\]

\[
\int v \otimes v w^{(1)} dv = -\frac{1}{\nu} \nabla_x \cdot \Pi^{(0)}_{nu} + \frac{1}{\nu} \nabla_x \cdot n u^{(0)} \frac{\Pi^{(0)}_{n}}{n} + ...
\]
Then Eq. (3) can be rewritten as

\[
\frac{\partial n}{\partial t} - \nabla_x \cdot n \frac{\nabla_x V}{\nu m} + \frac{\epsilon}{\nu} \nabla_x \cdot \nabla_x \cdot n \frac{\nabla_x V}{\nu m} + \frac{\nabla_x V}{\nu m} \]

\[
- \frac{\epsilon}{\nu} \nabla_x \cdot \nabla_x \frac{\nabla_x V}{\nu m} + \frac{\kappa \theta I}{m} + 2 \frac{\nabla_x V}{\nu m} \otimes \frac{\nabla_x V}{\nu m} + \frac{\hbar^2}{12 \nu \nu m} \nabla_x \otimes \nabla_x \nabla_x \cdot n \frac{\nabla_x V}{\nu m} + \frac{\epsilon}{\nu} \nabla_x \cdot \nabla_x \cdot n \frac{\nabla_x V}{\nu m}
\]

This is a drift equation with an $O(\epsilon)$-diffusive correction. Observe that by splitting the following term as

\[
\frac{\epsilon}{\nu} \nabla_x \cdot \frac{\nabla_x V}{\nu m} \nabla_x \cdot n \frac{\nabla_x V}{\nu m} = \frac{\epsilon}{\nu} \frac{\nabla_x \cdot \nabla_x V}{\nu m} \nabla_x \cdot n \frac{\nabla_x V}{\nu m} + \frac{\epsilon}{\nu} \frac{\nabla_x V}{\nu m} \nabla_x \cdot n \frac{\nabla_x V}{\nu m} + \frac{\epsilon}{\nu} \nabla_x \cdot n \frac{\nabla_x V}{\nu m}
\]

we derive the following high-field corrected version of the (classical) mobility coefficient $\mu_{\text{cl}}$:

\[
\mu_{\text{hf}} := \frac{1}{\nu m} \left( 1 + \frac{\epsilon}{\nu^2 m} \Delta_x V \right).
\]
High-field corrections to drift-collision balance system

Starting from

\[
\frac{\partial (nu)}{\partial t} + \nabla_x \cdot \int v \otimes vw \, dv + \frac{1}{\epsilon} \frac{\nabla_x V}{m} \int w \, dv = -\frac{\nu}{\epsilon} \int v w \, dv,
\]

\[
\frac{\partial W}{\partial t} + \nabla_x \cdot \int \frac{v^2}{2} w \, dv + \frac{1}{\epsilon} \frac{\nabla_x V}{m} \cdot (nu) = -\frac{\nu}{\epsilon} \int \frac{v^2}{2} w \, dv + \nu \epsilon W_{eq},
\]

we investigate two closure strategies to get corrected equations for \(u^{(0)}\), \(W\):

1. we substitute \(w \approx w^{(0)}\) in the \(O(1/\epsilon)\)-terms and \(w \approx w^{(0)} + \epsilon w^{(1)}\) in the remaining moments (drift-collision-balance closure),

2. we substitute \(w \approx w^{(0)} + \epsilon w^{(1)}\) everywhere (CE-corrected closure).

Remark: With 1. moment conservations hold due to drift-collision balance.
High-field corrections to drift-collision balance system.

Drift-collision-balance closure:

\[
\begin{align*}
\frac{\partial (n u^{(0)})}{\partial t} + \nabla_x \cdot \Pi^{(0)} + \frac{\epsilon}{\nu} \nabla_x \cdot \Pi^{(1)} &= 0, \\
\frac{\partial \mathcal{W}^{(0)}}{\partial t} + \nabla_x \cdot \mathcal{J}_{\mathcal{W}}^{(0)} + \frac{\epsilon}{\nu} \nabla_x \cdot \mathcal{J}_{\mathcal{W}}^{(1)} &= 0.
\end{align*}
\]

At $O(1)$ in $\epsilon$ drift terms, with $O(\epsilon)$-diffusive terms in $n u^{(0)}, \mathcal{W}^{(0)}$, respectively.

Chapman-Enskog-corrected closure:

\[
\begin{align*}
\frac{\partial (n u^{(0)})}{\partial t} + \nabla_x \cdot n u^{(0)} u^{(0)} + \frac{\epsilon}{\nu} \nabla_x \cdot \Pi^{(1)} &= 0, \\
\frac{\partial \mathcal{W}^{(0)}}{\partial t} + \nabla_x \cdot n u^{(0)} \frac{\mathcal{W}^{(0)}}{n} + \frac{\epsilon}{\nu} \nabla_x \cdot \mathcal{J}_{\mathcal{W}}^{(1)} &= 0.
\end{align*}
\]

At $O(1)$ in $\epsilon$ continuity equation multiplied by $u^{(0)}, \mathcal{W}^{(0)}/n$, respectively, with $O(\epsilon)$-diffusive terms in $n u^{(0)}, \mathcal{W}^{(0)}$, respectively.
\[ \Pi^{(1)} = \frac{\Pi^{(0)}}{n} + 2u^{(0)} \otimes u^{(0)} \nabla_x \cdot nu^{(0)} - 2u^{(0)} \otimes \nabla_x \Pi^{(0)} \]

- drift

\[ - \nabla_x \cdot n \frac{\hbar^2}{4m^3} \nabla_x \otimes \nabla_x \otimes \nabla_x V , \]

\[ J_W^{(1)} = \frac{J_W^{(0)}}{n} \nabla_x \cdot nu^{(0)} + u^{(0)}(W^{(1)} + \Pi^{(1)}) - \nabla_x \cdot \Pi^{(0)} W \]

\[ W^{(1)} = \frac{W^{(0)}}{n} + |u^{(0)}|^2 \nabla_x \cdot nu^{(0)} - u^{(0)} \cdot \nabla_x \Pi^{(0)} - \nabla_x \cdot \Pi^{(0)} \]

- drift+diffusion

\[ - \nabla_x \cdot n \frac{\hbar^2}{8m^3} \nabla_x \Delta_x V \]

\[ \Pi_W^{(0)} = \int v \otimes v \frac{v^2}{2} w_{eq} dv + \left[ 3\Pi^{(0)} \otimes u^{(0)} + n \frac{\hbar^2}{4m^3} \nabla_x \otimes \nabla_x \otimes \nabla_x V \right] \]

\[ + \left[ W^{(0)} + \Pi^{(0)} u^{(0)} + n \frac{\hbar^2}{8m^3} \nabla_x \Delta_x V \right] \otimes 2u^{(0)} . \]

- Standard diffusive terms and heat-flux \( \int v \otimes v (v^2/2) w_{eq} \) (moments up to 4th-order).
- High-field drift, diffusive terms and \( \mathcal{O}(\hbar^2)\)-high-field terms.
Summary

- We start from an $O(1)$-in-$\epsilon$ drift-collision balance model with unknown electron position and energy densities.

- The equations contain just drift terms, and in addition, $O(1)$-in-$\epsilon$ high-field corrections and $O(\hbar^2)$ quantum corrections due to the use of $\Theta[V]$.

- By applying the Chapman-Enskog procedure, we recover a system of equations for position and energy densities and fluid velocity, that contain standard diffusive terms as $O(\epsilon)$-corrections.

- Moreover, we obtain high-field corrections and $O(\hbar^2)$-high-field corrections due to the use of the pseudo-differential operator.

In conclusion, we obtain a highly-accurate quantum fluid-dynamical model for electron transport in high-field regime, since it contains moments up to $5^{th}$-order and high-field corrections peculiar of quantum transport.
Thanks for the attention!
Then the moments of $w^{(0)}$ are

\[ n = \int w^{(0)} dv , \]

\[ \mathcal{J}_n^{(0)} := n u^{(0)} := \int v w^{(0)} dv = -n \frac{\nabla_x V}{\nu m} , \]

\[ \Pi_n^{(0)} := \int v \otimes v w^{(0)} dv = n \frac{k\theta I}{m} + 2u^{(0)} \otimes u^{(0)} + \frac{\hbar^2}{12m^2k\theta} \]

\[ \mathcal{W}_n^{(0)} := \int \frac{v^2}{2} w^{(0)} dv = n \left( \frac{d^2k}{m} + |u^{(0)}|^2 + \frac{\hbar^2}{24m^2k\theta} \Delta_x V \right) , \]

\[ \Pi_{nu}^{(0)} := \int v \otimes v \otimes v w^{(0)} dv = 3u^{(0)} \otimes \Pi^{(0)} + n \frac{\hbar^2}{4m^3\nu} \nabla_x \otimes \nabla_x \]

\[ \mathcal{J}_W^{(0)} := \int v \frac{v^2}{2} w^{(0)} dv = \mathcal{W}^{(0)} + \Pi^{(0)} u^{(0)} + n \frac{\hbar^2}{8m^3\nu} \nabla_x \Delta_x V , \]

\[ \Pi_W^{(0)} := \int v \otimes v \frac{v^2}{2} w^{(0)} dv = \int v \otimes v \frac{v^2}{2} w_{eq} dv + 2\mathcal{W}^{(0)} + \]

\[ + \Pi^{(0)} |u^{(0)}|^2 + 2n \frac{\hbar^2}{4m^3\nu} \nabla_x \Delta_x V \otimes u^{(0)} + 2n \frac{\hbar^2}{4m^3\nu} \nabla_x \Delta_x V . \]