WASCOM 2007

Wave and Stability in Continuous Media

Scicli (Ragusa) - Hotel Baia Samuele July 1-6, 2007.

High-field quantum energy-transport model for semiconductors

Giovanni Borgioli

Dipartimento di Elettronica e Telecomunicazioni, University of Florence,
giovanni.borgioli@unifi.it

joint work with

G. Frosali and **C. Manzini**, Dipartimento di Matematica Applicata, University of Florence

Introduction

- Many devices work at high-field regimes: Drift-Diffusion models fail. Huge literature about "corrected" models (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

  $\Longrightarrow$ **quantum macroscopic models**.
- Quantum kinetic description: $w(x, v, t)$, $(x, v) \in \mathbb{R}^{2d}$, $t > 0$ is the electron quasi-distribution function. Wigner equation is the quantum equivalent of (Liouville) transport equation.
- Wigner-derived macroscopic models are analytically and numerically challenging.
- **Goal**: present a (rigorous) 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. $1/\kappa\beta$ enviroment temperature, V applied potential (also self-consistent).

$$\frac{\partial w}{\partial t} + v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w^{\mathrm{eq}}), \quad t > 0, \qquad w(t=0) = w_0,$$

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

with ν inverse relaxation-time, m effective mass, and $\mathcal{F} = \mathcal{F}_{v\to\eta}$ Fourier transform.
since, by Taylor expansion around x,

$$\frac{i}{\hbar}\left(V\left(x + \frac{\hbar\eta}{2m}\right) - V\left(x - \frac{\hbar\eta}{2m}\right)\right) = \frac{i\eta}{m}\cdot\nabla V(x) + \frac{i\eta^2\hbar^2}{24m^3}\,\eta\cdot\nabla\Delta V(x) + \mathcal{O}(\hbar^4),$$

then

$$\Theta[V]w(x,v) = -\frac{1}{m}\nabla V(x)\cdot\nabla_v w(x,v) + \frac{\hbar^2}{24m^3}\nabla\Delta V(x)\cdot\nabla_v\Delta_v w(x,v) + \mathcal{O}(\hbar^4)$$

Wigner equation: semiclassical limit

From the Taylor expansion of the pseudo-differential term with respect to η around x

$$\begin{aligned} \Theta[V]w &\xrightarrow{\hbar\to 0} -\frac{1}{m}\nabla_x V(x)\cdot\nabla_v w && \text{Vlasov operator.} \\ \Theta[V]w &= -\frac{1}{m}\nabla_x V(x)\cdot\nabla_v w + \mathcal{O}(\hbar^2)\,. \end{aligned}$$

Fact:

$$\Longrightarrow \quad \int v^k\,\Theta[V]w(x,v)\,dv \;=\; -(1/m)\int v^k\,\nabla V(x)\cdot\nabla_v w(x,v)\,dv\,, \quad k=0,1,2$$

$\Longrightarrow$ quantum corrections due to $\Theta[V]$ appear for $i \geq 3$.

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

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

The thermal equilibrium state

$$w^{\mathrm{eq}}(x,v,t) = n(x,t)C\,e^{-\beta m v^2/2}\left\{1+\hbar^2\left[-\frac{\beta^2\,\Delta V(x)}{24m}+\frac{\beta^3}{24}\sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V(x)}{\partial x_r x_s}\right]\right\}$$

$w^{\mathrm{eq}}(x,v,t)$, $\mathcal{O}(\hbar^2)$-accurate local thermal equilibrium distribution function (with β, V assigned),

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

$$\begin{aligned}
\int w^{\mathrm{eq}}(x,v,t)\,dv &= n(x,t) \;:=\; \int w(x,v,t)\,dv\,,\\
\int v\,w^{\mathrm{eq}}(x,v,t)\,dv &= 0\,,\\
\int v^2\,w^{\mathrm{eq}}(x,v,t)\,dv &= \left(\frac{3\,\kappa\theta}{m}+\frac{\hbar^2}{12\kappa\theta m^2}\Delta V(x)\right) n(x,t)
\end{aligned}$$

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

The electron equilibrium energy density depends on t ONLY through n.

Derivation of quantum macroscopic models

Questions:

- what are the differences in using $-(1/m)\,\nabla_x V(x)\cdot\,\nabla_v$ in spite of $\Theta[V]$ for the derivation of quantum macroscopic models?

  Remark: quantum corrections due to w^{eq}, which is $\mathcal{O}(\hbar^2)$-accurate, appear already in 2^{nd}-order moments:
$$\int v \otimes v\, w^{\mathrm{eq}}\, dv \;=\; \frac{nI}{\beta m} + \frac{\beta\hbar^2}{12m^2}\, n\, \nabla_x \otimes \nabla_x V\,.$$

- And in high-field regimes?

The Macroscopic Quantities

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

$$
\begin{aligned}
u = u(x,t) \quad &:= \quad \frac{1}{n}\int v\, w(x,v,t)\, dv \\
\mathcal{W} = \mathcal{W}(x,t) \quad &:= \quad \int \frac{v^2}{2}\, w(x,v,t)\, dv
\end{aligned}
$$

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}, from the expressions for the moments of w^{eq} we deduce

$\Longrightarrow$ **the fluid velocity is zero**, i.e. $u^{\mathrm{eq}}(x,t) \equiv 0$

The Equilibrium Energy

At the thermodynamical equilibrium the energy density equals

$$\mathcal{W}^{\mathrm{eq}}(x,t) \;=\; \frac{n(x,t)}{2}\left(\frac{3\kappa\theta}{m} + \frac{\hbar^2}{12m^2\kappa\theta}\Delta_x V(x)\right) \;=\; \mathcal{W}_i^{\mathrm{eq}}(x,t)\,.$$

- The kinetic energy is zero and in the expression for $\mathcal{W}_i^{\mathrm{eq}}$ we can recognize the classical term proportional to the temperature (the phonon one!) with the additional one which depends on the quantum correction $F^{\hbar}$ to the classical Maxwellian F.
- We stress that in the state of thermodynamical equilibrium w^{eq} the function $\mathcal{W}_i^{\mathrm{eq}}$ depends on time just through the function n, since we assume both θ and V constants with respect to time.

High-field Wigner-BGK equation

$$\epsilon\, w_t + \epsilon\, v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w^{\rm eq})\,, \quad t > 0\,, \qquad w(t=0) = w_0\,,$$

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 enviroment are the dominant mechanisms in the evolution and balance each other.
At the leading order, $\epsilon = 0$, the solution of $(\nu - \Theta[V])w = \nu w^{\rm eq}$ is

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

The inverse operator $(\nu - \Theta[V])^{-1}$ is defined in the Fourier space as the multiplication by the factor $\nu(\nu - i\delta V(x,\eta))^{-1}$, which exists and is bounded for all V since $\nu > 0$.

Moments at the Leading Order

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

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

$$\begin{aligned}
\int w^{(0)} dv &= n \\
\int v\, w^{(0)} dv &= -\frac{\nabla_x V}{\nu m} n \\
\int v \otimes v\, w^{(0)} dv &= \left(\frac{\kappa\theta\mathcal{I}}{m} + 2\frac{\nabla_x V}{\nu m} \otimes \frac{\nabla_x V}{\nu m} + \frac{\hbar^2}{12 m^2 \kappa\theta} \nabla_x \otimes \nabla_x V \right) n \\
\int v \frac{v^2}{2} w^{(0)} dv &= -\frac{\nabla_x V}{\nu m} \left(\frac{d\, k\theta}{2m} + \frac{|\nabla_x V|^2}{\nu^2 m^2} + \frac{\hbar^2}{24 m^2 k\theta} \Delta_x V \right) n + \frac{\hbar^2}{8 m^3 \nu} \nabla_x \Delta_x V\, n
\end{aligned}$$

We remark that, at the leading order, $u^{(0)} = -\dfrac{\nabla_x V}{\nu m}(x)$ is a nonzero-fluid velocity state. The velocity field is constant: in the high-field regime the fluid velocity reaches its saturation value.

Kinetic Energy at the Leading Order

The kinetic energy $\mathcal{K}^{(0)} = \frac{n}{2}(x,t)\frac{|\nabla_x V|^2}{(\nu m)^2}(x)$, as a consequence

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

In the internal energy it appears a contribute due the external field, which is peculiar of the high-field assumption:

$$\frac{n}{2}\frac{|\nabla_x V|^2}{(\nu m)^2},$$

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

$$\mathcal{W}_{\mathrm{w}}^{\mathrm{eq}} \; = \; \mathcal{W}_{\mathrm{w},i}^{\mathrm{eq}} + \mathcal{K}_{\mathrm{w}}^{\mathrm{eq}} = \frac{n}{2}\left(\frac{3\kappa\theta}{m} + \frac{\hbar^2}{12 m^2 \kappa\theta}\Delta_x V\right) + \frac{n}{2}\mathrm{w}^2\,.$$

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 enviroment.

Remark

- A nonzero fluid velocity generally only affects the kinetic term of the energy, but in the high-field regime, where $u = -\dfrac{\nabla_x V}{\nu m}$, this term also appears in the internal energy.
- The fact that the internal energy density at the physical regime of interest, $\mathcal{W}_i^{(0)}$, is different from the equilibrium internal energy density, both in case of a zero-fluid velocity, $\mathcal{W}^{\mathrm{eq}}$, and in case of nonzero-fluid velocity w, $\mathcal{W}_{\mathrm{w},i}^{\mathrm{eq}}$, induced us to consider the internal energy as the second macroscopic function of interest for our investigation.
- The function $\mathcal{W}_i^{(0)}$ depends on time just through the function n, whereas the fluid velocity $u^{(0)}$ does not depend on time.

At high-field regime, the system is completely characterized by the velocity field (determined by the applied potential), by the temperature θ, due to the contact with phonons, and by the position density n, which is the only one subject to time-evolution.

From high-field Wigner-BGK equation we can obtain evolution equations for n and $\mathcal{W}^{(0)}$ by considering $w \simeq w^{(0)}$ and taking v-moments.

Then the energy density $\mathcal{W}^{(0)}$ can change on time only because of *transport*. More explicitly,

$$
\begin{aligned}
\frac{\partial n}{\partial t} - \nabla_x \cdot \left(n \frac{\nabla_x V}{\nu m} \right) &= 0\,, \\
\frac{\partial \mathcal{W}^{(0)}}{\partial t} - \nabla_x \cdot \left(\mathcal{W}^{(0)} \frac{\nabla_x V}{\nu m} \right) + \nabla_x \cdot \left(\frac{\hbar^2}{8 m^3 \nu} \nabla_x \Delta_x V \, n \right) &= 0\,.
\end{aligned}
$$

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 in the two equations respectively only as $O(\epsilon)$ corrections via the Chapman-Enskog procedure.

Redistributing the energy density as

$$\mathcal{W}^{(0)} = \int \frac{|v-u^{(0)}|^2}{2} w^{(0)}\, dv + \frac{n|u^{(0)}|^2}{2} = \mathcal{W}_{\mathrm{i}}^{(0)} + \frac{n}{2}\frac{|\nabla_x V|^2}{(\nu m)^2}\,,$$

with

$$\mathcal{W}_{\mathrm{i}}^{(0)} = \frac{n(x,t)}{2}\left(\frac{3\kappa\theta}{m} + \frac{|\nabla_x V|^2(x)}{(\nu m)^2} + \frac{\hbar^2}{12 m^2 \kappa\theta}\Delta_x V(x)\right)\ ,$$

Consequently, the equations read as follows:

$$\begin{aligned} \frac{\partial n}{\partial t} - \nabla_x \cdot \left(n \frac{\nabla_x V}{\nu m}\right) &= 0\,, \\ \frac{\partial \mathcal{W}_{\mathrm{i}}^{(0)}}{\partial t} - \nabla_x \cdot \left(\mathcal{W}_{\mathrm{i}}^{(0)} \frac{\nabla_x V}{\nu m}\right) + \nabla_x \cdot \left(\frac{\hbar^2}{8 m^3 \nu} \nabla_x \Delta_x V\, n\right) &= 0\,. \end{aligned}$$

Next steps: we shall derive via a Chapman-Enskog procedure corrections of $\mathcal{O}(\epsilon)$ for the previous equations, in order to picture a physical regime "close to" the high-field one. We shall obtain modifications to the evolution equations for the unknown n and $\mathcal{W}$, coming from the inclusion of contributions of order ϵ in the computation of the fluxes.

The Chapman-Enskog procedure

The procedure consists of two steps:

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

$$\frac{\partial w}{\partial t} = \frac{\partial w}{\partial n}\frac{\partial n}{\partial t}\,. \tag{1}$$

Secondly, we assume that the macroscopic unknown n is an $\mathcal{O}(1)$ 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. We obtain 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 $\dfrac{\partial w}{\partial t}$ in (1) as

$$\frac{\partial w}{\partial t} = \frac{\partial w}{\partial n}\Big(-\nabla_x \cdot \int vw dv\Big) \,.$$

By substituting this expression in the Wigner equation, we obtain

$$\epsilon \left(\frac{\partial w}{\partial n}\Big(-\nabla_x \cdot \int vw dv\Big)\right) + \epsilon\, v \cdot \nabla_x w = \Theta[V]w - \nu(w - w_{\mathrm{eq}}) \,,$$

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

At the 0**-th order in** ϵ, we obtain

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

whose solution is given formally by

$$\begin{aligned} w^{(0)} &= (\nu - \Theta[V])^{-1}\, \nu w^{\mathrm{eq}} \\ &= \mathcal{F}^{-1}\left(\frac{\nu \mathcal{F} w^{\mathrm{eq}}}{\nu - i\delta V(x,\eta)}\right)(x,v,t) = n(x,t) M(x,v)\,, \end{aligned}$$

where

$$M(x,v) := \mathcal{F}^{-1}\left(\frac{\nu \mathcal{F}(F + \hbar^2 F^{\hbar})}{\nu - i\delta V(x,\eta)}\right)(x,v)\,.$$

At the first order in ϵ

$$\frac{\partial w^{(0)}}{\partial n}\Big(- \nabla_x \cdot \int v w^{(0)} dv\Big) + v \cdot \nabla_x w^{(0)} = (\Theta[V] - \nu) w^{(1)}\,,$$

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

$$M \nabla_x \cdot \left(n \,\frac{\nabla_x V}{\nu m}\right) + v \cdot \nabla_x w^{(0)} = (\Theta[V] - \nu) w^{(1)}\,,$$

Then we have

$$\boxed{w^{(1)} = \nabla_x \cdot \left(n \, \frac{\nabla_x V}{\nu m} \right) (\Theta[V] - \nu)^{-1} M + (\Theta[V] - \nu)^{-1} (v \cdot \nabla_x (n\, M)) \ .}$$

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 $\mathcal{O}(\epsilon)$ for the continuity equation.

$$\frac{\partial n}{\partial t} + \nabla_x \cdot \int v w^{(0)} dv + \epsilon \nabla_x \cdot \int v w^{(1)} dv = 0\,. \tag{2}$$

In order to write Eq. (2) in a more explicit form, we need the moments of $w^{(1)}$:

$$\begin{aligned}
\int w^{(1)} dv &= 0 \\
\int v\, w^{(1)} dv &= -\frac{1}{\nu} \nabla_x \cdot \left(n \left(\frac{\kappa \theta \mathcal{I}}{m} + 2 \frac{\nabla_x V}{\nu m} \otimes \frac{\nabla_x V}{\nu m} + \frac{\hbar^2}{12 m^2 \kappa \theta} \nabla_x \otimes \nabla_x V \right) \right) \\
&\quad + \frac{1}{\nu} \nabla_x \cdot \left(n \, \frac{\nabla_x V}{\nu m} \right) \frac{\nabla_x V}{\nu m}
\end{aligned}$$

Then Eq. (2) can be rewritten as

$$\boxed{\frac{\partial n}{\partial t} - \nabla_x \cdot \left(n \frac{\nabla_x V}{\nu m} \right) + \frac{\epsilon}{\nu} \nabla_x \cdot \left(\frac{\nabla_x V}{\nu m} \nabla_x \cdot \left(n \frac{\nabla_x V}{\nu m} \right) \right)}$$

$$\boxed{- \frac{\epsilon}{\nu} \nabla_x \cdot \nabla_x \left(\left(\frac{\kappa \theta \mathcal{I}}{m} + 2 \frac{\nabla_x V}{\nu m} \otimes \frac{\nabla_x V}{\nu m} + \frac{\hbar^2}{12 m^2 \kappa \theta} \nabla_x \otimes \nabla_x V \right) n \right) = 0 \,.}$$

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

$$\frac{\epsilon}{\nu} \nabla_x \cdot \left(\frac{\nabla_x V}{\nu m} \nabla_x \cdot \left(n \frac{\nabla_x V}{\nu m} \right) \right) = \frac{\epsilon}{\nu} \frac{\Delta_x V}{\nu m} \nabla_x \cdot \left(n \frac{\nabla_x V}{\nu m} \right) + \frac{\epsilon}{\nu} \frac{\nabla_x V}{\nu m} \cdot \Delta_x \left(n \frac{\nabla_x V}{\nu m} \right) \,,$$

we derive the following high-field corrected version of the (classical) mobilty coefficient $\mu_{\mathrm{cl}} = 1/(\nu m)$

$$\mu_{\mathrm{hf}} := \frac{1}{\nu m} \left(1 + \frac{\epsilon}{\nu} \Delta_x V \right) \,.$$

Corrections to the conservation equations

We want to get $\mathcal{O}(\epsilon)$-corrections for the equation for the energy density $\mathcal{W}$. We start from

$$\epsilon\,\frac{\partial \mathcal{W}}{\partial t} + \epsilon\,\nabla_x\cdot \int v\frac{v^2}{2}w\,dv + \frac{\nabla_x V}{m}\cdot(n\,u) = -\nu(\mathcal{W} - \mathcal{W}_{\mathrm{eq}})\,,$$

that is the 2nd-order moment of the high-field Wigner-BGK equation. Two “closure” strategies are feasible, then we shall obtain two corrected version the system for n and $\mathcal{W}$.

First closure: We assume that the energy conservation holds due to the field effect, namely, we say that the field balances the effect of the inelastic component of the collisions. Explicitly, this consists in considering $\mathcal{W} \approx \mathcal{W}^{(0)}$ in the $\mathcal{O}(1/\epsilon)$-part.
We get

$$\frac{\partial \mathcal{W}}{\partial t} - \nabla_x\cdot\left(\mathcal{W}^{(0)}\frac{\nabla_x V}{\nu m}\right) + \nabla_x\cdot\left(\frac{\hbar^2}{8m^3\nu}\nabla_x\Delta_x V\,n\right) + \epsilon\,\nabla_x\cdot\int v\frac{v^2}{2}w^{(1)}\,dv\,. \qquad (3)$$

Second closure: The first one corresponds to assume

$$\mathcal{W} \approx \mathcal{W}^{(0)} + \epsilon\, \mathcal{W}^{(1)},$$

equivalently, we are correcting the drift-collision balance assumption at the energy-level. Then we have

$$\frac{\partial \mathcal{W}}{\partial t} + \nabla_x \cdot \int v \frac{|v|^2}{2} w^{(0)}\, dv + \epsilon\, \nabla_x \cdot \int v \frac{v^2}{2} w^{(1)}\, dv + \frac{\nabla_x V}{m} \cdot \int v\, w^{(1)}\, dv = -\nu \int \frac{|v|^2}{2} w^{(1)}\, dv \,. \tag{4}$$

In order to get more explicit expressions of Eq. (4), we compute the following additional moment of $w^{(1)}$.

$$\nu \int \frac{|v|^2}{2}\, w^{(1)}\, dv \quad = \quad \left(-\nabla_x \cdot \left(\frac{n \nabla_x V}{\nu m} \right) \frac{\mathcal{W}^{(0)}}{n} \right) - \frac{\nabla_x V}{m} \cdot \int v\, w^{(1)} - \nabla_x \cdot \int v \frac{|v|^2}{2} w^{(0)}\, dv$$

Accordingly, Eq. (4) becomes

$$\frac{\partial \mathcal{W}}{\partial t} - \nabla_x \cdot \left(\frac{n \nabla_x V}{\nu m} \right) \frac{\mathcal{W}^{(0)}}{n} + \epsilon\, \nabla_x \cdot \int v \frac{v^2}{2} w^{(1)}\, dv = 0 \,.$$

Thanks for the attention!

RIGOROUS ASYMPTOTIC ANALYSIS
of the high-field Quantum Drift-Diffusion equation [Manzini, Frosali 06]

$$\epsilon\, w_t + \epsilon\, v \cdot \nabla_x w - \Theta[V]w = -\nu(w - w^{\mathrm{eq}})\,, \quad t > 0\,, \qquad w(t=0) = w_0\,,$$

- By a "modified" Chapman-Enskog expansion [Mika, Banasiak] up to 1^{st}-order in ϵ, we obtain a Quantum Drift-Diffusion equation with unknown n and field-dependent corrections,
- We prove *rigorously* high-field QDD is $\mathcal{O}(\epsilon^2)$-accurate approximation of high-field Wigner-BGK,
- We treat at the same time the *initial layer* part that provides initial datum for high-field QDD.

Abstract formulation:

$$\boxed{\epsilon\, \frac{dw}{dt}(t) = \epsilon\, Sw(t) + \mathcal{A}w(t) + \mathcal{C}w(t), \quad \forall\, t > 0\,,} \tag{5}$$

where $w(t), w_0 : (x, v) \in \mathbb{R}^{2d} \mapsto \mathbb{R}\,,$

$$Sw = -v\cdot \nabla_x w\,, \quad \mathcal{A}w := \Theta[V]w, \quad \mathcal{C}w := -\nu\,(w - w^{\mathrm{eq}})\,.$$

Define X_k : the subspace of $L^2(\mathbb{R}^{2d})$, s.t.

$$\|w\|^2_{X_k} = \int_{\mathbb{R}^{2d}} |w(x,v)|^2 (1+|v|^{2k})\, dx\, dv\,, \quad \text{with } 2k > d$$

$$w \in X_k \iff \mathcal{F}_v w \in L^2_x \otimes H^k_\eta \hookrightarrow L^2_x \otimes L^\infty_\eta$$

$\Longrightarrow$

- $n[w](x,t) := \int w(x,v,t)\, dv \in L^2_x$ with $\|n[w]\|_{L^2_x} \le C\, \|w\|_{X_k}$,
- $\forall\, V \in H^k_x\,, \quad \mathcal{A} + \mathcal{C} \in \mathcal{B}(X_k)\,.$

The problem for $\epsilon = 0$

$$\epsilon = 0 \;\Rightarrow\; \quad 0 = \mathcal{A}w + \mathcal{C}w \quad \Leftrightarrow \quad (\nu - \Theta[V])w = \nu\, w^{\mathrm{eq}}$$

The solution is $w = n[w] M$, with

$$M(x,v) := \nu\, (\nu - \Theta[V])^{-1} \left[\mathrm{e}^{-\beta m v^2/2} (1 + \hbar^2 F(V(x), v, \beta)) \right].$$

The compressed Chapman-Enskog procedure

Definition $\mathcal{P} : X_k \longrightarrow \ker(\mathcal{A}+\mathcal{C})$ and $\mathcal{Q} : X_k \longrightarrow (\ker(\mathcal{A}+\mathcal{C}))^\perp$

$$\mathcal{P}w := M \int w(x,v)\, dv \;\equiv M\, n[w] \;=: \varphi\,, \qquad \mathcal{Q}w := (\mathcal{I}-\mathcal{P})w \;=: \psi$$

Decompose the unknown $w = \varphi + \psi$ and from (5) derive two evolution equations for φ and ψ with $\varphi(0) = \varphi_0 = \mathcal{P}w_0\,,\; \psi(0) = \psi_0 = \mathcal{Q}w_0$.

Idea: Correct the evolution equation for φ with the one for ψ.

1. leave φ UNEXPANDED,
2. distinguish "bulk" from "initial layer" parts:

$$\varphi(t) = \bar{\varphi}(t) + \tilde{\varphi}\left(\frac{t}{\epsilon}\right) = M\, n(t) + \tilde{\varphi}\left(\frac{t}{\epsilon}\right)\,, \qquad \psi(t) = \bar{\psi}(t) + \tilde{\psi}\left(\frac{t}{\epsilon}\right)\,, \qquad (6)$$

3. expand $\bar{\psi}, \tilde{\varphi}, \tilde{\psi}$ as powers of ϵ

Expansion:

$$\bar{\psi}(t) = \bar{\psi}_0(t) + \epsilon\,\bar{\psi}_1(t) + \epsilon^2\,\bar{\psi}_2(t) + \dots\,,$$
$$\tilde{\varphi}\left(\frac{t}{\epsilon}\right) = \tilde{\varphi}_0\left(\frac{t}{\epsilon}\right) + \epsilon\,\tilde{\varphi}_1\left(\frac{t}{\epsilon}\right) + \epsilon^2\,\tilde{\varphi}_2\left(\frac{t}{\epsilon}\right) + \dots\,,$$
$$\tilde{\psi}\left(\frac{t}{\epsilon}\right) = \tilde{\psi}_0\left(\frac{t}{\epsilon}\right) + \epsilon\,\tilde{\psi}_1\left(\frac{t}{\epsilon}\right) + \epsilon^2\,\tilde{\psi}_2\left(\frac{t}{\epsilon}\right) + \dots$$

Substitute (6) in the evolution equations: the *approximate* problem has unknown

$$\boxed{\bar{\varphi}, \bar{\psi}_0, \bar{\psi}_1, \tilde{\varphi}_0, \tilde{\varphi}_1, \tilde{\psi}_0, \tilde{\psi}_1.}$$

We get the "diffusion-like" equation

$$\frac{\partial \bar{\varphi}}{\partial t} = \mathcal{P}S\mathcal{P}\bar{\varphi} - \epsilon\mathcal{P}S\mathcal{Q}(\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q})^{-1}\mathcal{Q}S\mathcal{P}\bar{\varphi}$$

and the equations for the other unknowns.

Rigorous analysis

Main Thm.: $w_0 \in H^4_{k+1}$, V smooth. Then, $\forall\, T$, $0 < T < \infty$, $\exists\, C$ independent of ϵ s.t.

$$\Big\| \underbrace{\varphi(t) + \psi(t)}_{\equiv w(t)} - \Big(\underbrace{\bar{\varphi}(t)}_{\equiv M\, n(t)} + \epsilon\, \bar{\psi}_1(t) + \tilde{\psi}_0(t/\epsilon) + \epsilon\, \tilde{\varphi}_1(t/\epsilon) + \epsilon\, \tilde{\psi}_1(t/\epsilon) \Big) \Big\|_{X_k} \leq C\epsilon^2 , \quad 0 \leq t \leq T .$$

Steps:

1. well-posedness of $\dfrac{\partial \bar{\varphi}}{\partial t} = \mathcal{P}S\mathcal{P}\bar{\varphi} - \epsilon \mathcal{P}S\mathcal{Q}(\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q})^{-1}\mathcal{Q}S\mathcal{P}\bar{\varphi}$, with $\bar{\varphi} \equiv M\, n$,

2. $\bar{\psi}_1(t) = (\nu - \Theta[V])^{-1} \mathcal{Q}S\mathcal{P}(M\, n(t))$, then

$$\|\partial_t \bar{\psi}_1(t)\|_{H^1_k} \sim \|\partial_t \nabla n(t)\|_{H^1_x} \qquad \|\mathcal{Q}S\mathcal{Q}\bar{\psi}_1(t)\|_{H^1_k} \sim \|\nabla \cdot \nabla n(t)\|_{H^1_x} ,$$

   regularity of the solution $n \implies$ regularity and behaviour w.r.t. $t \to 0^+$ of $\bar{\psi}_1$,

3. existence, regularity and behaviour w.r.t. $t \to 0^+$ of $\tilde{\psi}_0$, $\tilde{\varphi}_1$, $\tilde{\psi}_1$, precisely

$$\|S\tilde{\varphi}_1(t/\epsilon)\|_{X_k}, \|S\tilde{\psi}_1(t/\epsilon)\|_{X_k} \sim \mathrm{e}^{-\nu_k t/\epsilon} \qquad \text{with} \quad \nu_k > 0 .$$

High-field QDD equation

$$\boxed{\frac{\partial n}{\partial t} - \mathcal{D}n - \mathcal{G}n - \mathcal{E}n = 0\,, \quad t > 0\,, \quad n(t=0)}$$

$$\mathcal{D}n = \epsilon\,\nabla \cdot (\mathsf{D}\nabla n)\,, \quad \mathcal{G}n = \epsilon\,\nabla \cdot (\mathsf{W}\,n)\,, \quad \mathcal{E}n = \nabla \cdot (\mathsf{F}\,n)$$

$$\mathsf{D} := \frac{1}{\nu}\left(\frac{\mathcal{I}}{\beta m} + \frac{\nabla V}{\nu m} \otimes \frac{\nabla V}{\nu m} + \frac{\beta \hbar^2}{12m}\nabla \otimes \nabla V\right),$$

$$\mathsf{W} := \frac{1}{\nu}\left(2\frac{\nabla \otimes \nabla V}{\nu m} + \frac{\Delta V}{\nu m}\right)\frac{\nabla V}{\nu m} + \frac{\beta \hbar^2}{12 m \nu}\nabla \cdot \nabla \otimes \nabla V, \quad \mathsf{F} := \frac{\nabla V}{\nu m}\,.$$

Remark: singularly perturbed parabolic equation

Assumption: V smooth and s.t. $\exists\, c > 0$ s.t. $\mathsf{D}(x)\, y \otimes y \geq c|y|^2\,, \quad \forall\, x, y \in \mathbb{R}^d\,.$

Propositions: Regularity estimates, Well-posedness of the QDD equation.