Comunicazione orale all’interno del minisimposio: M1 Advanced modelling of semiconductor devices

Corrected Quantum Drift-Diffusion equation via Compressed Chapman-Enskog expansion

Giovanni Frosali and Chiara Manzini
Dipartimento di Matematica Applicata “G.Sansone”
Università di Firenze - Via S.Marta 3 I-50139 Firenze, Italy
giovanni.frosali@unifi.it, chiara.manzini@unifi.it

One of the most important aspects of quantum theory is the derivation of simple approximate models providing a hydrodynamic description of the transport of charged carriers. Quantum drift-diffusion equations, e.g., are both subject of diverse mathematical studies ([4] and the Refs. therein) and used by engineers in many practical simulations. Our aim is the derivation of a quantum drift-diffusion equation via the modified (compressed) Chapman–Enskog method [3], as the preliminary step towards a rigorous asymptotic analysis of the quantum transport equation, in case a strong external electric field and a relaxation-time collisional operator are included. Therefore, the Wigner equation for the quasi-distribution function \( w = w(x,v,t) \) is modified.

\[
\frac{\partial w}{\partial t} + v \cdot \nabla w - \Theta[V]w = -\nu(w - w_{eq}), \quad (x,v) \in \mathbb{R}^{2d}, \ t > 0,
\]

where the potential \( V \) enters through the pseudo-differential operator \( \Theta[V] \) defined by

\[
(\Theta[V]w)(x,v,t) = \frac{i}{(2\pi)^{d/2}} \int_{\mathbb{R}^{d}} \delta V(x,\eta) \mathcal{F}w(x,\eta,t)e^{i\eta \cdot v} d\eta,
\]

with \( \delta V(x,\eta) := \frac{1}{\hbar} \left( V(x + \frac{\hbar \eta}{2m}) - V(x - \frac{\hbar \eta}{2m}) \right) \) and \( \mathcal{F}f(\eta) \), which denotes the Fourier transform of \( w \) from the variable \( v \) to the variable \( \eta \). We can introduce a small parameter \( \epsilon \) related to the mean free path, which refers to the relaxation to thermodynamical equilibrium and to the presence of a strong field. Accordingly, in dimensionless form

\[
\frac{\partial w}{\partial t} + v \cdot \nabla w - \frac{1}{\epsilon} \Theta[V]w = -\frac{w - w_{eq}}{\epsilon}, \quad (x,v) \in \mathbb{R}^{2d}, \ t > 0. \quad (1)
\]
We shall describe the equilibrium state by the $O(h^2)$-quantum corrected thermodynamical equilibrium function calculated by Wigner in [6] (cf. [2] for an updated discussion). Precisely, we can write the Wigner thermal equilibrium function as

\[ w_{eq}(x, v) = n(x, t) \left( F(v) + h^2 F^{(2)}(x, v) \right) + O(h^4) , \quad F(v) := \left( \frac{\beta m}{2\pi} \right)^{d/2} e^{-\beta m v^2/2}, \]

\[ F^{(2)}(x, v) := F(v) \left[ -\frac{\beta^2}{24m} \sum_{r=1}^{d} \frac{\partial^2 V}{\partial x_r^2} + \frac{\beta^3}{24} \sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V}{\partial x_r \partial x_s} \right], \]

where $n(x, t) = n[w](x, t) := \int w(x, v, t) dv$ is the position density, $\beta \equiv 1/kT$, $T$ is the (constant) temperature and $k$ is the Boltzmann constant (cf. [1]).

We shall consider the Hilbert space $X_k = L^2(\mathbb{R}^d, (1 + |v|^2)dx dv; \mathbb{R})$ and write (1) in the abstract form

\[ \epsilon \frac{dw}{dt} = \epsilon S w + A w + C w, \quad \lim_{t \to 0^+} \|w(t) - w_0\|_{X_k} = 0 \quad (2) \]

with

\[ A w := \Theta [V] w, \quad C w := -(w - \Omega w), \quad \Omega w = n(F + h^2 F^{(2)}) \]

and the free-streaming operator $Su = -v \cdot \nabla, D(S) = \{u \in X_k | Su \in X_k\}$.

The main ingredient of the compressed Chapman-Enskog expansion, as proposed in [3], is the study of the problem (2) with $\epsilon = 0$, i.e. of the equation $(A + C) f = 0$ in the space $X_k$. We can state that, for any fixed $x \in \mathbb{R}^d$

\[ \ker(A + C) := \{cM(v), c \in \mathbb{R}\} \subset X_k^v := L^2(\mathbb{R}^d, (1 + |v|^{2k})dv; \mathbb{R}) \]

with

\[ M(x, v) = \mathcal{F}^{-1} \left\{ \frac{\mathcal{F}F(\eta)}{1 - i\delta V(x, \eta)} \left( 1 - \frac{\beta^2 h^2}{24m} \sum_{r,s=1}^{d} \eta_r \eta_s \frac{\partial^2 V(x)}{\partial x_r \partial x_s} \right) \right\}(x, v). \quad (3) \]

Moreover, for all $h \in X_k^v$, $(A + C) u = h$ has a solution if and only if $\int h(v) dv = 0$. According to the previous considerations, we can decompose the space $X_k$ as

\[ X_k = (X_k)_M \oplus (X_k)^0 \]

where $(X_k)_M$ is the eigenspace spanned by $M$ and

\[ (X_k)^0 = \left\{ f \in X_k \left| \int f(v) dv = 0 \right. \right\}. \]
Let \( \mathcal{P} \) be the corresponding spectral projection from \((X_k)\) into \((X_k)\), defined by \( \mathcal{P} f = M \int f(v) \, dv \) and \( \mathcal{Q} = I - \mathcal{P} \). Accordingly, we decompose the unknown function \( w \in X_k \) as \( w = \varphi + \psi = \mathcal{P} w + \mathcal{Q} w \), where \( \varphi \) is called the hydrodynamic part and \( \psi \) is called the kinetic part of \( w \). Observe that for all \( w \in X_k, \mathcal{P} w = M n[w] \).

Operating formally on both sides of Eq. (2 with the projections \( \mathcal{P} \) and \( \mathcal{Q} \), we obtain the following system

\[
\begin{align*}
\frac{\partial \varphi}{\partial t} & = \mathcal{P} S \mathcal{P} \varphi + \mathcal{P} \mathcal{Q} \psi \\
\frac{\partial \psi}{\partial t} & = \mathcal{Q} S \mathcal{P} \varphi + \mathcal{Q} \mathcal{Q} \psi + \frac{1}{\epsilon} \mathcal{Q}(\mathcal{A} + \mathcal{C}) \mathcal{Q} \psi 
\end{align*}
\]

with initial conditions

\[
\varphi(0) = \varphi_0 = \mathcal{P} f_0, \quad \psi(0) = \psi_0 = \mathcal{Q} f_0.
\]

The compressed asymptotic expansion consists in splitting the unknown functions \( \varphi \) and \( \psi \) into the sum of the “bulk” parts \( \bar{\varphi} \) and \( \bar{\psi} \) and of the initial layer parts \( \tilde{\varphi} \) and \( \tilde{\psi} \), which take account of the rapid changes of \( f \) for small times \( t = \frac{t}{\epsilon} \). Then the bulk hydrodynamic part \( \bar{\varphi} \) is left unexpanded and the other parts are expanded in series of \( \epsilon \). By disregarding terms of order \( \epsilon^2 \), we recover the following equation for the unexpanded function \( \bar{\varphi}(x,v,t) \)

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

\( \bar{\varphi}(x,v,t) \) can still be written as the product \( \bar{\varphi}(x,v,t) = M(x,v) n(x,t) \), since we shall consider the contribution of the initial layer part \( \bar{\varphi} \) via an appropriate initial condition. After some algebra manipulations, we write Eq. (5) in the following form

\[
\frac{\partial n}{\partial t} = - \nabla \cdot \left( n \int vM dv \right) - \epsilon \nabla \cdot \left[ \left( \int v \otimes D_2 dv \right) \nabla n + n \int v D_1 dv \right]
\]

where \( D_2 \) and \( D_1 \) are explicitly determined by solving appropriate equations containing the operator \( \mathcal{Q}(\mathcal{A} + \mathcal{C}) \mathcal{Q} \). We remark that the solution of Eq. (6) is the correction up to order \( \epsilon^2 \) of the solution \( n \) of the continuity equation, in case of strong field.

We can calculate the coefficient in the operator \( \mathcal{P} S \mathcal{P} \) defined above

\[
\int vM(x,v) \, dv = - \nabla V(x),
\]
the diffusion tensor $D$

$$D := \int v \otimes D_2 \, dv = \frac{I}{\beta} + \nabla V \otimes \nabla V - \frac{\beta \hbar^2}{12m} (\nabla \otimes \nabla)V + O(\hbar^4),$$

with $I$ identity tensor, and

$$\int v D_1(x,v) \, dv = (\nabla \otimes \nabla)V \, \nabla V - \frac{\beta \hbar^2}{12m} \nabla \cdot (\nabla \otimes \nabla)V + O(\hbar^4).$$

Finally, Eq. (6) looks like

$$\frac{\partial n}{\partial t} - \nabla \cdot (n \nabla V) - \frac{\epsilon}{\beta} \Delta n - \epsilon \nabla \cdot (n \nabla V \nabla n) - \epsilon \nabla \cdot [n (\nabla \otimes \nabla)V \, \nabla V] + \frac{\epsilon \beta \hbar^2}{12m} \nabla \cdot [(\nabla \otimes \nabla)V \nabla n + n \nabla \cdot (\nabla \otimes \nabla)V] = 0$$

and we can recognize the drift and the diffusion terms, two terms due to the strong field assumption (cf. [5]) and the terms due to the (quantum) Bohm potential (cf. [1]). We shall give a rigorous proof of the results up to now formally derived. In particular, we study the well-posedness for the initial parts of our problem. We shall also prove regularity of the solution of the drift-diffusion equation, starting from sufficiently smooth initial value. Finally we can prove that the asymptotic expansion up to the first order gives an approximation of order $\epsilon^2$ to the solution of the exact problem.

REFERENCES


