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

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

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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 by a BGK operator, that indicates relaxation in a time $1/\nu$ to the equilibrium state w_{eq}. Precisely, the Wigner equation for the quasi-distribution function $w = w(x, v, t)$ is

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

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

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

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 η. We can introduce a small parameter ϵ 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

$$\frac{\partial w}{\partial t} + v \cdot \nabla w - \frac{1}{\epsilon}\Theta[V]w \;\; = \;\; -\frac{w - w_{\text{eq}}}{\epsilon}, \quad (x,v) \in \mathbb{R}^{2d},\ t > 0. \qquad (1)$$

We shall describe the equilibrium state by the $O(\hbar^2)$-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

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

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

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

$$\epsilon\,\frac{dw}{dt} = \epsilon\, Sw + \mathcal{A}w + \mathcal{C}w, \qquad \lim_{t\to 0^+} \|w(t) - w_0\|_{X_k} = 0 \tag{2}$$

with

$$\mathcal{A}w := \Theta[V]w, \qquad \mathcal{C}w := -(w - \emptyset w)\,, \quad \Omega w = n(F + \hbar^2 F^{(2)})$$

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

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 $(\mathcal{A}+\mathcal{C})f = 0$ in the space X_k. We can state that, for any fixed $x \in \mathbb{R}^d$

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

with

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

Moreover, for all $h \in X_k^v$, $(\mathcal{A}+\mathcal{C})u = h$ 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

$$(X_k)^0 = \left\{ f \in X_k \,\middle|\, \int f(v)\,dv = 0 \right\}.$$

Let $\mathcal{P}$ be the corresponding spectral projection from (X_k) into $(X_k)_M$, defined by $\mathcal{P}f = M\int f(v)\,dv$ and $\mathcal{Q} = \mathcal{I} - \mathcal{P}$. Accordingly, we decompose the unknown function $w \in X_k$ as $w = \varphi + \psi = \mathcal{P}w + \mathcal{Q}w$, where φ is called the hydrodynamic part and ψ is called the kinetic part of w. Observe that for all $w \in X_k, \mathcal{P}w = Mn[w]$.
Operating formally on both sides of Eq. (2 with the projections $\mathcal{P}$ and $\mathcal{Q}$, we obtain the following system

$$\left\{ \begin{array}{rcl} \dfrac{\partial \varphi}{\partial t} & = & \mathcal{PSP}\varphi + \mathcal{PSQ}\psi \\ \dfrac{\partial \psi}{\partial t} & = & \mathcal{QSP}\varphi + \mathcal{QSQ}\psi + \frac{1}{\epsilon}\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\psi \end{array} \right. \tag{4}$$

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 φ and ψ 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 ϵ. By disregarding terms of order ϵ^2, we recover the following equation for the unexpanded function $\bar{\varphi}(x, v, t)$

$$\frac{\partial \bar{\varphi}}{\partial t} = \mathcal{PSP}\bar{\varphi} - \epsilon \mathcal{PSQ}(\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q})^{-1}\mathcal{QSP}\bar{\varphi}\,. \tag{5}$$

$\bar{\varphi}(x, v, t)$ 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 $\tilde{\varphi}$ via an appropriate initial condition. After some algebra manipulations, we write Eq. (5) in the following form

$$\begin{aligned} \frac{\partial n}{\partial t} = & - \nabla\cdot \left(n \int vM dv \right) \\ & - \epsilon \nabla\cdot \left[\left(\int v \otimes D_2\, dv \right) \nabla n + n \int v D_1\, dv \right] \end{aligned} \tag{6}$$

where D_2 and D_1 are esplicitly 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 ϵ^2 of the solution n of the continuity equation, in case of strong field.
We can calculate the coefficient in the operator $\mathcal{PSP}$ defined above

$$\int vM(x, v) dv \quad = \quad -\nabla V(x)\,, \tag{7}$$

the diffusion tensor D

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

with $\mathcal{I}$ 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

$$\frac{\partial n}{\partial t} - \nabla \cdot (n \nabla V) - \frac{\epsilon}{\beta} \Delta n - \epsilon \nabla \cdot (\nabla V \otimes \nabla V \, \nabla n)$$

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

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 ϵ^2 to the solution of the exact problem.

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