DERIVATION OF A QUANTUM HYDRODYNAMIC MODEL IN THE HIGH-FIELD CASE

G. BORGIOLI*, G. FROSALI†, C. MANZINI†

* *Dip. di Elettronica e Telecomunicazioni,* † *Dip. di Matematica Applicata, Università di Firenze, Via S.Marta 3, I-50139 Firenze, Italy*
**E-mail: giovanni.borgioli@unifi.it*

A fluid-dynamical set of equations is derived starting from a quantum kinetic description of transport in high-field regime.

1. Introduction and formulation of the scaled problem

We derive a hydrodynamical model for a quantum system evolving in high-field regime, namely when advection and dissipative terms are dominant and have the same order of magnitude. To this aim we consider a rescaled version of the Wigner equation with unknown the quasi-distribution function $w = w(x, v, t), (x, v) \in \mathbb{R}^{2d}$, $t > 0$, describing the time-evolution of a quantum system with d degrees of freedom, under the effect of an external potential $V = V(x), x \in \mathbb{R}^d$ and a "collisional" term $Q(w)$. It reads

$$\epsilon\partial_t w + \epsilon v \cdot \nabla_x w - \Theta[V]w \;=\; Q(w)\,, \quad (x, v) \in \mathbb{R}^{2d}, \quad t > 0. \tag{1}$$

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

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

where

$$\delta V(x, \eta) := \frac{1}{\hbar}\left[V\left(x + \frac{\hbar\eta}{2m}\right) - V\left(x - \frac{\hbar\eta}{2m}\right)\right]$$

and ϵ is a parameter corresponding to the Knudsen number. $\mathbf{F}f(\eta) \equiv [\mathbf{F}_{v\to\eta}f](\eta)$ denotes the Fourier transform of w from v to η. In the Fourier-transformed space $\mathbb{R}^d_x \times \mathbb{R}^d_\eta$ the operator $\Theta[V]$ is the multiplication operator by the function $i\,\delta V$; in symbols,

$$\mathbf{F}\left(\Theta[V]w\right)(x, \eta) = i\,\delta V(x, \eta)\mathbf{F}w(x, \eta)\,. \tag{3}$$

We choose the collisional term in the relaxation-time BGK form, i.e. $Q(w) = -\nu(w - w_{\rm eq})$. It describes the dissipative mechanism due to the interaction with the environment, which leads the system to a state $w_{\rm eq}$ of thermodynamical equilibrium with temperature $1/k\beta$. Explicitly,

$$\begin{aligned} w_{\rm eq}(x,v,t) &= n(x,t)\left(\frac{\beta m}{2\pi}\right)^{d/2} e^{-\beta m v^2/2} \\ &\times \left\{1 + \hbar^2 \frac{\beta^2}{24}\left[-\frac{1}{m}\Delta V(x) + \beta \sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V(x)}{\partial x_r x_s}\right] + O(\hbar^4)\right\} . \end{aligned} \quad (4)$$

This is obtained by inserting in the Wigner thermodynamical equilibrum function[8] the parameter $c = c(x,t)$ and then by assuming

$$\int w_{\rm eq}(x,v,t)\,dv \;=\; \int w(x,v,t)\,dv \;=:\; n[w](x,t) \equiv n(x,t)\,. \quad (5)$$

The version of Wigner equation (1) under examination corresponds to the case in which a "strong" external potential is included. Accordingly the potential characteristic time t_V and the mean free time t_C between interactions of the system with the background are assumed to be comparable and small. The Knudsen number ϵ is inserted in order to identify terms of the same order of magnitude. Since dissipative interaction and advection terms coexist during the evolution, the high-field relaxation-time state shall be determined by considering the joint actions of collisions and external field. The corresponding distribution function is the solution of Eq.1 for $\epsilon = 0$ and it shall be adopted to close the system for the fluid-dynamical moments of the Wigner function

$$\begin{aligned} n(x,t) &:= \int_{R_v^d} w(x,v,t)\,dv\,, \quad nu(x,t) \;:=\; \int_{R_v^d} v\, w(x,v,t)\,dv\,, \\ e(x,t) &:= \int_{R_v^d} \frac{1}{2} m|v|^2\, w(x,v,t)\,dv\,. \end{aligned} \quad (6)$$

Let us rewrite the right-hand side part of Eq. (1) as

$$Q(w) := -(\nu\, w - \Omega\, w)\,,$$

where the operator Ω is defined by

$$\Omega w(x,v) = \nu\, n[w](x)\left[F(v) + \hbar^2 F^{(2)}(x,v)\right]\,,$$

the function $F(v)$ is the normalized Maxwellian $F(v) := \left(\frac{\beta m}{2\pi}\right)^{d/2} e^{-\beta m v^2/2}$ and $F^{(2)}$ is the $O(\hbar^2)-$coefficient in w_{eq}

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

2. The high-field relaxation-time function

Let us denote by $M = M(x,v)$ the solution of the following equation

$$\theta[V]w + Qw = 0 \tag{7}$$

In Ref. 7 it is proved that exists a unique solution M with $\int M(x,v,t)\,dv = \int w(x,v,t)\,dv$, by setting the problem in the Hilbert space $L^2(\mathbb{R}^{2d}; 1+|v|^{2k})$ with $2k > d$, provided V is regular enough ($V \in H^{k+2}$, e.g.). By taking formally the moments $(mv, mv\otimes v, mv|v|^2)$ of (7), it is possible to compute the corresponding moments of the relaxation-time function M. For brevity, we omit the proof here.

Lemma 2.1. *Let M be the solution of Eq.* (7) *such that* $\int M(x,v,t)\,dv = \int w(x,v,t)\,dv = n[w](x,t)$. *Then*

$$\int vM\,dv = -n\frac{\nabla V}{\nu\, m} := nu_M\,, \tag{8}$$

$$\int v\otimes mvM\,dv = n\frac{\mathcal{I}}{\beta} + 2mnu_M\otimes u_M + \frac{\beta\hbar^2}{12m} n\nabla\otimes\nabla V\,, \tag{9}$$

$$\int \frac{1}{2}m|v|^2 M\,dv = n\frac{d}{2\beta} + mnu_M^2 + \frac{\beta\hbar^2}{24m} n\Delta V\,, \tag{10}$$

$$\int \frac{1}{2}mv|v|^2 M\,dv = -\frac{\hbar^2}{8m} n\Delta u_M + u_M \int v\otimes mvM\,dv + u_M\int\frac{1}{2}m|v|^2 M\,dv\,.$$

The moments of the function M can be compared with the corresponding ones of the shifted-Maxwellian.[3] To the high-field relaxation-time distribution function is associated the fluid velocity in (8), accordingly the expression for the energy density $e = e(x,t)$ calculated at relaxation-time is

$$\int \frac{1}{2}m|v|^2 M\,dv = \frac{1}{2}mnu_M^2 - \frac{1}{2}\mathrm{tr}\mathbf{P}_M\,,$$

since it is natural to define the pressure tensor $\mathbf{P}_M$ as

$$\mathbf{P}_M := -n\frac{\mathcal{I}}{\beta} - mnu_M\otimes u_M - \frac{\beta\hbar^2}{12m} n\nabla\otimes\nabla V\,, \tag{11}$$

in analogy with Gardner.[3] The high-field assumption yields the additional tensor

$$-mnu_M \otimes u_M = -mn\frac{\nabla V}{\nu\, m} \otimes \frac{\nabla V}{\nu\, m}$$

in the pressure term. Moreover, by comparing the expression (11) with the one computed with the shifted-Maxwellian, the heat-flux term q can be defined as

$$q := -\frac{\hbar^2}{8m} n\Delta u_M + mnu_M \left(u_M \otimes u_M\right) . \tag{12}$$

Again, the heat-flux term, in the high-field case, consists of the expected quantum term and an additional one which is cubic in the fluid velocity. Next, we shall give another motivation for the definitions of the pressure and the heat-flux terms in the high-field case.

3. Derivation of the high-field QHD system

In this section we shall derive the QHD system, in the high field case. Starting from Eq. (1) with $\epsilon > 0$ and multiplying by $1, mv, \frac{1}{2}m|v|^2$ and integrating in dv, one gets

$$\begin{aligned}
\partial_t n + \nabla_x \cdot (nu) &= \tfrac{1}{\epsilon} \textstyle\int Q(w)\, dv \\
\partial_t (mnu) + \nabla_x \cdot \textstyle\int mv \otimes vw\, dv + \tfrac{1}{\epsilon} \textstyle\int mv\Theta[V] w\, dv &= \tfrac{1}{\epsilon} \textstyle\int mvQ(w)\, dv \\
\partial_t e + \nabla_x \cdot \textstyle\int \tfrac{1}{2} mv|v|^2 w\, dv + \tfrac{1}{\epsilon} \textstyle\int \tfrac{1}{2} m|v|^2 \Theta[V] w\, dv &= \tfrac{1}{\epsilon} \textstyle\int \tfrac{1}{2} m|v|^2 Q(w)\, dv
\end{aligned} \tag{13}$$

where n, nu, e are defined in (6). We use the relaxation-time distribution function M to close the $\mathcal{O}(\frac{1}{\epsilon})$ terms. Since M satisfies Eq. (7), that is the Wigner equation with $\epsilon = 0$, Eqs. (13) reduce immediately to

$$\begin{aligned}
\partial_t n + \nabla_x \cdot (nu) &= 0\, , \\
\partial_t (mnu) + \nabla_x \cdot \int mv \otimes vw\, dv &= 0\, , \\
\partial_t e + \nabla_x \cdot \int \frac{1}{2} mv|v|^2 w\, dv &= 0\, ,
\end{aligned} \tag{14}$$

where n, u and e are the unknown functions. Then we still need to close the integral terms. Eq. (8) indicates the fluid velocity computed at relaxation time. Accordingly, the velocity momentum can be expressed in terms of the deviation from the relaxation-time velocity, that is,

$$\begin{aligned}
n\ u = \int vw\, dv \ &= \ \int \left(v - \frac{1}{n}\int vM\right) w\, dv + \frac{1}{n}\int vM\, dv \int w\, dv \\
&= \int (v - u_M)\, w\, dv + nu_M\, .
\end{aligned}$$

Analogously, the tensor $\int mv \otimes vw\,dv$ can be written as

$$\int mv \otimes vw\,dv = \int m\,(v-u_M) \otimes (v-u_M)\,w\,dv + \int (mv \otimes v - m\,(v-u_M) \otimes (v-u_M))\,w\,dv$$

and, by some manipulations in the same spirit of the calculations in Ref. 5, it becomes

$$\int mv \otimes vw\,dv = \int m\,(v-u_M) \otimes (v-u_M)\,w\,dv + mnu \otimes u - \frac{m}{n} \int (v-u_M)\,w\,dv \otimes \int (v-u_M)\,w\,dv\,. \tag{15}$$

We shall use the function M to close the previous expression: let us define

$$\mathbf{P}_M := -\int m\,(v-u_M) \otimes (v-u_M)\,M dv = -\int mv \otimes vM(x,v)\,dv + mnu_M \otimes u_M = -n\frac{\mathcal{I}}{\beta} - mnu_M \otimes u_M - \frac{\beta\hbar^2}{12m} n\nabla \otimes \nabla V\,, \tag{16}$$

where the last equality is obtained by (9). The definition of the tensor $\mathbf{P}_M$ is consistent with classical kinetic theory[6] (apart from the sign that is a matter of convention) and with the quantum case.[4] Moreover, it coincides with (11), given in analogy with Gardner.[3] Thus (15) reads

$$\int mv \otimes vw\,dv = mnu \otimes u - \mathbf{P}_M\,, \tag{17}$$

and (16) has to be compared with the corresponding results obtained in Ref. 1 and Ref. 2, respectively. In the same spirit,

$$\int \frac{1}{2} mv|v|^2 w\,dv = \int \frac{1}{2} m\,(v-u_M)\,|v-u_M+u_M|^2\,w\,dv + u_M \int \frac{1}{2} m|v|^2 w\,dv = \int \frac{1}{2} m\,(v-u_M)\,|v-u_M|^2\,w\,dv + (e\mathcal{I} - \mathbf{P}_M)u + |u_M|^2 \int \frac{1}{2} m\,(v-u_M)\,w\,dv\,. \tag{18}$$

By using M and defining

$$q_M := \int \frac{1}{2} m\,(v-u_M)\,|v-u_M|^2\,M\,dv\,, \tag{19}$$

(18) becomes

$$\int \frac{1}{2} mv|v|^2 w\,dv = q_M + (e\mathcal{I} - \mathbf{P}_M)u\,. \tag{20}$$

The expression (19) can be rewritten as

$$q_M = \frac{1}{2}\left[\int mv|v|^2 M\,dv - 2u_M \int v\otimes mvM\,dv + |u_M|^2 \int mvM\,dv \right. \tag{21}$$
$$\left. -\; u_M \int m|v|^2 M\,dv + 2u_M\otimes u_M \int mvM\,dv - mnu_M|u_M|^2\right]$$

and, by using Lemma 2.1,

$$q_M \;=\; -\frac{\hbar^2}{8m} n\Delta u_M + mnu_M\left(u_M\otimes u_M\right)\,. \tag{22}$$

The definition (19) of the heat flux is consistent with the classical and quantum literature, moreover it coincides with (12), previously introduced in analogy with Gardner.[3]

Finally, by using in Eqs. (14) the expressions (17) for the moment $\int v\otimes mvw\,dv$ and (20) for $\int \frac{1}{2}mv|v|^2 w\,dv$, we derive

$$\begin{aligned} \partial_t n + \nabla_x\cdot(nu) &= 0\,,\\ \partial_t(mnu) + \nabla_x\cdot mnu\otimes u - \nabla_x\cdot \mathbf{P}_M &= 0\,,\\ \partial_t e + \nabla_x\cdot(eu) - \nabla_x\cdot(\mathbf{P}_M u) + \nabla_x\cdot q_M &= 0\,. \end{aligned} \tag{23}$$

In conclusion, we remark that, unlike Ref. 3, the high-field relaxation-time function is adopted for the closure procedure. Accordingly, pressure tensor and heat-flux differ from the quantum (standard) ones in terms that are quadratic and cubic, respectively, in the ϵ^0 order velocity field u_M.

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