

Derivation of viscous correction terms for the isothermal quantum Euler model

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Abstract

The aim of this paper is to compute viscous correction terms for the isothermal quantum Euler system of Degond, Gallego, Méhats (SIAM Multiscale Model Simul., **6**, 2007). We derive this model by using a Chapman-Enskog expansion up to order 1. In a last part, we consider a situation where the flow is nearly irrotational in order to get a simplified model.

1 Introduction.

This paper is the continuation of a program of work initiated in 2003 in [9]. Extending Levermore's moments method [16] to a quantum context, P. Degond and C. Ringhofer derived hydrodynamical models from Chapman-Enskog expansions around quantum local equilibriums. Next, after this work, an entropic quantum drift-diffusion model was derived in [8], numerically discretized in [11] and discussed in the context of quantum transport in electronic nanostructures in [4]. In [6], an isothermal quantum Euler system was derived, recovering at a semiclassical asymptotics a model obtained in [14]. Extended models were also discussed in [2, 5].

All these models were obtained –formally– by applying a hydrodynamic or a diffusive scaling to a Wigner equation with ad-hoc relaxation operators and performing the limit as the mean free path converges to zero. In

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this paper, we are interested in the next order approximation of the hydrodynamic limit. In the classical setting, it is well-known [1] that this leads to the viscous correction to the Euler equations, i.e. to the Navier-Stokes system. Here, we apply the same idea in the quantum setting in order to derive the first order correction to the isothermal Euler equation of [6]. By analogy, we shall call *quantum Navier-Stokes system* the obtained model. A viscous model has been considered in ([13], [3]) where existence theorems are proved. It consists in two conservation equations for mass and current coupled with the Poisson equation.

Let us shortly present the approach. From the Wigner equation, integrations with respect to the momentum variable $p \in \mathbb{R}^3$ lead to equations for the first two moments $n(t, x)$ (the mass density) and $n(t, x)u(t, x)$ (the current density), both densities being functions of the space variable $x \in \mathbb{R}^3$ and the time variable $t \in \mathbb{R}$:

$$\partial_t n + \operatorname{div}(nu) = 0, \quad (1)$$

$$\partial_t(nu) + \operatorname{div}(nu \otimes u + \mathbb{P}) + n\nabla V = 0, \quad (2)$$

where V denotes an applied potential. Of course, this system of equations is not closed, since the pressure tensor \mathbb{P} is still expressed in terms of the microscopic Wigner function $f(t, x, p)$:

$$\mathbb{P} = \int_{\mathbb{R}^d} (p - u)(p - u) f(t, x, p) \frac{dp}{(2\pi\hbar)^3}, \quad (3)$$

where \hbar is the dimensionless Planck constant. The Wigner function $f(t, x, p)$ can be seen as a quantum extension of the phase-space Boltzmann distribution function, though $f(t, x, p)$ is not a positive function.

In ([15],[12], [10]), by using this procedure, full hydrodynamical systems are derived.

In [6], an isothermal quantum Euler system was derived by closing the system of moments as follows. The expression (3) of \mathbb{P} is simply replaced by another one in terms of n and nu :

$$\mathbb{P} = \int_{\mathbb{R}^d} (p - u)(p - u) f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}, \quad (4)$$

where $f_{n,nu}^{eq}$ is the so-called local equilibrium, depending only on n and nu in a non local (and non explicit) way – see Definition 1. Equivalently, this isothermal quantum Euler model can be obtained as the limit $\varepsilon \rightarrow 0$ of the following quantum BGK equation in a hydrodynamic scaling:

$$\partial_t f + p \cdot \nabla_x f + \Theta(V)f = \frac{1}{\varepsilon}(f_{n,nu}^{eq} - f).$$

In the present paper, in order to obtain a Navier-Stokes model, f will be formally expanded up to first order around the local equilibrium $f_{n,nu}^{eq}$ as $f = f_{n,nu}^{eq} + \varepsilon f_1$.

The outline of the paper is the following. In Section 2, the quantum Navier-Stokes model is derived and formulated in Theorem 1. Then, Section 3 is devoted to some simplifications of this model when the flow is assumed to be nearly irrotational: Proposition 1 is a reformulation of the quantum Navier-Stokes model in this situation.

2 Derivation of the model

In this section we first recall some backgrounds about the Wigner equation and we present the model derived in the general situation.

2.1 Notations and background.

By a density operator, we shall always mean a positive, Hermitian, trace-class operator acting on $L^2(\mathbb{R}^3)$. Let us recall the definition of the first moments of a density operator ϱ , i.e. the mass density n and the current density nu . These quantities are defined by duality, considering scalar test functions ϕ and vector ones Φ . We set

$$\forall \phi \in C_0^\infty(\mathbb{R}^3) \quad \int n \phi dx = \text{Tr}\{\varrho \phi\}, \quad (5)$$

$$\begin{aligned} \forall \Phi \in C_0^\infty(\mathbb{R}^3)^3 \quad \int nu \cdot \Phi dx &= \text{Tr}\{\varrho W^{-1}[p \cdot \Phi]\} \\ &= -i\hbar \text{Tr}\left\{\varrho \left(\Phi \cdot \nabla + \frac{1}{2}(\nabla \cdot \Phi)\right)\right\} \end{aligned} \quad (6)$$

Note that an immediate consequence of (5) and (6) is the following property which will be useful later:

$$\forall \Phi \quad -\frac{i}{\hbar} \text{Tr}\{\varrho(\Phi \cdot \nabla)\} = \int nu \cdot \Phi dx + \frac{i\hbar}{2} \int n \nabla \cdot \Phi dx. \quad (7)$$

In (6), W^{-1} denote the inverse Wigner transform (or Weyl quantization). Let us recall the definitions of the Wigner transform and the inverse Wigner transform. The Wigner transform maps operators on $L^2(\mathbb{R}^3)$ onto symbols, ie $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ functions of the classical position and momentum variables $(x, p) \in \mathbb{R}^3 \times \mathbb{R}^3$. More precisely, one defines the integral kernel of the

operator ϱ to be the distribution $\underline{\varrho}(x, x')$ such that ϱ operates on any function $\psi(x) \in L^2(\mathbb{R}^3)$ as follows:

$$\varrho\psi(x) = \int \underline{\varrho}(x, x')\psi(x')dx'.$$

Then, the Wigner transform $W[\varrho](x, p)$ is defined by:

$$W[\varrho](x, p) = \int \underline{\varrho}\left(x - \frac{1}{2}\eta, x + \frac{1}{2}\eta\right) e^{\frac{i\eta \cdot p}{\hbar}} d\eta. \quad (8)$$

The Wigner transform can be inverted and its inverse (called Weyl quantization) is defined for any function $f(x, p)$ as the operator acting on $\psi(x) \in L^2(\mathbb{R}^3)$ as:

$$W^{-1}[f]\psi(x) = (2\pi\hbar)^{-3} \int f\left(\frac{x+y}{2}, p\right) \psi(y) e^{\frac{ip \cdot (x-y)}{\hbar}} dp dy. \quad (9)$$

We have also the following Parseval property: for any operators ρ and σ in $\mathcal{L}^2 = \{\varrho : \text{Tr}(\varrho\varrho^\dagger) < \infty\}$:

$$\text{Tr}(\rho\sigma^\dagger) = \int W[\rho]\overline{W[\sigma]} \frac{dx dp}{(2\pi\hbar)^3}, \quad (10)$$

where the bar means complex conjugation. We also recall the cyclicity of the trace, where a, b, c are three operators:

$$\text{Tr}\{[a, b]c\} = \text{Tr}\{[c, a]b\} = \text{Tr}\{[b, c]a\}.$$

In quantum statistical mechanics, the Von Neumann entropy is defined by:

$$S(\varrho) = \text{Tr}(\varrho \ln \varrho - \varrho). \quad (11)$$

In order to deal with isothermal problems, we introduce the quantum free energy defined by:

$$G(\varrho) = TS(\varrho) + E(\varrho) = \text{Tr}(T(\varrho \ln \varrho - \varrho) + \mathcal{H}\varrho). \quad (12)$$

where \mathcal{H} is the Hamiltonian defined by

$$\mathcal{H} = -\frac{\hbar^2}{2}\Delta + V. \quad (13)$$

For simplicity, the potential $V = V(t, x)$ applied to the system of particles is assumed to be given, independent of the particles.

In this paper, we suppose that the particle system interacts with a thermal bath and that the mass n and the current nu are conserved by this interaction. Following [9], [8], [6], we shall model this interaction via a relaxation operator constructed according to a principle of free energy minimization. To this aim, we define the *local thermal equilibrium* associated to n and nu , at temperature T through the following formal procedure.

Definition 1. *Let the scalar function $n(x) \geq 0$ and the vectorial function $nu(x)$ be given. Consider the following constrained minimization problem:*

$$\min \{G(\varrho) \text{ such that } \varrho \text{ is a density operator satisfying (5) and (6)}\}. \quad (14)$$

The solution, if it exists, is called the local equilibrium density operator associated to n and nu . Lagrange multiplier theory for the constrained problem (14) (see [9], [6]) shows that there exist a scalar function A and a vector function B , both real valued and defined on \mathbb{R}^3 , such that this local equilibrium density operator takes necessarily the form:

$$\varrho_{n,nu}^{eq} = \exp\left(-\frac{1}{T} H(A, B)\right), \quad (15)$$

where $H(A, B)$ is the following modified Hamiltonian:

$$H(A, B) = W^{-1} \left[\frac{1}{2}(p - B)^2 + A \right] = \frac{1}{2} (i\hbar\nabla + B)^2 + A. \quad (16)$$

The local equilibrium Wigner function associated to n and nu is the Wigner transform of $\varrho_{n,nu}^{eq}$:

$$f_{n,nu}^{eq} = W[\varrho_{n,nu}^{eq}].$$

2.2 Derivation of the quantum Navier-Stokes system

Let us now introduce the quantum BGK equation, by adding a relaxation operator to the quantum Liouville equation. This operator, denoted by $\mathcal{Q}(\varrho)$, describes the collisions between the particles and a surrounding environment at temperature T . In this paper, we choose this collision operator equal to the simplest quantum BGK operator that can be constructed according to the minimization problem (14):

$$i\hbar\partial_t\varrho = [\mathcal{H}, \varrho] + i\hbar\frac{\varrho_{n,nu}^{eq} - \varrho}{\varepsilon}, \quad (17)$$

where, for all t , the local equilibrium $\varrho_{n,nu}^{eq}(t)$ is defined thanks to Definition 1 from the density $n(t, \cdot)$ and the current $(nu)(t, \cdot)$ associated to $\varrho(t)$ through (5), (6).

Let us now expand ϱ around $\varrho_{n,nu}^{eq}$ as follows:

$$\varrho = \varrho_{n,nu}^{eq} + \varepsilon \varrho_1.$$

By inserting this expansion of ϱ into the equation (17), we get the relation defining ϱ_1

$$\varrho_1 = -\partial_t \varrho_{n,nu}^{eq} + \frac{i}{\hbar} [\mathcal{H}, \varrho_{n,nu}^{eq}].$$

By using a Wigner transformation of the equation (17), we get the following Wigner-BGK equation

$$\partial_t f + p \cdot \nabla_x f - \Theta(V) f = \frac{f_{n,nu}^{eq} - f}{\varepsilon} \quad (18)$$

with

$$\Theta(V) f = \frac{i}{(2\pi)^3} \int_{\mathbb{R}^6} \frac{V(t, x + \frac{\hbar}{2}\eta) - V(t, x - \frac{\hbar}{2}\eta)}{\hbar} f(x, p') e^{i(p-p') \cdot \eta} d\eta dp'. \quad (19)$$

The Wigner transformation of the expansion of ϱ gives $f = f_{n,nu}^{eq} + \varepsilon f_1$. Hence f_1 has the expression

$$f_1 = -\partial_t f - p \cdot \nabla_x f + \Theta(V) f$$

and, formally,

$$f_1 = -\partial_t f_{n,nu}^{eq} - p \cdot \nabla_x f_{n,nu}^{eq} + \Theta(V) f_{n,nu}^{eq} + \mathcal{O}(\varepsilon). \quad (20)$$

Moreover, by considering the first moments of (18) with respect to p , we obtain

$$\partial_t \int f \frac{dp}{(2\pi\hbar)^3} + \text{div} \int p f \frac{dp}{(2\pi\hbar)^3} = 0$$

and

$$\partial_t \int f p \frac{dp}{(2\pi\hbar)^3} + \text{div} \int p \otimes p f \frac{dp}{(2\pi\hbar)^3} + n \nabla_x V = 0.$$

The last equation can be rewritten

$$\partial_t(nu) + \text{div} \int p \otimes p f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3} + n \nabla_x V = -\varepsilon \text{div} \int p \otimes p f_1 \frac{dp}{(2\pi\hbar)^3}.$$

Then (20) gives formally

$$\begin{aligned} \partial_t(nu) + \operatorname{div} \int p \otimes p f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3} + n\nabla_x V \\ = \varepsilon \operatorname{div} \int p \otimes p \left(\partial_t f_{n,nu}^{eq} + p \cdot \nabla_x f_{n,nu}^{eq} - \Theta(V) f_{n,nu}^{eq} \right) \frac{dp}{(2\pi\hbar)^3} + \mathcal{O}(\varepsilon^2). \end{aligned}$$

The isothermal quantum Navier-Stokes system is simply the model obtained when the $\mathcal{O}(\varepsilon^2)$ term is dropped in this equation:

$$\partial_t n + \operatorname{div}(nu) = 0, \quad (21)$$

$$\begin{aligned} \partial_t(nu) + \operatorname{div} \int p \otimes p f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3} + n\nabla_x V \\ = \varepsilon \operatorname{div} \int p \otimes p \left(\partial_t f_{n,nu}^{eq} + p \cdot \nabla_x f_{n,nu}^{eq} - \Theta(V) f_{n,nu}^{eq} \right) \frac{dp}{(2\pi\hbar)^3}, \quad (22) \end{aligned}$$

where $f_{n,nu}^{eq}$ is still defined from n and nu through Definition 1.

Let us now simplify this system. Equation (22) contains moments of order 2 and 3 of the equilibrium function $f_{n,nu}^{eq}$ which might not be easy to handle. Denote

$$\Pi_{ij} = \int p_i p_j f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}, \quad \mathbb{Q}_{ijk} = \int p_i p_j p_k f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}. \quad (23)$$

Using commutator properties as in [6] and [5], one can express $\operatorname{div}\Pi$ in terms of n , nu , A and B only. We recall from [6] that:

$$(\operatorname{div}\Pi)_i = \sum_j \partial_j \Pi_{ij} = \sum_j \partial_{x_j} (nu_i B_j) + \sum_j n(u_j - B_j) \partial_{x_i} B_j - n \partial_{x_i} A. \quad (24)$$

Similarly, we shall express $\sum_{j,k} \mathbb{Q}_{ijk}$ in terms of n , nu , A , B and Π only. This is the aim of the following theorem:

Theorem 1. *The above defined isothermal quantum Navier-Stokes system (21), (22) is formally equivalent to the following system, up to terms of order $\mathcal{O}(\varepsilon^2)$:*

$$\partial_t n + \operatorname{div}(nu) = 0, \quad (25)$$

$$\partial_t(nu_i) + \sum_{j=1}^3 \left(\partial_{x_j} (nu_i B_j) + n(u_j - B_j) \partial_{x_i} B_j \right) + n \partial_{x_i} (V - A) = \varepsilon S_i \quad (26)$$

where A and B are related to n and nu via Definition 1 and where S_i is equal to:

$$\begin{aligned}
S_i = & - \sum_{k=1}^3 \sum_{j=1}^3 \partial_{x_k} (\partial_{x_j} (nu_i B_j) B_k - n \partial_{x_j} (u_j - B_j) \partial_{x_i} B_j B_k) \\
& - \sum_{k=1}^3 \sum_{j=1}^3 \partial_{x_i} B_k \left(\partial_{x_j} (nu_k B_j) + n \partial_{x_j} (u_j - B_j) \partial_{x_k} B_j \right) \\
& - \sum_{k=1}^3 \partial_{x_k} (n \partial_{x_i} (V - A) B_k) + \sum_{k=1}^3 (\partial_{x_k} (nu_i \partial_t B_k) + \partial_{x_i} \partial_t B_k nu_k) \\
& - \sum_{k=1}^3 n \partial_{x_i} B_k \partial_{x_k} (V - A) + \sum_{k=1}^3 nu_k \partial_{x_i} \left(A + \frac{B^2}{2} \right) - n \partial_{x_i} \partial_t \left(A + \frac{B^2}{2} \right) \\
& - \sum_{j=1}^3 \sum_{j=1}^3 \partial_{x_j} \left(\partial_{x_j} \left(A + \frac{B^2}{2} \right) nu_i + \partial_{x_i} \left(A + \frac{B^2}{2} \right) nu_j \right) \\
& + \sum_{j=1}^3 \sum_{k=1}^3 \partial_{x_j} (\partial_{x_k} (B_k \Pi_{ij}) + \partial_{x_j} B_k \Pi_{ik} + \partial_{x_i} B_k \Pi_{jk}) \\
& - \frac{\hbar^2}{4} \sum_{j=1}^3 \sum_{k=1}^3 \partial_{x_j} \partial_{x_k} (n \partial_{x_i} \partial_{x_j} B_k) + \sum_{j=1}^3 \partial_{x_j} \left(\partial_{x_j} V nu_i + \partial_{x_i} V nu_j \right), \quad (27)
\end{aligned}$$

the tensor Π being defined by (23).

Proof. From (24), we deduce directly that the l.h.s. of (22) can be rewritten as the l.h.s. of (26). To prove the theorem, it remains to consider the r.h.s. of (22), which is

$$-\varepsilon \operatorname{div} \int p \otimes p f_1 \frac{dp}{(2\pi\hbar)^3} = \varepsilon g_1 + \varepsilon g_2 + \varepsilon g_3,$$

where we have set, for $i = 1, 2, 3$,

$$(g_1)_i = \sum_{j=1}^3 \partial_t \partial_{x_j} \int p_i p_j f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}, \quad (28)$$

$$(g_2)_i = \sum_{j=1}^3 \sum_{k=1}^3 \partial_{x_j} \partial_{x_k} \int p_i p_j p_k f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}, \quad (29)$$

$$(g_3)_i = - \sum_{j=1}^3 \partial_{x_j} \int p_i p_j \Theta(V) f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^3}. \quad (30)$$

The expressions of g_1 , g_2 and g_3 are given in the following lemmas whose proof is in the appendix. By summing up these expressions, the proof of the theorem is complete. \square

Lemma 1. *The quantity g_3 defined by (30) can be written*

$$(g_3)_i = \sum_{j=1}^3 \partial_{x_j} \left(\partial_{x_j} V n u_i + \partial_{x_i} V n u_j \right). \quad (31)$$

Lemma 2. *The quantity g_2 defined in (29) has the following expression:*

$$\begin{aligned} (g_2)_i &= - \sum_{j=1}^3 \sum_{k=1}^3 \partial_{x_j} \left(\partial_{x_j} \left(A + \frac{B^2}{2} \right) n u_i + \partial_{x_i} \left(A + \frac{B^2}{2} \right) n u_j \right) \\ &\quad + \sum_{j=1}^3 \sum_{k=1}^3 \partial_{x_j} \left(\partial_{x_k} (B_k \Pi_{ij}) + \partial_{x_j} B_k \Pi_{ik} + \partial_{x_i} B_k \Pi_{jk} \right) \\ &\quad - \frac{\hbar^2}{4} \sum_{j=1}^3 \sum_{k=1}^3 \partial_{x_j} \partial_{x_k} (n \partial_{x_i} \partial_{x_j} B_k). \end{aligned} \quad (32)$$

Lemma 3. *Up to $\mathcal{O}(\varepsilon)$ terms, the quantity g_1 defined in (28) has the following expression:*

$$\begin{aligned} (g_1)_i &= - \sum_{k=1}^3 \sum_{j=1}^3 \partial_{x_k} \left(\partial_{x_j} (n u_i B_j) B_k - n \partial_{x_j} (u_j - B_j) \partial_{x_i} B_j B_k \right) \\ &\quad - \sum_{k=1}^3 \sum_{j=1}^3 \partial_{x_i} B_k \left(\partial_{x_j} (n u_k B_j) + n \partial_{x_j} (u_j - B_j) \partial_{x_k} B_j \right) \\ &\quad - \sum_{k=1}^3 \partial_{x_k} (n \partial_{x_i} (V - A) B_k) + \sum_{k=1}^3 \left(\partial_{x_k} (n u_i \partial_t B_k) + \partial_{x_i} \partial_t B_k n u_k \right) \\ &\quad - \sum_{k=1}^3 n \partial_{x_i} B_k \partial_{x_k} (V - A) + \sum_{k=1}^3 n u_k \partial_{x_i} \left(A + \frac{B^2}{2} \right) \\ &\quad - n \partial_{x_i} \partial_t \left(A + \frac{B^2}{2} \right). \end{aligned} \quad (33)$$

3 The system in the irrotational case

In this part we focus on the special case of irrotational flows, which enables to simply notably the system obtained in Theorem 1. Indeed, it has been

shown in [6], [5] that when $\nabla \times u = 0$ then the quantity B defined in Definition 1 is nothing but the velocity u itself.

In the case of the isothermal quantum Euler equation, i.e. when we make $\varepsilon = 0$ in (26), it has been shown in [6] that when the initial data is irrotational, then the solution remains irrotational for all time. Unfortunately, it is not clear whether this property remains true for the quantum Navier-Stokes equations (25), (26). Instead, we have the following property: if $(\nabla \times u)(t = 0) = \mathcal{O}(\varepsilon)$ then we have $(\nabla \times u)(t) = \mathcal{O}(\varepsilon)$, which implies $B = u + \mathcal{O}(\varepsilon)$. In such situation, the model obtained by replacing B by u in the r.h.s. of (26) will only differ from (26) by $\mathcal{O}(\varepsilon^2)$ terms, and thus will remain consistent with our theory.

Proposition 1. *Assume that $(\nabla \times u)(t = 0) = \mathcal{O}(\varepsilon)$. Then, for all time, we have $(\nabla \times u)(t) = \mathcal{O}(\varepsilon)$ and the following system is formally equivalent to (25), (26), up to $\mathcal{O}(\varepsilon^2)$ terms:*

$$\partial_t n + \operatorname{div}(nu) = 0 \quad (34)$$

$$\partial_t(nu_i) + \sum_{j=1}^3 \left(\partial_{x_j}(nu_i B_j) + n(u_j - B_j)\partial_{x_i} B_j \right) + n\partial_{x_i}(V - A) = \varepsilon \tilde{S}_i \quad (35)$$

where

$$\begin{aligned} \tilde{S}_i &= \sum_{j=1}^3 \sum_{k=1}^3 \left(\partial_{x_j}(\partial_{x_j} u_k \mathbb{P}_{ik}) + \partial_{x_j}(\partial_{x_i} u_k \mathbb{P}_{jk}) + \partial_{x_j x_k}^2(\mathbb{P}_{ij} u_k) \right) \\ &+ \sum_{k=1}^3 \partial_{x_k}(nu_k)\partial_{x_i} A - n\partial_{x_i}(\partial_t A) - \frac{\hbar^2}{4} \sum_{k=1}^3 \sum_{j=1}^3 \partial_{x_j} \partial_{x_k}(n\partial_{x_i} \partial_{x_j} u_k) \end{aligned} \quad (36)$$

and where \mathbb{P} is the following tensor:

$$\mathbb{P} = \int_{\mathbb{R}^d} (p - u)(p - u) f_{n,nu}^{eq} \frac{dp}{(2\pi\hbar)^d}.$$

Proof. If $B = u + \mathcal{O}(\varepsilon)$, then (25), (26) yield

$$\partial_t u_i + \sum_{k=1}^3 u_k \partial_{x_k} u_i + \partial_{x_i}(V - A) = \mathcal{O}(\varepsilon). \quad (37)$$

So $\partial_t \frac{u^2}{2}$ reads

$$\partial_t \frac{u^2}{2} = - \sum_{j=1}^3 \sum_{k=1}^3 (u_j u_k \partial_{x_k} u_j) - \sum_{j=1}^3 u_j \partial_{x_j}(V - A) + \mathcal{O}(\varepsilon).$$

Let us replace B by u in the expression (27) of S_i . The terms depending on V vanish:

$$\begin{aligned} & -\partial_{x_k}(nu_k \partial_{x_i} V) - \partial_{x_k}(nu_i \partial_{x_k} V) + \partial_{x_i}(-\partial_{x_k} V) nu_k - n\partial_{x_k} V \partial_{x_i} u_k \\ & + n\partial_{x_i}(u_k \partial_{x_k} V) + \partial_{x_k}(\partial_{x_k} V nu_i) + \partial_{x_k}(\partial_{x_i} V nu_k) = 0. \end{aligned}$$

Let X be defined by

$$\begin{aligned} X &= -\partial_{x_k}(\partial_{x_j}(nu_j u_i) u_k) - \partial_{x_k}(nu_i u_j \partial_{x_j} u_k) - \partial_{x_i}(u_j \partial_{x_j} u_k) nu_k \\ & - \partial_{x_i} u_k \partial_{x_j}(nu_k u_j) + \partial_{x_j}(nu_j) u_k \partial_{x_i} u_k + n\partial_{x_i}(u_k \partial_{x_j} u_k u_j) \\ & + \partial_{x_j}(u_k \partial_{x_j} u_k nu_i) + \partial_{x_j}(u_k \partial_{x_i} u_k nu_j). \end{aligned}$$

and consider the terms depending on the stress tensor Π :

$$\begin{aligned} Y &= \partial_{x_j}(\partial_{x_j} u_k nu_i u_k) + \partial_{x_j}(\partial_{x_i} u_k nu_j u_k) + \partial_{x_j x_k}^2(nu_i u_j u_k) \\ & + \partial_{x_j}(\partial_{x_j} u_k \mathbb{P}_{ik}) + \partial_{x_j}(\partial_{x_i} u_k \mathbb{P}_{jk}) + \partial_{x_j x_k}^2(\mathbb{P}_{ij} u_k). \end{aligned}$$

Straightforward calculations lead to

$$X + Y = \partial_{x_j}(\partial_{x_j} u_k \mathbb{P}_{ik}) + \partial_{x_j}(\partial_{x_i} u_k \mathbb{P}_{jk}) + \partial_{x_j x_k}^2(\mathbb{P}_{ij} u_k).$$

Furthermore, the terms depending on A become

$$\begin{aligned} & \partial_{x_k}(n \partial_{x_i} A u_k) + \partial_{x_k}(nu_i \partial_{x_i} A) + \partial_{x_i}(\partial_{x_k} A) nu_k \\ & + n\partial_{x_k} A \partial_{x_i} u_k + \partial_{x_k}(nu_k) \partial_{x_i} A - n\partial_{x_i}(u_k \partial_{x_k} A) \\ & - \partial_{x_k}(\partial_{x_k} A nu_i) - \partial_{x_k}(\partial_{x_i} A nu_k) - n\partial_{x_i}(\partial_t A) \\ & = \partial_{x_k}(nu_k) \partial_{x_i} A - n\partial_{x_i}(\partial_t A). \end{aligned}$$

Hence (36) follows. \square

Remark 1. *The semi-classical limit of (36) leads to the classical isothermal Navier-Stokes equation. Indeed, in that case, \mathbb{P}_{ij} , A and B have the expressions [6]*

$$\mathbb{P}_{ij} = nT \delta_{ij}, \quad A = -T \ln(n), \quad B = u.$$

So we obtain

$$\sum_{k=1}^3 \sum_{j=1}^3 \partial_{x_j}(\partial_{x_j} u_k \mathbb{P}_{ik} + \partial_{x_i} u_k \mathbb{P}_{jk}) = \sum_{j=1}^3 \partial_{x_j}((\partial_{x_j} u_i + \partial_{x_i} u_j) nT),$$

$$\begin{aligned}
-n\partial_{x_i}(\partial_t A) &= -T\partial_{x_i}(\operatorname{div}(nu)) + \frac{T}{n}\partial_{x_i}n \operatorname{div}(nu), \\
\operatorname{div}(nu) \partial_{x_i} A &= -\operatorname{div}(nu) \frac{T}{n} \partial_{x_i} n, \\
\sum_{j=1}^3 \partial_{x_j}(\operatorname{div}(u \mathbb{P}_{ij})) &= T \partial_{x_i} \operatorname{div}(nu),
\end{aligned}$$

and we get finally

$$\tilde{S}_i = \sum_{j=1}^3 \partial_{x_j} \left((\partial_{x_j} u_i + \partial_{x_i} u_j) n T \right). \quad (38)$$

Appendix.

Proof of Lemma 1.

Let f be given. Then we have

$$\int p_i p_j \Theta(V) f \frac{dp}{(2\pi\hbar)^3} = -(\partial_{\eta_i} \partial_{\eta_j} \widehat{\Theta(V)} f)(t, x, 0).$$

But from (19), it holds that

$$\widehat{\Theta(V)} f = \imath \frac{V(t, x + \frac{\hbar}{2}\eta) - V(t, x - \frac{\hbar}{2}\eta)}{\hbar} \hat{f}(t, x, \eta).$$

Hence

$$\begin{aligned}
\int p_i p_j \Theta(V) f dp &= -\imath \partial_{x_i} \left(\frac{1}{2} \partial_{x_j} V(t, x + \frac{\hbar}{2}\eta) + \frac{1}{2} \partial_{x_j} V(t, x - \frac{\hbar}{2}\eta) \hat{f} \right. \\
&\quad \left. + \frac{V(t, x + \frac{\hbar}{2}\eta) - V(t, x - \frac{\hbar}{2}\eta)}{\hbar} \partial_{\eta_j} \hat{f} \right) \Big|_{\eta=0}.
\end{aligned}$$

So

$$\int p_i p_j \Theta(V) f \frac{dp}{(2\pi\hbar)^3} = -\imath \left(\partial_{x_j} V \partial_{\eta_i} \hat{f} + \partial_{x_i} V \partial_{\eta_j} \hat{f} \right)(t, x, 0).$$

Then

$$\int p_i p_j \Theta(V) f \frac{dp}{(2\pi\hbar)^3} = -\partial_{x_j} V n u_i - \partial_{x_i} V n u_j,$$

where

$$n = \int f \frac{dp}{(2\pi\hbar)^3}, \quad nu = \int fp \frac{dp}{(2\pi\hbar)^3},$$

and (31) follows. \square

Proof of Lemma 2.

Recall the definition (23) of \mathbb{Q} . We claim that, for all i and j ,

$$\begin{aligned} \sum_{k=1}^3 \partial_{x_k} \mathbb{Q}_{ijk} &= -\partial_{x_i} \left(A + \frac{B^2}{2} \right) nu_j - \partial_{x_j} \left(A + \frac{B^2}{2} \right) nu_i \\ &\quad + \sum_{k=1}^3 \left(\partial_{x_i} B_k \Pi_{jk} + \partial_{x_j} B_k \Pi_{ik} + \partial_{x_k} (B_k \Pi_{ij}) \right) \\ &\quad - \frac{\hbar^2}{4} \sum_{k=1}^3 \partial_{x_k} (n \partial_{x_i} \partial_{x_j} B_k). \end{aligned} \quad (39)$$

From (39), we deduce (32) and the proof of Lemma 2 is complete.

Let us prove (39). To this aim, we recall a useful commutator lemma that was established in [5]. Let us first introduce some notations. If $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3$ is a multi-index (with \mathbb{N} the set of natural integers), we denote

$$p^\alpha = p_1^{\alpha_1} p_2^{\alpha_2} p_3^{\alpha_3}, \quad \partial_x^\alpha = \partial / \partial x_1^{\alpha_1} \partial / \partial x_2^{\alpha_2} \partial / \partial x_3^{\alpha_3}, \quad |\alpha| = \alpha_1 + \alpha_2 + \alpha_3,$$

$$\sum_{0 \leq \gamma \leq \alpha} = \sum_{\gamma_1=0}^{\alpha_1} \sum_{\gamma_2=0}^{\alpha_2} \sum_{\gamma_3=0}^{\alpha_3} \quad \text{and} \quad \binom{\alpha}{\gamma} = \binom{\alpha_1}{\gamma_1} \binom{\alpha_2}{\gamma_2} \binom{\alpha_3}{\gamma_3},$$

where $\binom{\alpha_i}{\gamma_i}$ are the binomial coefficients.

Lemma 4 (Lemma 3.4 of [5]). *Let $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3$ and $\beta = (\beta_1, \beta_2, \beta_3) \in \mathbb{N}^3$ be two multi-indices and let $\lambda(x)$ and $\mu(x)$ be any smooth real or complex valued functions. Let us denote $[\lambda p^\alpha, \mu p^\beta]_\hbar$ the symbol associated to the commutator of the operators $W^{-1}(\lambda p^\alpha)$ and $W^{-1}(\mu p^\beta)$, i.e.:*

$$[\lambda p^\alpha, \mu p^\beta]_\hbar = W \left(\left[W^{-1}(\lambda p^\alpha), W^{-1}(\mu p^\beta) \right] \right). \quad (40)$$

The following formal expansion holds:

$$[\lambda p^\alpha, \mu p^\beta]_\hbar = \sum_{k=0}^{[(|\alpha+\beta|-1)/2]} i\hbar^{2k+1} \left(-\frac{1}{4} \right)^k [\lambda p^\alpha, \mu p^\beta]_{2k+1}, \quad (41)$$

with

$$[\lambda p^\alpha, \mu p^\beta]_{2k+1} = \sum_{\substack{0 \leq \gamma \leq \alpha, 0 \leq \zeta \leq \beta \\ |\gamma + \zeta| = 2k+1}} (-1)^{|\gamma|} \binom{\alpha}{\gamma} \binom{\beta}{\zeta} (\partial_x^\zeta \lambda) (\partial_x^\gamma \mu) p^{\alpha + \beta - \gamma - \zeta}, \quad (42)$$

where $[\cdot]$ denotes the floor function.

Let $\mu(x)$ be a given test function. From Lemma 4, we compute:

$$\sum_{k=1}^3 \partial_{x_k} \mu p_i p_j p_k = \frac{i}{\hbar} \left[\frac{|p|^2}{2}, \mu p_i p_j \right]_{\hbar}. \quad (43)$$

Hence, an integration by parts gives

$$\begin{aligned} \int \mu \sum_{k=1}^3 \partial_{x_k} \mathbb{Q}_{ijk} dx &= - \sum_{k=1}^3 \int \partial_{x_k} \mu p_i p_j p_k f_{n,nu}^{eq} \frac{dx dp}{(2\pi\hbar)^3} \\ &= - \frac{i}{\hbar} \int \left[\frac{|p|^2}{2}, \mu p_i p_j \right]_{\hbar} f_{n,nu}^{eq} \frac{dx dp}{(2\pi\hbar)^3} \\ &= - \frac{i}{\hbar} \int W \left(\left[-\frac{\hbar^2}{2} \Delta, W^{-1}(\mu p_i p_j) \right] \right) f_{n,nu}^{eq} \frac{dx dp}{(2\pi\hbar)^3}. \end{aligned}$$

Now, using the Parseval property (10) and observing that

$$-\frac{\hbar^2}{2} \Delta = H(A, B) - W^{-1} \left(-B \cdot p + A + \frac{B^2}{2} \right),$$

where $H(A, B)$ is defined by (16), we get

$$\begin{aligned} \int \mu \sum_{k=1}^3 \partial_{x_k} \mathbb{Q}_{ijk} dx &= - \frac{i}{\hbar} \text{Tr} \left(\left[-\frac{\hbar^2}{2} \Delta, W^{-1}(\mu p_i p_j) \right] \varrho_{n,nu}^{eq} \right) \\ &= - \frac{i}{\hbar} \text{Tr} \left(\left[H(A, B) - W^{-1} \left(-B \cdot p + A + \frac{B^2}{2} \right), W^{-1}(\mu p_i p_j) \right] \varrho_{n,nu}^{eq} \right) \\ &= \frac{i}{\hbar} \text{Tr} \left(\left[W^{-1} \left(-B \cdot p + A + \frac{B^2}{2} \right), W^{-1}(\mu p_i p_j) \right] \varrho_{n,nu}^{eq} \right) \\ &= \frac{i}{\hbar} \int \left[-B \cdot p + A + \frac{B^2}{2}, \mu p_i p_j \right]_{\hbar} f_{n,nu}^{eq} \frac{dx dp}{(2\pi\hbar)^3} \end{aligned}$$

where we used the cyclicity of the trace and the crucial fact that, by (15), $\varrho_{n,nu}^{eq}$ commutes with the operator $H(A, B)$.

Let us now compute $\left[-B \cdot p + A + \frac{B^2}{2}, \mu p_i p_j\right]_{\hbar}$. From Lemma 4, we deduce

$$\left[A + \frac{B^2}{2}, \mu p_i p_j\right]_{\hbar} = i\hbar \left(\partial_{x_i} \left(A + \frac{B^2}{2} \right) p_j + \partial_{x_j} \left(A + \frac{B^2}{2} \right) p_i \right) \mu,$$

and that

$$[B \cdot p, \mu p_i p_j]_{\hbar} = i\hbar [B \cdot p, \mu p_i p_j]_1 - \frac{i\hbar^3}{4} [B \cdot p, \mu p_i p_j]_3,$$

with

$$\begin{aligned} [B \cdot p, \mu p_i p_j]_1 &= \sum_{k=1}^3 [B_k p_k, \mu p_i p_j]_1 \\ &= \sum_{k=1}^3 (\partial_{x_i} B_k \mu p_j p_k + \partial_{x_j} B_k \mu p_i p_k - B_k \partial_{x_k} \mu p_i p_j) \end{aligned}$$

and

$$[B \cdot p, \mu p_i p_j]_3 = \sum_{k=1}^3 [B_k p_k, \mu p_i p_j]_3 = - \sum_{k=1}^3 \partial_{x_i} \partial_{x_j} B_k \partial_{x_k} \mu.$$

Hence,

$$\begin{aligned} -[B \cdot p, \mu p_i p_j]_{\hbar} &= -i\hbar \sum_{k=1}^3 (\partial_{x_i} B_k p_j p_k + \partial_{x_j} B_k p_i p_k) \mu \\ &\quad - i\hbar \sum_{k=1}^3 \left(\frac{\hbar^2}{4} \partial_{x_i} \partial_{x_j} B_k - B_k p_i p_j \right) \partial_{x_k} \mu. \end{aligned}$$

We get finally, after an integration by parts,

$$\begin{aligned}
& \int \mu \sum_{k=1}^3 \partial_{x_k} \mathbb{Q}_{ijk} dx \\
&= - \int \left(\partial_{x_i} \left(A + \frac{B^2}{2} \right) p_j + \partial_{x_j} \left(A + \frac{B^2}{2} \right) p_i \right) \mu f_{n,nu}^{eq} \frac{dx dp}{(2\pi\hbar)^3} \\
&\quad + \int \sum_{k=1}^3 (\partial_{x_i} B_k p_j p_k + \partial_{x_j} B_k p_i p_k) \mu f_{n,nu}^{eq} \frac{dx dp}{(2\pi\hbar)^3} \\
&\quad - \int \sum_{k=1}^3 \partial_{x_k} \left(\left(\frac{\hbar^2}{4} \partial_{x_i} \partial_{x_j} B_k - B_k p_i p_j \right) f_{n,nu}^{eq} \right) \mu \frac{dx dp}{(2\pi\hbar)^3} \\
&= - \int \left(\partial_{x_i} \left(A + \frac{B^2}{2} \right) nu_j + \partial_{x_j} \left(A + \frac{B^2}{2} \right) nu_i \right) \mu dx \\
&\quad + \int \sum_{k=1}^3 (\partial_{x_i} B_k \Pi_{jk} + \partial_{x_j} B_k \Pi_{ik}) \mu dx \\
&\quad - \int \sum_{k=1}^3 \partial_{x_k} \left(\frac{\hbar^2}{4} n \partial_{x_i} \partial_{x_j} B_k - B_k \Pi_{ij} \right) \mu dx.
\end{aligned}$$

Therefore, since this expression holds true for all function $\mu(x)$, one can identify (39).

Proof of Lemma 3.

From (24), we deduce

$$\begin{aligned}
(g_1)_i &= \partial_t (\operatorname{div} \Pi)_i \\
&= \sum_{k=1}^3 \partial_{x_k} (\partial_t (nu_i) B_k) + \sum_{k=1}^3 \partial_{x_k} (nu_i \partial_t B_k) + \sum_{k=1}^3 \partial_{x_i} \partial_t B_k nu_k \\
&\quad + \sum_{k=1}^3 \partial_{x_i} B_k \partial_t (nu_k) - \partial_t n \partial_{x_i} \left(A + \frac{B^2}{2} \right) - n \partial_{x_i} \partial_t \left(A + \frac{B^2}{2} \right).
\end{aligned} \tag{44}$$

But according to (21), (22), we have

$$\begin{aligned}
\partial_t n &= -\operatorname{div}(nu), \\
\partial_t (nu_i) &= - \sum_{j=1}^3 \partial_{x_j} (nu_i B_j) - n \sum_{j=1}^3 \partial_{x_j} (u_j - B_j) \partial_{x_i} B_j - n \partial_{x_i} (V - A) + \mathcal{O}(\varepsilon).
\end{aligned}$$

So, neglecting the $\mathcal{O}(\varepsilon)$ terms, we get the following relations:

$$\begin{aligned}\partial_t(nu_i)B_k &= -\sum_{j=1}^3 \partial_{x_j}(nu_i B_j)B_k - n \sum_{j=1}^3 \partial_{x_j}(u_j - B_j)\partial_{x_i}B_j B_k \\ &\quad - n\partial_{x_i}(V - A)B_k,\end{aligned}$$

$$\begin{aligned}\sum_{k=1}^3 \partial_{x_i}B_k \partial_t(nu_k) &= \sum_{k=1}^3 \partial_{x_i}B_k \left(-\sum_{j=1}^3 \partial_{x_j}(nu_k B_j) - n \sum_{j=1}^3 \partial_{x_j}(u_j - B_j)\partial_{x_k}B_j \right. \\ &\quad \left. - n\partial_{x_k}(V - A) \right)\end{aligned}$$

and

$$\partial_t n \partial_i \left(A + \frac{1}{2} B^2 \right) = - \sum_{k=1}^3 (nu_k) \partial_{x_i} \left(A + \frac{1}{2} B^2 \right)$$

which enable to simplify (44) and gives (33).

References

- [1] C. Bardos, F. Golse, D. Levermore, *Fluid dynamic limits of kinetic equations. I. Formal derivations*. J. Statist. Phys. **63** (1991), no. 1-2, 323–344.
- [2] J.-P. Bourgade, P. Degond, F. M ehats, C. Ringhofer, *On quantum extensions to classical Spherical Harmonics Expansion / Fokker-Planck models*, J. Math. Phys. **47** (2006), no. 4, 043302
- [3] L. Chen, M. Dreher, *The viscous model of quantum hydrodynamics in several dimensions*, Math. Models Methods Appl. Sci. **17** (2007) 1065–1093.
- [4] P. Degond, S. Gallego, F. M ehats, *An entropic Quantum Drift-Diffusion model for electron transport in resonant tunneling diodes*, J. Comput. Phys. **221** (2007), 226–249.
- [5] P. Degond, S. Gallego, F. M ehats. *On Quantum Hydrodynamic and Quantum Energy Transport Models*, Commun. Math.Sci. **5** (2007), no. 4, 887-908.
- [6] P. Degond, S. Gallego, F. M ehats. *Isothermal quantum hydrodynamics: derivation, asymptotic analysis and simulation*, SIAM Multiscale Model. Simul. **6** (2007), no.1, 246-272.

- [7] P. Degond, F. Méhats, C. Ringhofer, *Quantum hydrodynamic models derived from the entropy principle*, Contemp. Math. **371** (2005), 107–331.
- [8] P. Degond, F. Méhats, C. Ringhofer, *Quantum energy-transport and drift-diffusion models*, J. Stat. Phys. **118** (2005), no. 3-4, 625–665.
- [9] P. Degond, C. Ringhofer, *Quantum Moment Hydrodynamics and the Entropy Principle*, J. Stat. Phys. **112** (2003), no. 3-4, 587–628.
- [10] D. Ferry, J.-R. Zhou. *Form of the quantum potential for use in hydrodynamic equations for semiconductor device modeling*, Phys. Rev. B **48** (1993) 7944-7950.
- [11] S. Gallego, F. Méhats, *Entropic discretization of a quantum drift-diffusion model*, SIAM J. Numer. Anal. **43** (2005), no. 5, 1828–1849.
- [12] C. Gardner, *The quantum hydrodynamic model for semiconductor devices*, SIAM J. Appl. Math. **54** (1994), no. 2, 409–427.
- [13] M. P. Gualdani and A. Jüngel: *Analysis of the viscous quantum hydrodynamic equations for semiconductors*. Europ. J. Appl. Math. **15** (2004), 577–595.
- [14] A. Jüngel, D. Matthes, *A derivation of the isothermal quantum hydrodynamic equations using entropy minimization*, Z. Angew. Math. Mech. **85** (2005), 806–814.
- [15] A. Jngel, D. Matthes and J.P. Milisic. *Derivation of new quantum hydrodynamic equations using entropy minimization*, SIAM J. Appl. Math. **67** (2006), 46–68.
- [16] C. D. Levermore, *Moment closure hierarchies for kinetic theories*, J. Stat. Phys. **83** (1996), 1021–1065.