A new derivation of the quantum Navier-Stokes equations in the Wigner-Fokker-Planck approach

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Abstract A quantum Navier–Stokes system for the particle, momentum, and energy densities are formally derived from the Wigner–Fokker–Planck equation using a moment method. The viscosity term depends on the particle density with a shear viscosity coefficient which equals the quantum diffusion coefficient of the Fokker–Planck collision operator. The main idea of the derivation is the use of a so-called osmotic momentum operator, which is the sum of the phase-space momentum and the gradient operator. In this way, a Chapman–Enskog expansion of the Wigner function, which typically leads to viscous approximations, is avoided. Moreover, we show that the osmotic momentum emerges from local gauge theory.

Keywords Quantum Navier–Stokes model · Wigner–Fokker–Planck equations · moment method · osmotic momentum · local gauge transformation

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1 Introduction

Dissipative quantum models aim for describing a quantum system together with a reservoir, which absorbs the energy lost by the system. Examples are active re-

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gions and contacts in semiconductor devices [2], spin chains with thermal noise [14], or open Bose–Einstein condensates [1]. These models are typically based on the master equation in Lindblad form [17], the Schrödinger-Langevin equation [19], or collisional Wigner equations [2,17]. Due to their high numerical complexity, simpler macroscopic models have been derived in recent years.

One strategy is to introduce the Wigner–Weyl transform of the density matrix, which defines the Wigner function $w(x, p, t)$ in the phase-space variables $(x, p) \in \mathbb{R}^6$ and time $t > 0$, and to write the master equation in terms of the Wigner function, leading to the Wigner equation

$$\partial_t w + p \cdot \nabla_x w + \theta_\hbar[V]w = L_{\mathrm{BGK}}[w] + L_{\mathrm{FP}}[w], \quad (x, p) \in \mathbb{R}^6, \ t > 0, \qquad (1)$$

with the initial condition $w(\cdot, \cdot, 0) = w_0$ in $\mathbb{R}^6$. Here, $\theta_\hbar[V]$ is the nonlocal potential operator

$$(\theta_\hbar[V]w)(x, p, t) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} (\delta V)(x, y, t) e^{iy \cdot (p-p)/\hbar} dp \ dy,$$

which models the influence of the electric potential $V(x, t)$, and

$$(\delta V)(x, y, t) = \frac{i}{\hbar} \left(V\left(x + \frac{y}{2}, t\right) - V\left(x - \frac{y}{2}, t\right) \right).$$

The operators on the right-hand side of (1) describe collisions and are explained in Section 2. By slight abuse of notation, $\hbar$ denotes the scaled reduced Planck constant, although the above equations are scaled (see [13, Appendix] for details of the scaling). For mathematical results on the Wigner–Fokker–Planck model, we refer to [3,4].

By formal integration of the Wigner equation over the momentum space, evolution equations for the particle density n, moment density nu, and energy density ne, defined by

$$(n, nu, ne) = \int_{\mathbb{R}^3} \left(1, p, \frac{1}{2}|p|^2\right) w \, dp, \qquad (2)$$

can be derived. However, higher-order moments appear which cannot be expressed in terms of the moments (n, nu, ne), which is called the closure problem. It can be solved by assuming that the Wigner function in the higher-order moments can be approximated by the quantum equilibrium distribution $M[w]$ (see Section 2 for a definition). In this way, quantum hydrodynamic equations were derived [10, 12], whose numerical solution is less demanding than for Wigner models. When a Chapman–Enskog expansion around the quantum equilibrium is applied, $w = M[w] + \alpha g$, where g is some first-order correction and $\alpha > 0$ is some parameter, diffusive corrections are obtained.

This procedure was recently applied by Brull and Méhats [6] to the Wigner–BGK equation (named after Bhatnagar, Gross, and Krook [5]), which equals (1) with $L_{\mathrm{FP}}[w] = 0$, leading to nonlocal quantum Navier–Stokes equations, consisting of the mass conservation equation and the momentum balance equation. Local equations are realized by approximating the quantum equilibrium up to order $O(\hbar^4)$, yielding a density-dependent viscosity in the stress tensor. The full model, including the energy equation, was derived in [18].

In this paper, we present an alternative derivation of the quantum Navier–Stokes model by starting from the Wigner–Fokker–Planck equation and by just applying a moment method. The first advantage of our ansatz is that we can avoid the Chapman–Enskog expansion, which simplifies significantly the derivation. The second advantage is that the viscosity coefficient can be identified with the quantum diffusion coefficient of the operator $L_{\text{FP}}[w]$, which is proportional to the de Broglie wavelength and whose numerical value can be easily determined. On the other hand, the viscosity coefficient in [6,18] equals the scaled relaxation time in the BGK operator and it may be less easier to determine its numerical value.

In principle, the moment method just gives zeroth-order approximations of the moments. It may appear surprising why we obtain viscous corrections *without* applying a (first-order) Chapman–Enskog expansion. The reason is that we calculate the moments not in the momentum variable p but employing the moment operator

$$\eta = p - D_{qq}\nabla_x \tag{3}$$

(see (5) below for an expression of D_{qq}). This definition is related to the osmotic velocity of Nelson [25, Formula (26)] and to the deformed momentum of Mosna, Hamilton, and Delle Site [24, Formula (8)]. We show in Section 2.4 that (3) originates from a local gauge transformation in the Schrödinger picture. Then, introducing the η-moments

$$(n, nu_\eta, ne_\eta) = \int_{\mathbb{R}^3} \left(1, \eta, \frac{1}{2}|\eta|^2\right) w\,dp, \tag{4}$$

where $|\eta|^2 = \eta \cdot \eta$, new quantum Navier–Stokes equations for (n, nu_η, ne_η) are derived with a viscosity term essentially coming from the expression $D_{qq}\int_{\mathbb{R}^3}(\nabla_x \otimes p + p \otimes \nabla_x)w\,dp$ up to terms of order $O(\hbar^4)$, where "$\otimes$" denotes the tensor product (see Theorem 1 below).

When we apply the moment method to the Wigner–Fokker–Planck equation (1) using the p-moments (2), we obtain quantum hydrodynamic equations including the diffusion operators $\alpha\Delta_x n$, $\alpha\Delta_x(nu)$, and $\alpha\Delta_x(ne)$, respectively, in the moment equations [13,20]. There is a surprising connection between the quantum Navier–Stokes model and these quantum hydrodynamic equations. Indeed, introducing the new velocity $v = u - \alpha\nabla_x \log n$, the latter model can be formulated as the former one if $\hbar > \alpha = D_{qq}$ [16]. It holds

$$nu_\eta = \int_{\mathbb{R}^3} \eta w\,dp = \int_{\mathbb{R}^3} pw\,dp - D_{qq}\nabla_x \int_{\mathbb{R}^3} w\,dp = nu - D_{qq}\nabla_x n = nv,$$

and thus, the velocities u_η and v coincide for $n > 0$. Hence, it may be expected that the quantum Navier–Stokes system follows from the Wigner–Fokker–Planck equation by means of the above momentum operator. In this paper, we show that this expectation is correct although the two models, either derived from the Wigner–BGK equation or from the Wigner–Fokker–Planck model, have different stress tensors and energies (see Section 2 for a discussion).

The paper is organized as follows. In Section 2, we detail the Wigner–Fokker–Planck model (1) and present a model hierarchy involving the Wigner equation and its moment models as well as our main result. The η-moment equations are derived in Section 3 and their closure is performed in Section 4.

2 Model hierarchy, main result, and discussion

In this section, we make precise the Wigner–Fokker–Planck model and the definition of the quantum equilibrium, present a model hierarchy, give our main result, and discuss the osmotic momentum.

2.1 Definition of the collision operators

The collision operator on the right-hand side of (1) consists of two terms. The dominant term is of BGK type,

$$L_{\mathrm{BGK}}[w] = \frac{1}{\alpha}(M[w] - w),$$

where $\alpha > 0$ is the relaxation time and $M[w]$ denotes the quantum equilibrium [9]. In order to define $M[w]$, we assume that the collision operator L_{BGK} conserves mass, momentum, and energy,

$$\int_{\mathbb{R}^3} \left(1, p, \frac{1}{2}|p|^2\right) L_{\mathrm{BGK}}[w]\, dp = 0.$$

Then, according to Degond and Ringhofer [9], given a Wigner function w and the corresponding moments (2), the quantum equilibrium is defined (if it exists) as the maximizer of the quantum free energy (or quantum entropy) subject to the constraints $(n, nu, ne) = {}_{\mathbb{R}^3}(1, p, \frac{1}{2}|p|^2)M[w]\, dp$:

$$M[w](x, p, t) = \mathrm{Exp}\left(A(x, t) - \frac{|p - U(x, t)|^2}{2T(x, t)}\right).$$

The functions A, U, and T are the Lagrange multipliers of the constrained extremal problem, $\mathrm{Exp}(w) = W(\exp W^{-1}(w))$ is the quantum exponential defined in [9], and W and W^{-1} are the Wigner transform and its inverse operator, respectively [2, 15]. The multiplier U is linked to the velocity u by the relation $U = u + O(\hbar^2)$ and it holds $U = u$ for irrotational flows [15, p. 295]. The rigorous solvability of the constrained maximization problem is a delicate issue. A unique maximizer of the quantum entropy in the one-dimensional setting subject to a given local particle density was proven recently in [23].

The second collision term in (1) is the Fokker–Planck operator

$$L_{\mathrm{FP}}[w] = D_{pp}\Delta_p w + 2\lambda \,\mathrm{div}_p(pw) + 2D_{pq}\,\mathrm{div}_x(\nabla_p w) + D_{qq}\Delta_x w,$$

which models the dissipative interaction of an electron ensemble with an idealized heat bath consisting of an ensemble of harmonic oscillators [8]. The parameters are the friction coefficient $\lambda > 0$, the decoherence coefficient $D_{pp} > 0$, and the system-to-bath diffusion parameters $D_{pq} > 0$ and $D_{qq} > 0$. In particular, the diffusion coefficient

$$D_{qq} = \frac{\lambda \hbar^2}{6mk_BT_0} \tag{5}$$

plays the role of the viscosity (see Theorem 1 below), where m is the (effective) mass of the electrons and k_BT_0 the thermal energy. When the quantum diffusion

parameters vanish, $D_{pq} = D_{qq} = 0$, we obtain the Caldeira–Leggett operator [7]. This operator, however, does not satisfy the Lindblad condition $D_{pp}D_{qq} - D_{pq}^2 \geq \lambda^2/4$ which is a generic condition for quantum systems to preserve complete positivity of the density matrix along the evolution [2].

2.2 A model hierarchy

Let w be a solution to the Wigner–Fokker–Planck equation (1) and let the particle density n, momentum nu, and energy density ne be given by (2). When integrating the Wigner–BGK equation (1) with $L_{\text{FP}}[w] = 0$ over the momentum space, closing the moment equations by $M[w]$, performing a Chapman–Enskog expansion $w = M[w] + \alpha g$, and expanding $M[w]$ in powers of $\hbar^2$, the (local) *quantum Navier–Stokes equations* up to $O(\hbar^4)$

$$\partial_t n + \text{div}_x(nu) = 0, \tag{6}$$

$$\partial_t(nu) + \text{div}_x(nu \otimes u + P) - n\nabla_x V = \text{div}_x S, \tag{7}$$

$$\partial_t(ne) + \text{div}_x\big((P + ne\mathbb{I})u + q\big) - nu \cdot \nabla_x V = \text{div}_x(Su), \quad x \in \mathbb{R}^3,\ t > 0, \tag{8}$$

are obtained (see Arrow 1 in Figure 1), where $\mathbb{I}$ is the identity matrix in $\mathbb{R}^{3 \times 3}$,

$$ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\hbar^2}{24}n\Delta_x \log n, \quad P = nT\mathbb{I} - \frac{\hbar^2}{12}n\nabla_x^2 \log n$$

are the energy density and quantum stress tensor, respectively, and

$$q = -\frac{5}{2}\alpha nT\nabla T - \frac{\hbar^2}{24}n(\Delta_x u + 2\nabla_x \text{div}_x u), \quad S = 2\alpha nT\left(D(u) - \frac{1}{3}\text{div}_x u\mathbb{I}\right) \tag{9}$$

are the quantum heat flux and viscous stress tensor, respectively [18]. Furthermore, $\nabla_x^2 \log n$ is the Hessian of $\log n$ and $D(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$ the symmetric velocity gradient. The initial conditions are given by $(n, nu, ne)(\cdot, 0) = (n_0, nu_0, ne_0)$, where

$$(n_0, nu_0, ne_0) = \int_{\mathbb{R}^3}\left(1, p, \frac{1}{2}|p|^2\right)w_0 dp. \tag{10}$$
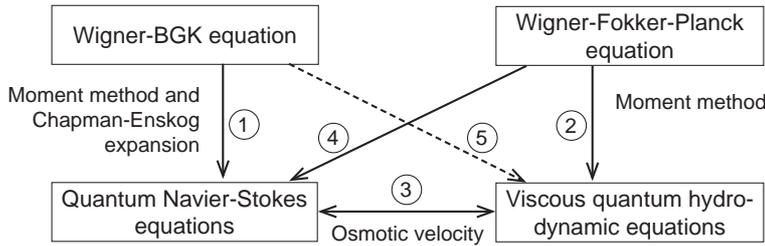
Fig. 1 Macroscopic quantum models derived from the Wigner–BGK or Wigner–Fokker–Planck equations. The derivation expressed by Arrow 4 is new.

On the other hand, when integrating the Wigner–Fokker–Planck equation (1) with $L_{\mathrm{BGK}}[w] = 0$ over the momentum space, closing the moment equations by $M[w]$, and expanding the quantum equilibrium in powers of $\hbar^2$, the *viscous quantum hydrodynamic equations* up to $O(\hbar^4)$

$$\partial_t n + \operatorname{div}_x(nu) = D_{qq}\Delta_x n, \tag{11}$$

$$\partial_t(nu) + \operatorname{div}_x(nu \otimes u + P + 2D_{pq}n\mathbb{I}) - n\nabla_x V = -2\lambda nu + D_{qq}\Delta_x(nu), \tag{12}$$

$$\partial_t(ne) + \operatorname{div}_x\big((P + ne\mathbb{I} + 2D_{pq}n\mathbb{I})u\big) - nu \cdot \nabla_x V \tag{13}$$
$$= 3D_{pp}n - 4\lambda ne + D_{qq}\Delta_x(ne),$$

with initial conditions (10) are derived (Arrow 2 in Figure 1).

As explained in the introduction, there is a surprising connection between the above models (6)–(8) and (11)–(13) by means of the transformation $u_\eta = u - \alpha\nabla_x \log n$, where $\alpha = D_{qq}$ (Arrow 3 in Figure 1). The expression $D_{qq}\nabla_x \log n$ is known as the osmotic velocity, see [25]. This motivates the introduction of the momentum operator $\eta = p - D_{qq}\nabla_x$ (see Section 2.4). One may expect that the quantum Navier–Stokes system can be derived from the Wigner–Fokker–Planck equation (1) if we define the moments by using η instead of p, see definition (4). Theorem 1 below shows that this is indeed the case (Arrow 4 in Figure 1).

We expect that a viscous quantum hydrodynamic model can be derived from the Wigner–BGK equation using a similar transformation (Arrow 5 in Figure 1) but this is not of our interest since we cannot expect a simplification of the derivation from the Wigner–Fokker–Planck equation.

2.3 Main result and discussion

Now we can state our main result.

Theorem 1 *Let w_α be a (smooth) solution to the Wigner–Fokker–Planck equation (1). Then the limit function $w = \lim_{\alpha \to 0} w_\alpha$ solves, up to terms of order $O(\hbar^4)$, the quantum Navier-Stokes equations*

$$\partial_t n + \operatorname{div}_x(nu_\eta) = 0, \tag{14}$$

$$\partial_t(nu_\eta) + \operatorname{div}_x\big(nu_\eta \otimes u_\eta + P_\eta\big) + n\nabla_x V = -2\lambda nu_\eta + \operatorname{div}_x S_\eta, \tag{15}$$

$$\partial_t(ne_\eta) + \operatorname{div}_x\big((P_\eta + ne_\eta\mathbb{I})u_\eta + q_\eta\big) + D_{qq}n\Delta_x V - nu_\eta \cdot \nabla_x V \tag{16}$$
$$= 3D_{pp}n - 4\lambda ne_\eta + \operatorname{div}_x(S_\eta u_\eta), \quad x \in \mathbb{R}^3, \ t > 0,$$

where (n, nu_η) is given by (4), and we have assumed that $A(u_\eta) = \frac{1}{2}(\nabla u_\eta - \nabla u_\eta^\top) = O(\hbar^2)$ and $\nabla_x \log T = O(\hbar^2)$ with T being defined in (17) below. Furthermore, the modified quantum stress tensor P_η, the quantum heat flux q_η, the viscous stress tensor S_η, and the energy density ne_η are given by

$$P_\eta = n\big(T + 2(D_{pq} + \lambda D_{qq})\big)\mathbb{I} - \frac{\hbar^2}{12}n\nabla_x^2 \log n,$$

$$q_\eta = -\frac{\hbar^2}{24}n\big(\Delta_x u_\eta + 2\nabla_x \operatorname{div}_x u_\eta\big), \quad S_\eta = 2D_{qq}nD(u_\eta),$$

$$ne_\eta = \frac{3}{2}nT + \frac{1}{2}n|u_\eta|^2 - \frac{\hbar^2}{24}n\Delta_x \log n - D_{qq}n\,\mathrm{div}_x u_\eta. \tag{17}$$

The initial conditions are, up to terms of order $O(\hbar^4)$, given by

$$(n, nu_\eta, ne_\eta)(\cdot, 0) = (n_0, nu_0 - D_{qq}\nabla_x n_0, ne_0 - D_{qq}\,\mathrm{div}_x(nu_0)) \quad in\ \mathbb{R}^3,$$

where (n_0, nu_0, ne_0) is defined in (10).

The operator $\frac{1}{2}|\eta|^2$ is defined by

$$\tfrac{1}{2}|\eta|^2 = \tfrac{1}{2}|p|^2 - D_{qq}p\cdot\nabla_x + \tfrac{1}{2}D_{qq}^2\Delta_x = \tfrac{1}{2}|p|^2 - D_{qq}\eta\cdot\nabla_x - \tfrac{1}{2}D_{qq}^2\Delta_x.$$

Notice that we have employed the same notation for ne_η, defined by (4) and (17). Since both expressions only differ up to terms of order $O(\hbar^4)$ and the above system is derived up to terms of the same order, no confusion can occur.

The model of Theorem 1 can be interpreted as follows. Equations (14)–(16) are the balance equations of the particle, momentum, and energy densities. The stress tensor P_η consists of the pressure nT, which expresses the Boyle law for ideal gases, the increase $2(D_{pq} + \lambda D_{qq})$ to the temperature due to quantum diffusion, and the quantum tensor $-(\hbar^2/12)n\nabla_x^2\log n$. Beside the term $2(D_{pq} + \lambda D_{qq})n$, the quantum stress tensor P_η corresponds to the expression derived in other quantum fluid models [15].

The general expression of the viscous stress tensor S can be formulated as

$$S = 2\mu D(u) + \left(\zeta - \frac{2}{3}\mu\right)\mathrm{div}_x u\mathbb{I},$$

where μ is the shear viscosity and ζ the bulk viscosity. In the model of [18], the bulk viscosity vanishes, $\zeta = 0$; in our model, we have $\zeta = \frac{2}{3}\mu$. The quantum heat flux in [18] contains the stabilizing Fourier term $-\frac{5}{2}\alpha nT\nabla_x T$ (see (9)), which comes from the Chapman–Enskog expansion and is missing in the above model.

The energy density ne_η is the sum of the thermal energy $\frac{3}{2}nT$, the kinetic energy $\frac{1}{2}n|u_\eta|^2$, and two quantum contributions. When integrated over space, the energy density becomes (after an integration by parts)

$$\int_{\mathbb{R}^3} ne_\eta\,dx = \int_{\mathbb{R}^3}\left(\frac{3}{2}nT + \frac{1}{2}n|u_\eta|^2\right)dx + \frac{\hbar^2}{6}\int_{\mathbb{R}^3}|\nabla_x\ \overline{n}|^2 dx$$
$$- D_{qq}\int_{\mathbb{R}^3} n\,\mathrm{div}_x u_\eta\,dx.$$

The third term can be interpreted as the Fisher information, whereas the last term describes the work due to compression and vanishes for incompressible fluids. According to (16), the energy dissipation becomes

$$\frac{d}{dt}\int_{\mathbb{R}^3} ne_\eta\,dx = 3D_{pp}\int_{\mathbb{R}^3} n\,dx - 4\lambda\int_{\mathbb{R}^3} ne_\eta\,dx - D_{qq}\int_{\mathbb{R}^3} n\Delta_x V\,dx$$
$$+ \int_{\mathbb{R}^3} nu_\eta\cdot\nabla_x V\,dx.$$

The first term expresses the increase of total mass due to the decoherence coefficient D_{pp}. The second term describes energy relaxation with rate 4λ. The last two terms can be understood when assuming that the electric potential is self-consistently coupled to the Poisson equation

$$\lambda_D^2 \Delta_x V = n - C(x),$$

where λ_D is the scaled Debye length and $C(x)$ models fixed charged background ions. By integrating by parts and using (14), we find that

$$\int_{\mathbb{R}^3} n u_\eta \cdot \nabla_x V dx = \int_{\mathbb{R}^3} \partial_t n V dx = \lambda_D^2 \int_{\mathbb{R}^3} \Delta_x \partial_t V V dx = -\frac{\lambda_D^2}{2} \frac{d}{dt} \int_{\mathbb{R}^3} |\nabla_x V|^2 dx.$$

Hence, the last two terms of the energy dissipation are written as

$$-\frac{D_{qq}}{\lambda_D^2} \int_{\mathbb{R}^3} n(n - C(x)) dx - \frac{\lambda_D^2}{2} \frac{d}{dt} \int_{\mathbb{R}^3} |\nabla_x V|^2 dx.$$

Whereas the second term expresses energy fluctuation due to electric forces, the first one, which is bounded from below, is an effect of the quantum dissipation.

2.4 Osmotic momentum

We wish to elucidate the origin of the kinetic momentum operator (3) and to relate it to similar expressions in the literature. First, we discuss the relation between (3) and the deformed momentum operator of [24]. For simplification, we consider a single quantum state given by the wave function ψ. Let $\mathrm{P} = -i\hbar\nabla_x$ be the quantum momentum operator. The idea of [24] is to introduce the deformed momentum operator $\mathrm{P}_u \psi = (\mathrm{P} - iu)\psi$ for some real function u and the corresponding kinetic energy

$$T_u = \frac{1}{2} \int_{\mathbb{R}^3} (\mathrm{P}_u \psi)^* (\mathrm{P}_u \psi) dx,$$

where ψ^* denotes the complex conjugate of ψ.

The formal minimizer of $u \quad T_u$ equals the osmotic velocity $u_c = -(\hbar/2) \nabla_x \log n$, where $n = |\psi|^2$ is the particle density. This leads to the deformed momentum operator

$$\mathrm{P}_c = \mathrm{P} + \frac{i\hbar}{2} \nabla_x \log n.$$

We remark that the notion "osmotic velocity" appears first in the work of Nelson, see [25, Formula (26)]. We wish to formulate the above operator in terms of the moments of the Wigner function. To this end, we define the Wigner function of a single state by

$$w(x, p, t) = (2\pi\hbar)^3 \int_{\mathbb{R}^3} \psi\left(x + \frac{y}{2}\right)^* \psi\left(x - \frac{y}{2}\right) e^{-iy \cdot p/\hbar} dy.$$

A computation shows that the (macroscopic) particle and momentum densities become [15, Lemma 11.2]

$$n = |\psi|^2 = \int_{\mathbb{R}^3} w\,dp, \tag{18}$$

$$nu = \mathrm{Re}(\psi^* P\,\psi) = -\frac{i\hbar}{2}\left(\psi^* \nabla_x \psi - \nabla_x \psi^* \psi\right) = \int_{\mathbb{R}^3} pw\,dp. \tag{19}$$

The deformed momentum operator equals

$$\psi^* P_c\,\psi = \psi^*\left(P + \frac{i\hbar}{2}\nabla_x \log n\right)\psi = \psi^* P\,\psi + \frac{i\hbar}{2}\nabla_x n,$$

and the (macroscopic) deformed momentum density equals the original momentum density,

$$\mathrm{Re}(\psi^* P_c\,\psi) = \mathrm{Re}(\psi^* P\,\psi) = \int_{\mathbb{R}^3} pw\,dp.$$

In other words, the deformed momentum does not "see" the osmotic velocity part since it is complex.

We claim that the osmotic velocity emerges from gauge field theory [11, Chapter 1]. Given the quantum state ψ, we introduce the local gauge transformation

$$\phi = e^{-i\theta}\psi,$$

where $\theta = D_{qq}\log n/\hbar$ is the gauge function. The corresponding covariant derivative

$$D_x \psi = \nabla_x \psi - i\nabla_x \theta\,\psi = \nabla_x \psi - i\frac{D_{qq}}{\hbar}(\nabla_x \log n)\psi$$

has the property $\nabla_x(e^{-i\theta}\psi) = e^{-i\theta}D_x\psi$. The transformed state ϕ and ψ have the same particle density but the momentum density changes according to

$$nv := \mathrm{Re}(\phi^* P\,\phi) = \mathrm{Re}(\psi^* P\,\psi) - \hbar|\psi|^2\nabla_x \theta = nu - D_{qq}n\nabla_x \log n,$$

which is the sum of the momentum density (19) and the osmotic momentum. In terms of the Wigner function we find that, by (18) and (19),

$$nv = \int_{\mathbb{R}^3} pw\,dp - D_{qq}\nabla_x \int_{\mathbb{R}^3} w\,dp = \int_{\mathbb{R}^3}(p - D_{qq}\nabla_x)w\,dp = \int_{\mathbb{R}^3}\eta w\,dp,$$

which motivates the definition (3) of the operator η.

The gauge transformation explains the new energy estimate derived in [16]. Indeed, the Lagrangian density of ψ equals

$$L_\psi = \frac{\hbar^2}{2}|\nabla_x \psi|^2 - V|\psi|^2.$$

When ψ can be decomposed in terms of the amplitude and phase according to $\psi = \sqrt{n}\exp(iS/\hbar)$ for some velocity potential S, the local Lagrangian density

$$L_\psi = \frac{\hbar^2}{2}|\nabla_x \sqrt{n}|^2 + \frac{1}{2}n|\nabla_x S|^2 - nV$$

is the sum of the quantum, kinetic, and electric energy. The transformed local Lagrangian density becomes, after a straightforward calculation,

$$L_\phi = \frac{\hbar^2}{2}|\nabla_x \phi|^2 - V|\phi|^2 = \frac{\hbar^2}{2}|D_x \psi|^2 - V|\psi|^2$$
$$= L_\psi + \frac{D_{qq}^2}{2}n|\nabla_x \log n|^2 - D_{qq}nu \cdot \nabla_x \log n.$$

When $\psi = \bar{n}\exp(iS/\hbar)$, we have $u = \nabla_x S$, and the transformed Lagrangian density can be rewritten as

$$L_\phi = \frac{\hbar^2}{2}|\nabla_x \bar{n}|^2 + \frac{1}{2}n|u - D_{qq}\nabla_x \log n|^2 - nV = \frac{\hbar^2}{2}|\nabla_x \bar{n}|^2 + \frac{1}{2}n|v|^2 - nV$$

being the sum of the quantum, kinetic, and electric energy but involving the new velocity $v = u - D_{qq}\nabla_x \log n$ (see formula (1.9) in [16]).

3 The η-moment equations

In this section, we derive the moment equations in the variable η, defined in (3). First, we recall the expressions for the moments of the potential operator (see Lemmas 12.9 and 13.2 in [15]). We use the following notation

$$\langle g \rangle = \int_{\mathbb{R}^3} g(p)dp \quad \text{for functions } g(p).$$

Lemma 1 *The moments of the potential operator $\theta_\hbar[V]$ are as follows:*

$$\langle \theta_\hbar[V] \rangle = 0, \quad \langle p\theta_\hbar[V]w \rangle = -n\nabla_x V, \quad \langle \tfrac{1}{2}|p|^2\theta_\hbar[V]w \rangle = -nu \cdot \nabla_x V. \quad (20)$$

As a consequence, the moments in the η-variable become

$$\langle \eta\,\theta_\hbar[V]w \rangle = -n\nabla_x V, \quad \langle \tfrac{1}{2}|\eta|^2\theta_\hbar[V]w \rangle = -nu_\eta \cdot \nabla_x V + D_{qq}n\Delta_x V. \quad (21)$$

The Wigner equation (1) in the osmotic momentum writes as

$$\partial_t w + \eta \cdot \nabla_x w + \theta_\hbar[V]w = L_{\text{BGK}}[w] + L_\eta[w], \quad (22)$$

where the modified Fokker–Planck operator is given by

$$L_\eta[w] = D_{pp}\Delta_p w + 2\lambda \operatorname{div}_p(pw) + 2D_{pq}\operatorname{div}_x(\nabla_p w).$$

Then, introducing the moments in terms of η (the particle density n does not change in the η-formulation),

$$nu_\eta = \langle \eta w \rangle = nu - D_{qq}\nabla_x n, \quad (23)$$
$$ne_\eta = \langle \tfrac{1}{2}|\eta|^2 w \rangle = ne - D_{qq}\operatorname{div}_x(nu) + \tfrac{1}{2}D_{qq}^2\Delta_x n \quad (24)$$
$$= ne - D_{qq}\operatorname{div}_x(nu_\eta) - \tfrac{1}{2}D_{qq}^2\Delta_x n,$$

the η-moment equations read as follows.

Lemma 2 *Let w be a solution to the Wigner–Fokker–Planck equation* (1). *The η-moments (n, nu_η, ne_η), defined in* (23)–(24)*, solve the following hydrodynamic equations:*

$$\partial_t n + \operatorname{div}_x(nu_\eta) = 0, \tag{25}$$

$$\partial_t(nu_\eta) + \operatorname{div}_x \ \eta \otimes \eta w \ - n\nabla_x V + 2(D_{pq} + \lambda D_{qq})\nabla_x n = -2\lambda nu_\eta, \tag{26}$$

$$\partial_t(ne_\eta) + \operatorname{div}_x \ \tfrac{1}{2}\eta|\eta|^2 w \ + 2(D_{pq} + \lambda D_{qq})\operatorname{div}_x(nu_\eta) + D_{qq}n\Delta_x V \tag{27}$$
$$- nu_\eta \cdot \nabla_x V = 3D_{pp}n - 4\lambda ne_\eta.$$

Proof Integrating the Wigner equation (22) over the momentum space and observing that $L_{\mathrm{BGK}}[w] = L_\eta[w] = 0$ immediately gives (25). Next, we apply η to (22) and integrate over p:

$$\partial_t(nu_\eta) + \operatorname{div}_x \ \eta \otimes \eta w \ + \ \eta\theta_\hbar[V]w \ = \ \eta L_\eta[w] \ .$$

The right-hand side becomes

$$\eta L_\eta[w] \ = \ pL_\eta[w] \ - D_{qq}\nabla_x \ L_\eta[w] \ = -2\lambda nu - 2D_{pq}\nabla_x n$$
$$= -2\lambda nu_\eta - 2(D_{pq} + \lambda D_{qq})\nabla_x n.$$

Together with the first identity in (21), we obtain (26). Finally, applying $\frac{1}{2}|\eta|^2$ to (22) and integrating over p leads to

$$\partial_t(ne_\eta) + \operatorname{div}_x \ \tfrac{1}{2}\eta|\eta|^2 w \ + \ \tfrac{1}{2}|\eta|^2\theta_\hbar[V]w \ = \ \tfrac{1}{2}|\eta|^2 L_\eta[w] \ . \tag{28}$$

We calculate the moment of $L_\eta[w]$:

$$\tfrac{1}{2}|\eta|^2 L_\eta[w] \ = \ \tfrac{1}{2}|p|^2 L_\eta[w] \ - D_{qq}\operatorname{div}_x \ pL_\eta[w] \ + \tfrac{1}{2}D_{qq}^2 \Delta_x \ L_\eta[w] \ .$$

The first summand equals

$$\tfrac{1}{2}|p|^2 L_\eta[w] \ = 3D_{pp}n - 4\lambda ne - 2D_{pq}\operatorname{div}_x(nu)$$
$$= 3D_{pp}n - 4\lambda ne_\eta - 2(D_{pq} + 2\lambda D_{qq})\operatorname{div}_x(nu_\eta)$$
$$- 2D_{qq}(D_{pq} + \lambda D_{qq})\Delta_x n;$$

the second summand becomes

$$-D_{qq}\operatorname{div}_x \ pL_\eta[w] \ = 2\lambda D_{qq}\operatorname{div}_x(nu) + 2D_{pq}D_{qq}\Delta_x n$$
$$= 2\lambda D_{qq}\operatorname{div}_x(nu_\eta) + 2D_{qq}(D_{pq} + \lambda D_{qq})\Delta_x n;$$

and the third summand vanishes. Adding these expressions leads to

$$\tfrac{1}{2}|\eta|^2 L_\eta[w] \ = 3D_{pp}n - 4\lambda ne_\eta - 2(D_{pq} + \lambda D_{qq})\operatorname{div}_x(nu_\eta).$$

Inserting this expression and the second identity in (21) into (28) proves the result.

4 Closure of the η-moment equations

Let w_α be a solution to the Wigner–Fokker–Planck equation (1) and let $(n, (nu_\eta)_\alpha, (ne_\eta)_\alpha)$ be the corresponding η-moments. The parameter α is the scaled relaxation time occuring in the BGK operator. In the limit $\alpha \to 0$, we obtain $L_{\mathrm{BGK}}[w] = 0$, where $w = \lim_{\alpha \to 0} w_\alpha$. This implies that $w = M[w]$ and the η-moments can be closed according to the formal limit $\alpha \to 0$:

$$
\begin{pmatrix} n_\alpha \\ (nu_\eta)_\alpha \\ (ne_\eta)_\alpha \end{pmatrix} = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \eta \\ \frac{1}{2}|\eta|^2 \end{pmatrix} w_\alpha dx \qquad \begin{pmatrix} n \\ nu_\eta \\ ne_\eta \end{pmatrix} = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \eta \\ \frac{1}{2}|\eta|^2 \end{pmatrix} M[w] dx.
$$

We notice that there exist other strategies to close the moment equations, for instance the shifted Maxwellian closure of Gardner [12] or the closure relations accounting for quantum mixtures in the wave-function picture [20–22].

We calculate now the moments $\langle \eta \otimes \eta M[w] \rangle$ and $\langle \frac{1}{2}\eta|\eta|^2 M[w] \rangle$.

Lemma 3 *Assuming that $\nabla_x \log T = O(\hbar^2)$ and $A(u_\eta) = \frac{1}{2}(\nabla u_\eta - \nabla u_\eta^\top) = O(\hbar^2)$, the following expansions hold:*

$$
\langle \eta \otimes \eta M[w] \rangle = nu_\eta \otimes u_\eta + P - 2D_{qq} nD(u_\eta) + O(\hbar^4), \tag{29}
$$

$$
\langle \tfrac{1}{2}\eta|\eta|^2 M[w] \rangle = q_\eta + (P + ne_\eta \mathbb{I})u_\eta - 2D_{qq}\mathrm{div}_x(nD(u_\eta)u_\eta) + O(\hbar^4), \tag{30}
$$

where $\nabla_x^2 \log n$ denotes the Hessian of $\log n$, $P = nT\mathbb{I} - (\hbar^2/12)n\nabla_x^2 \log n$ is the quantum stress tensor and $q_\eta = -(\hbar^2/24)n(\Delta_x u_\eta + 2\nabla_x \mathrm{div}_x u_\eta)$ is the quantum heat flux.

Proof First, we observe that

$$
\langle p \otimes p M[w] \rangle = P + nu \otimes u, \qquad \langle \tfrac{1}{2}p|p|^2 M[w] \rangle = q + (P + ne\mathbb{I})u,
$$

where $P = \langle (p-u) \otimes (p-u)M[w] \rangle$ is the quantum stress tensor and $q = \langle \frac{1}{2}(p - u)|p - u|^2 M[w] \rangle$ is the quantum heat flux in the p variable. Under the assumptions $\nabla \log T = O(\hbar^2)$ and $A(u) = A(u_\eta) = O(\hbar^2)$, P, q, and ne can be expanded in powers of $\hbar^2$ [18, Formulas (19)-(20)]:

$$
P = nT\mathbb{I} - \frac{\hbar^2}{12}n\nabla_x^2 \log n + O(\hbar^4), \tag{31}
$$

$$
q = -\frac{\hbar^2}{24}n(\Delta_x u + 2\nabla_x \mathrm{div}_x u) + O(\hbar^4), \tag{32}
$$

$$
ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\hbar^2}{24}n\Delta_x \log n + O(\hbar^4). \tag{33}
$$

Since $\langle M[w] \rangle = n$ and $\langle pM[w] \rangle = nu$, we find that

$$
\begin{aligned}
\langle \eta \otimes \eta M[w] \rangle &= \langle p \otimes p M[w] \rangle - 2D_{qq}\langle \nabla_x \otimes_s pM[w] \rangle + D_{qq}^2 \langle \nabla_x^2 M[w] \rangle \\
&= P + nu \otimes u - 2D_{qq}\nabla_x \otimes_s (nu) + D_{qq}^2 \nabla_x^2 n,
\end{aligned}
$$

where $a \otimes_s b = \frac{1}{2}(a \otimes b + b \otimes a)$ is the symmetric tensor product. Inserting the definition (23) of nu_η, a computation shows that

$$\eta \otimes \eta M[w] \ = P + nu_\eta \otimes u_\eta - 2D_{qq}nD(u_\eta) + D_{qq}^2 n\nabla_x \log n \otimes \nabla_x \log n,$$

where $D(u_\eta) = \frac{1}{2}(\nabla u_\eta + \nabla u_\eta^\top)$. The expansion (31) and the property $D_{qq}^2 = O(\hbar^4)$ (see (5)) then implies the first claim (29).

Next, we obtain

$$
\begin{aligned}
\tfrac{1}{2}\eta|\eta|^2 M[w] \ &= \ \tfrac{1}{2}p|p|^2 M[w] \ -D_{qq} \ p(p \cdot \nabla_x)M[w] \ + \tfrac{1}{2}D_{qq}^2\Delta_x \ pM[w] \\
&\quad -D_{qq}\nabla_x \ \tfrac{1}{2}|p|^2 M[w] \ +D_{qq}^2 \ \nabla_x(p \cdot \nabla_x)M[w] \\
&\quad -\tfrac{1}{2}D_{qq}^3\Delta_x\nabla_x \ M[w] \\
&= q + (P + ne\mathbb{I})u - D_{qq}\big(\mathrm{div}_x(P + nu \otimes u) + \nabla_x(ne)\big) \\
&\quad + \tfrac{1}{2}D_{qq}^2\big(\Delta_x(nu) + 2\nabla_x^2(nu)\big) - \tfrac{1}{2}D_{qq}^3\Delta_x\nabla_x n.
\end{aligned}
$$

Because of (31), $D_{qq}^2 = O(\hbar^4)$, $nu \otimes u = nu_\eta \otimes u_\eta + O(\hbar^2)$, and $ne = ne_\eta + O(\hbar^2)$ (see (24)), this expression simplifies to

$$
\begin{aligned}
\tfrac{1}{2}\eta|\eta|^2 M[w] \ &= q + (P + ne\mathbb{I})u - D_{qq}\big(\nabla_x(nT) + \mathrm{div}_x(nu_\eta \otimes u_\eta) \qquad (34) \\
&\quad + \nabla_x(ne_\eta)\big) + O(\hbar^4).
\end{aligned}
$$

We write q and $(P + ne\mathbb{I})u$ in terms of the η-moments:

$$q = -\frac{\hbar^2}{24}n\big(\Delta_x u_\eta + 2\nabla_x \mathrm{div}_x u_\eta\big) + O(\hbar^4),$$

$$(P + ne\mathbb{I})u = (P + ne_\eta\mathbb{I})u_\eta + D_{qq}(P + ne_\eta\mathbb{I})\nabla_x \log n + D_{qq}\mathrm{div}_x(nu_\eta)u_\eta + O(\hbar^4).$$

Inserting these expansions into (34) gives, since $\nabla_x T = O(\hbar^2)$,

$$
\begin{aligned}
\tfrac{1}{2}\eta|\eta|^2 M[w] \ &= -\frac{\hbar^2}{24}n\big(\Delta_x u_\eta + 2\nabla_x \mathrm{div}_x u_\eta\big) + (P + ne_\eta\mathbb{I})u_\eta \\
&\quad + D_{qq}\big((nT + ne_\eta)\nabla_x \log n + \mathrm{div}_x(nu_\eta)u_\eta - \nabla_x(nT) \\
&\quad - \mathrm{div}_x(nu_\eta \otimes u_\eta) - \nabla_x(ne_\eta)\big) + O(\hbar^4) \\
&= -\frac{\hbar^2}{24}n\big(\Delta_x u_\eta + 2\nabla_x \mathrm{div}_x u_\eta\big) + (P + ne_\eta\mathbb{I})u_\eta \\
&\quad - D_{qq}\big(nu_\eta \cdot \nabla_x u_\eta + n\nabla_x e\big) + O(\hbar^4).
\end{aligned}
$$

Finally, observing that

$$
\begin{aligned}
D_{qq}\big(nu_\eta \cdot \nabla_x u_\eta + n\nabla_x e\big) &= D_{qq}\Big(nu_\eta \cdot \nabla_x u_\eta + \frac{1}{2}n\nabla_x(|u_\eta|^2)\Big) + O(\hbar^4) \\
&= 2D_{qq}\mathrm{div}_x\big(nD(u_\eta)u_\eta\big) + O(\hbar^4),
\end{aligned}
$$

the claim (30) follows.

Theorem 1 now follows immediately from the η-moment equations (25)–(27) and Lemma 2. The expression for the energy density is a consequence of (24) and (33):

$$ne_\eta = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\hbar^2}{24}n\Delta_x \log n - D_{qq}\operatorname{div}_x(nu_\eta) + O(\hbar^4)$$

$$= \frac{3}{2}nT + \frac{1}{2}n|u_\eta|^2 - \frac{\hbar^2}{24}n\Delta_x \log n - D_{qq}n\operatorname{div}_x u_\eta + O(\hbar^4).$$

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