A derivation of the isothermal quantum hydrodynamic equations using entropy minimization

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Isothermal quantum hydrodynamic equations of order $\mathcal{O}(\hbar^2)$ using the quantum entropy minimization method recently developed by Degond and Ringhofer are derived. The equations have the form of the usual quantum hydrodynamic model including a correction term of order $\mathcal{O}(\hbar^2)$ which involves the vorticity. If the initial vorticity is of order $\mathcal{O}(\hbar)$, the standard model is obtained up to order $\mathcal{O}(\hbar^4)$. The derivation is based on a careful expansion of the quantum equilibrium obtained from the entropy minimization in powers of $\hbar^2$.

Dedicated to Prof. Herbert Gajewski in occasion of his 65th birthday

1 Introduction

It is well known since the early years of quantum mechanics that there exists a fluiddynamical formulation of the Schrödinger equation [19]. The derivation of such quantum hydrodynamic models from first principles has attracted recently a lot of interest in the mathematical and physical literature [4, 6, 8, 9]. This interest relies on the need of accurate and efficient simulations of quantum semiconductor devices like lasers and tunneling diodes. Indeed, the numerical solution of the (many-particle) Schrödinger or quantum Liouville equation is extremely time consuming, whereas fluid-type quantum models are computationally less expensive.

A simple derivation uses WKB wave functions $\psi = \sqrt{n}e^{iS/\varepsilon}$ for the particle density $n(x,t)$ and phase $S(x,t)$, where ε is the scaled Planck constant. Separating the real and imaginary part of the single-state Schrödinger equation gives Euler-type equations including the so-called Bohm potential $\Delta\sqrt{n}/\sqrt{n}$ as a quantum correction of order ε^2 (see, e.g., [12, 14, 15] for details). In the semi-classical limit $\varepsilon \to 0$, the classical pressureless Euler equations are obtained. This appraoch does not take into account many-particle effects and the model can be considered as a zero-temperature model. In order to incorporate temperature effects, we are aware of two approaches.

The first approach starts from a mixed-state Schrödinger-Poisson system consisting of a sequence of single-state Schrödinger equations to each of which an occupation probability is associated [12]. Defining the total particle and current densities as the superposition of all single-state densities, weighted by the occupation probabilities, fluid equations for the particle density, the current density and the energy tensor are derived, expressing the conservation of mass, momentum, and energy. However, the system of equations is not closed. The energy equation contains a heat flux vector which cannot be expressed in terms of the particle density, current density and energy only. Therefore, a closure condition is necessary. In the literature, several choices have been proposed, using a special ansatz for the heat flux [11] or assuming a constant temperature (isothermal case; [14]).

The second approach is based on the kinetic picture of quantum mechanics, described by the collisional (scaled) Wigner equation

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

where (x,p) are the position-momentum variables, $\Theta[V]$ is a pseudo-differential operator [20] defined by

$$(\Theta[V]w)(x,p,t) = \frac{i}{(2\pi)^{d/2}}\int_{\mathbb{R}^{2d}} \frac{1}{\varepsilon}\left[V\Big(x+\frac{\varepsilon}{2}\eta,t\Big) - V\Big(x-\frac{\varepsilon}{2}\eta,t\Big)\right] w(x,p',t)e^{i\eta\cdot(p-p')}d\eta dp',$$

and $Q(w)$ is a collision operator which will be specified in section 2. The electrostatic potential $V = V(x,t)$ is usually selfconsistently coupled to the particle density $\int w(x,p,t)dp$ via Poisson's equation but in this paper, we suppose that the

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potential is a given function since the coupling through Poisson's equation does not effect our analysis. We notice that the Schrödinger equation is formally equivalent to the Wigner equation without collisions.

Applying a moment method to (1), i.e. multiplying this equation by 1, p, and $|p|^2/2$ and integrating over the momentum space, we obtain formally the so-called moment equations for the first moments of the Wigner function w, namely the particle density $n = \langle w \rangle$, the fluiddynamical momentum $nu = \langle wp \rangle$, and the energy density $e = \langle w|p|^2/2 \rangle$, where we have used the notation $\langle f(p) \rangle = \int f(p)dp$ for functions $f(p)$. However, the moment equations contain the integral $\langle wp|p|^2/2 \rangle$ which generally cannot be expressed in terms of n, nu, and e only. Gardner used a "momentum-shifted" approximation of the quantum thermal equilibrium distribution derived by Wigner, w^*, as a closure function in the above system, i.e., he replaced w by w^* and calculated the corresponding moments [8] (also compare with [5]). Assuming that the spatial variations of the temperature are sufficiently small and taking into account only terms of order ε^2, the resulting equations lead to the quantum hydrodynamic model

$$\partial_t n + \mathrm{div}(nu) = 0, \tag{2}$$

$$\partial_t(nu) + \mathrm{div}(nu \otimes u) + \nabla(nT) - n\nabla V - \frac{\varepsilon^2}{6} n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right) = 0, \tag{3}$$

$$\partial_t e + \mathrm{div} \left(nu(e+T) - \frac{\varepsilon^2}{12} n((\nabla \otimes \nabla)\ln n)u \right) - nu \cdot \nabla V = 0, \qquad x \in \mathbb{R}^d,\ t > 0, \tag{4}$$

where $e = \frac{d}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\Delta \ln n$, with initial conditions for n, nu, and e. A related set of state equations which are nonlocal in the potential have been derived in [9, 10] by small-field asymptotics for quantum thermodynamical equilibria.

Another closure ansatz has been recently employed by Degond and Ringhofer [4] by extending Levermore's moment hierarchy [17] for classical gas dynamics to quantum systems. More precisely, the equilibrium function, which is chosen as a closure, is the minimum (or maximum according to the physical convention) of a quantum entropy functional $H(w)$ subject to the constraints that the moments of the equilibrium function are prescribed:

$$H(w^*) = \min \left\{ H(v) : \int_{\mathbb{R}^d} v(x,p) \begin{pmatrix} 1 \\ p \\ \frac{1}{2}|p|^2 \end{pmatrix} dp = \begin{pmatrix} n(x) \\ nu(x) \\ e(x) \end{pmatrix} \quad \text{for all } x \in \mathbb{R}^d \right\}.$$

A definition of the quantum entropy will be given in section 2. This approach yields quantum hydrodynamic equations including a pressure tensor and heat flux vector. Unfortunately, they cannot easily be expressed in terms of the particle density, momentum, and energy since the pressure and heat flux are nonlocal (i.e., their values at a given point x depend on the values of n, nu, and e at any other point).

Degond et al. [3] have derived more explicit expressions by expanding the quantum equilibrium w^* in powers of the scaled Planck constant ε. In this way, they have derived the quantum drift-diffusion and a quantum energy-transport model in the diffusion limit (i.e. replacing $x \to x/\delta$ and $t \to t/\delta^2$ for some $\delta > 0$ and then letting $\delta \to 0$). Here, the quantum equilibrium is the minimum of the entropy to the constraint of a given particle density, in the case of the quantum drift-diffusion model, and to the constraints of a given particle density and energy, in the case of the quantum energy-transport equations.

This paper is motivated by the formal resemblance between Wigner's equilibrium function employed by Gardner [8] and the quantum equilibrium of Degond et al. [3] (see Remark 3.3 for a detailed discussion). This observation allows us to derive an *isothermal* quantum hydrodynamic model by using quantum entropy minimization. The derivation of the full model is devoted to future work. We notice that this is the first derivation of an *explicit* quantum hydrodynamic model by this method.

More precisely, we derive the equations

$$\partial_t n + \mathrm{div}(nu) = 0, \qquad x \in \mathbb{R}^d,\ t > 0, \tag{5}$$

$$\partial_t(nu) + \mathrm{div}(nu \otimes u) + \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right) = \frac{\varepsilon^2}{12}\mathrm{div}(nU) + \mathcal{O}(\varepsilon^4), \tag{6}$$

where U is a tensor with components

$$U_{k\ell} = -\sum_{i=1}^{d} (\partial_i u_k - \partial_k u_i)(\partial_i u_\ell - \partial_\ell u_i)$$

and ∂_i denotes the partial derivative $\partial/\partial x_i$. The scaled temperature is $T = 1$. The tensor U vanishes if the velocity u is irrotational in the sense $\partial_i u_k - \partial_k u_i = 0$ for all i, $k = 1, \ldots, d$. In particular, it vanishes in one space dimension. In fact, it is enough to require that $U = \mathcal{O}(\varepsilon^2)$. We also prove that the usual quantum hydrodynamic equations (2)-(3) (with $T = 1$) are obtained up to order $\mathcal{O}(\varepsilon^4)$ if the vorticity is initially of order $\mathcal{O}(\varepsilon)$. In Remark 3.3 we explain the presence of the vorticity term in (6) by comparing the approach of Degond et al. with the approach of Gardner.

The isothermal quantum hydrodynamic model (2)-(3) with $T = 1$ has been analytically and numerically studied in, e.g., [7, 13, 16, 18]. The full model including the energy equation (4) has been numerically solved in, e.g., [1, 8].

This paper is organized as follows. In section 2 we make precise the definition of the quantum entropy and the quantum equilibrium and we state our main results. In section 3 we recall some technical lemmas from [3], and sections 4 and 5 are devoted to the proof of the main results.

2 Definitions and main results

We start with the collisional Wigner equation (1). We assume a hydrodynamic scaling, i.e., we introduce the following space and time scaling,

$$x' = \delta x, \quad t' = \delta t,$$

for some $\delta > 0$ which is assumed to be small compared to one. Then (1) becomes (omitting the primes)

$$\delta\partial_t w_\delta + \delta(p \cdot \nabla_x w_\delta - \Theta[V]w_\delta) = Q(w), \qquad t > 0, \tag{7}$$

$$w_\delta(x, p, 0) = w_I(x, p), \qquad (x, p) \in \mathbb{R}^{2d}. \tag{8}$$

The collision operator is given by the simple relaxation-time or “BGK” approach (with scaled relaxation time $\tau = 1$)

$$Q(w) = M[w] - w,$$

where $M[w]$ is a quantum analogue of the Maxwellian used in classical gas dynamics (also see Remark 5.1).

In order to define the quantum Maxwellian $M[w]$, we first introduce the Wigner transform. Let ρ be an operator on $L^2(\mathbb{R}^d)$ and $\widetilde{\rho}(x, x')$ its integral kernel, i.e.

$$(\rho\phi)(x) = \int_{\mathbb{R}^d} \widetilde{\rho}(x, x')\phi(x')dx' \qquad \text{for all } \phi \in L^2(\mathbb{R}^d).$$

Then the Wigner transform is defined by

$$W(\rho)(x, p) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \widetilde{\rho}\Big(x + \frac{\varepsilon}{2}\eta, x - \frac{\varepsilon}{2}\eta\Big) e^{i\eta \cdot p} d\eta.$$

Its inverse W^{-1}, also called Weyl quantization, is defined for any function $f(x, p)$ as an operator on $L^2(\mathbb{R}^d)$:

$$(W^{-1}(f)\phi)(x, p) = \int_{\mathbb{R}^d} f\Big(\frac{x + y}{2}\Big)\phi(y)e^{ip\cdot(x-y)/\varepsilon} dp dy \qquad \text{for all } \phi \in L^2(\mathbb{R}^d).$$

With these definitions we are able to introduce the *quantum exponential* and the *quantum logarithm* formally by

$$\text{Exp}\, w = W(\exp W^{-1}(w)), \quad \text{Ln}\, w = W(\ln W^{-1}(w)),$$

where exp and ln are the operator exponential and logarithm, respectively [3].

Now, the *relative quantum entropy* is given by

$$H(w) = \int_{\mathbb{R}^{2d}} w\Big(\text{Ln}\, w - 1 + \frac{|p|^2}{2} - V(x)\Big) dx dp.$$

Notice that this entropy is a scalar quantity with non-local spatial dependence on w, in contrast to the classical entropy which is defined pointwise in space. Finally, we define the quantum Maxwellian or quantum equilibrium $w^* = M[w]$ for some given function $w(x, p)$ as the solution of the constrained minimization problem

$$H(w^*) = \min\left\{H(v) : \int_{\mathbb{R}^d} v(x, p, t)\begin{pmatrix}1\\ p\end{pmatrix} dp = \begin{pmatrix}n(x, t)\\ nu(x, t)\end{pmatrix} \quad \text{for all } x \in \mathbb{R}^d,\ t > 0\right\}, \tag{9}$$

where

$$n(x, t) = \int_{\mathbb{R}^d} w(x, p, t)dp, \quad nu(x, t) = \int_{\mathbb{R}^d} w(x, p, t)p dp.$$

The solution w^* of the constrained minimization problem, if it exists, is given by

$$M[w](x, p, t) = w^*(x, p, t) = \text{Exp}\left(A(x, t) + B(x, t) \cdot p - \frac{|p|^2}{2}\right),$$

where $A(x, t)$ and $B(x, t)$ are some Lagrange multipliers. This completes the definition of the collision operator.

The moment equations are obtained from (1) by multiplication by 1, p, respectively, and integration over the momentum space. Noticing that

$$\int_{\mathbb{R}^d} \Theta[V] w dp = 0, \quad \int_{\mathbb{R}^d} \Theta[V] w p dp = -n\nabla V \qquad \text{for all } w(x,p)$$

and, by the definition of $M[w]$,

$$\int_{R^d} Q(w) dp = 0, \qquad \int_{R^d} Q(w) p dp = 0 \qquad \text{for all } w(x,p)$$

we obtain the moment equations

$$\partial_t \langle w \rangle + \text{div}\langle wp \rangle = 0, \qquad \partial_t \langle wp \rangle + \text{div}\langle wp \otimes p \rangle - \langle w \rangle \nabla V = 0, \tag{10}$$

where we recall that $\langle f(p) \rangle = \int f(p) dp$.

Our main result is as follows.

Theorem 2.1 *Let w_δ be a solution of (7)-(8). Then, formally, $w_\delta \to w = M[w]$ as $\delta \to 0$. Moreover, $n = \langle M[w] \rangle$ and $nu = \langle M[w]p \rangle$ are (formally) solutions of (5)-(6) with initial conditions*

$$n(x,0) = \langle w_I \rangle(x), \quad nu(x,0) = \langle w_I p \rangle(x), \qquad x \in \mathbb{R}^d.$$

Recall that the function $w^* = M[w]$ is formally defined by (9), where the moments are given by

$$\int_{\mathbb{R}^d} M[w](x,p,t) \begin{pmatrix} 1 \\ p \end{pmatrix} dp = \int_{\mathbb{R}^d} \lim_{\delta \to 0} w_\delta(x,p,t) \begin{pmatrix} 1 \\ p \end{pmatrix} dp.$$

We are able to show that the quantum hydrodynamic equations are satisfied up to oder $\mathcal{O}(\varepsilon^4)$ if the initial vorticity is of order $\mathcal{O}(\varepsilon)$. For this, let Curl u be the tensor with components $(\text{Curl}\, u)_{ij} = \partial_i u_j - \partial_j u_i$, $i, j = 1, \ldots, d$. Then we can write $U = -(\text{Curl}\, u)^\top (\text{Curl}\, u)$. Furthermore, we set

$$\|\text{Curl}\, u(t)\|^2_{L^2(\mathbb{R}^d)} = \sum_{i,j=1}^d \int_{\mathbb{R}^d} (\text{Curl}\, u)_{ij}(x,t)^2 dx.$$

Corollary 2.2 *Let (n,u) be a smooth solution to (5)-(6). We assume that u is bounded independently of ε in $L^\infty(0,\infty; C^{m+1}(\mathbb{R}^d))$, where $m \in \mathbb{N}$, $m > d/2$, and that the initial vorticity satisfies*

$$\|\text{Curl}\, u(0)\|_{H^m(\mathbb{R}^d)} = \mathcal{O}(\varepsilon).$$

Then, for $t > 0$,

$$\|\text{Curl}\, u(t)\|_{H^m(\mathbb{R}^d)} = \mathcal{O}(\varepsilon) \tag{11}$$

and (n, nu) solves formally

$$\begin{aligned} \partial_t n + \text{div}(nu) &= 0, \\ \partial_t(nu) + \text{div}(nu \otimes u) + \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right) &= \mathcal{O}(\varepsilon^4), \qquad x \in \mathbb{R}^d,\ t > 0. \end{aligned} \tag{12}$$

3 Some auxiliary lemmas

For the expansion of the quantum exponential we need some preparations.

Lemma 3.1 *The following identities hold:*

$$\begin{aligned} \int_{\mathbb{R}^d} e^{-|p|^2/2} dp &= (2\pi)^{d/2}, \\ \int_{\mathbb{R}^d} e^{-|p|^2/2} p_i p_j dp &= (2\pi)^{d/2} \delta_{ij}, \\ \int_{\mathbb{R}^d} e^{-|p|^2/2} p_i p_j p_k p_\ell dp &= (2\pi)^{d/2} (\delta_{ij}\delta_{k\ell} + \delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}). \end{aligned}$$

The following lemma is a consequence of [3, Prop. 5.3].

Lemma 3.2 *Let A, $B : \mathbb{R}^d \to \mathbb{R}$ be smooth functions and x, $p \in \mathbb{R}^d$. Then we can expand the quantum exponential as follows:*

$$\operatorname{Exp}\left(A(x) + B(x)\cdot p - \frac{|p|^2}{2}\right) = e^{A(x)+B(x)\cdot p-|p|^2/2}\Big[1 + \frac{\varepsilon^2}{8}\Big(\Delta A + \Delta B\cdot p + \partial_i B_j \partial_j B_i$$
$$- \frac{1}{3}(\partial_{ij}A + \partial_{ij}B\cdot p)(p_i - B_i)(p_j - B_j) - \frac{2}{3}\partial_i B_j (p_i - B_i)(\partial_j A + \partial_j B\cdot p)$$
$$+ \frac{1}{3}|\nabla(A + B\cdot p)|^2\Big)\Big] + \mathcal{O}(\varepsilon^4). \tag{13}$$

Here and in the following, we use Einstein's summation convention and the notation ∂_i for the partial derivative $\partial/\partial x_i$.

Remark 3.3 This paper is motivated by the resemblance between Wigner's equilibrium distribution [21, (25)]

$$w^*_{\mathrm{W}}(x,p) = e^{-V/T-|p|^2/2T}\left[1 + \frac{\varepsilon^2}{8T^2}\Big(-\Delta V + \frac{1}{3}|\nabla V|^2 + \frac{1}{3T}p_i p_j \partial_{ij}V\Big)\right] + \mathcal{O}(\varepsilon^4)$$

with (constant) temperature T and potential $V = V(x)$, and the quantum Maxwellian

$$w^*_{\mathrm{D}}(x,p) = \operatorname{Exp}\left(A(x,t) - \frac{|p|^2}{2T}\right) = e^{A-|p|^2/2T}\left[1 + \frac{\varepsilon^2}{8T}\Big(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3T}p_i p_j \partial_{ij}A\Big)\right] + \mathcal{O}(\varepsilon^4)$$

employed by Degond et al. [3] as a closure function in the derivation of the quantum drift-diffusion model. Both formulas coincide if we identify the Lagrange parameter A with the "potential" $-V/T$. In fact, both approximations are essentially derived in the same way since Wigner approximates the operator $\exp(H/T)$, which is related to the quantum exponential, H being the Schrödinger operator.

For his derivation of the quantum hydrodynamic model, Gardner employed the "shifted" equilibrium distribution [8, (24)]

$$w^*_{\mathrm{G}}(x,p) = C(x,t)e^{-V/T-|p-u|^2/2T}\left[1 + \frac{\varepsilon^2}{8T^2}\Big(-\Delta V + \frac{1}{3}|\nabla V|^2 + \frac{1}{3T}\partial_{ij}V(p_i-u_i)(p_j-u_j)\Big)\right] + \mathcal{O}(\varepsilon^4)$$

with temperature $T = T(x,t)$ which is assumed to vary slowly in x, i.e., he replaced p by the "shifted" momentum $p-u$. This approach is motivated by the classical Maxwellian derived, for instance by minimizing the classical thermodynamic entropy subject to given moments of density, momentum, and energy [17]. The "density" C, the temperature T, and the velocity u are the Lagrange multipliers arising from the solution of the constrained minimization problem. The equilibrium function w^*_{G} differs from the approximation of the quantum exponential (13), since the Lagrange multipliers A and B arising from (9) (recall that the temperature is constant in (9)) give rise to additional terms in the approximation of the quantum Maxwellian not present in the heuristic approach of Gardner. Only for $B = 0$ and $u = 0$ we obtain the same formulas (if $T = 1$). Therefore, the vorticity term in the momentum equation (6) is a purely quantum mechanical effect. Its presence is justified by the expansion of the quantum exponential taking care of the Lagrange multipliers from (9).

4 Proof of Theorem 2.1

We expand the first moments of the quantum exponential.

Lemma 4.1 *It holds:*

$$\begin{aligned} n &= \int_{\mathbb{R}^d} \operatorname{Exp}\left(A(x) + B(x)\cdot p - \frac{|p|^2}{2}\right)dp \\ &= (2\pi)^{d/2}e^{A+|B|^2/2}\left[1 + \frac{\varepsilon^2}{24}\Big(2\Delta(A + \tfrac{1}{2}|B|^2) + |\nabla(A+\tfrac{1}{2}|B|^2)|^2 + \partial_i B_j(\partial_i B_j - \partial_j B_i)\Big)\right] + \mathcal{O}(\varepsilon^4). \end{aligned}$$

In particular,

$$n = (2\pi)^{d/2}e^{A+|B|^2/2} + \mathcal{O}(\varepsilon^2). \tag{14}$$

In the following, we suppress the dependence on t since it is only a parameter in the formulas.

P r o o f. The lemma follows after integration of the $\mathcal{O}(\varepsilon^2)$ expansion of the quantum exponential given by Lemma 3.2. For the calculation it is convenient to write the quantum exponential in terms of the difference $p - B$,

$$\operatorname{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right) = e^{A+|B|^2/2-|p-B|^2/2}\left(1 + \frac{\varepsilon^2}{8}F(p-B)\right) + \mathcal{O}(\varepsilon^4),$$

where

$$\begin{aligned} F(p-B) &= \Delta A + \frac{1}{3}|\nabla A|^2 + \Delta B\cdot(p-B) + \Delta B\cdot B + \partial_i B_j \partial_j B_i - \frac{1}{3}(\partial_{ij}A + \partial_{ij}B\cdot B)(p_i-B_i)(p_j-B_j) \\ &\quad - \frac{1}{3}\partial_{ij}B\cdot(p-B)(p_i-B_i)(p_j-B_j) - \frac{2}{3}\partial_i B_j(p_i-B_i)(\partial_j + \partial_j B\cdot B) \\ &\quad - \frac{2}{3}\partial_i B_j(p_i-B_i)\partial_j B\cdot(p-B) + \frac{1}{3}\partial_i B\cdot(p-B)\partial_i B\cdot(p-B) + \frac{1}{3}\partial_i B\cdot B\partial_i B\cdot B \\ &\quad + \frac{1}{3}\partial_i B\cdot(p-B)\partial_i B\cdot B + \frac{1}{3}\partial_i B\cdot B\partial_i B\cdot(p-B) + \frac{2}{3}\partial_i A\partial_i B\cdot(p-B) + \frac{2}{3}\partial_i A\partial_i B\cdot B. \end{aligned}$$

Thus, by Lemma 3.1,

$$\begin{aligned} n &= e^{A+|B|^2/2}\int_{\mathbb{R}^d} e^{-|p-B|^2/2}\Big(1+\frac{\varepsilon^2}{8}F(p-B)\Big)dp + \mathcal{O}(\varepsilon^4) \\ &= (2\pi)^{d/2}e^{A+|B|^2/2} + \frac{\varepsilon^2}{8}e^{A+|B|^2/2}\int_{\mathbb{R}^d} e^{-|q|^2/2}F(q)dq + \mathcal{O}(\varepsilon^4), \end{aligned}$$

and the conclusion follows by computing the last integral, taking into account Lemma 3.1. □

Lemma 4.2 *It holds for* $k=1,\ldots,d$*:*

$$nu_k = \int_{\mathbb{R}^d} \operatorname{Exp}\left(A(x)+B(x)\cdot p - \frac{|p|^2}{2}\right)p_k dp = nB_k + \frac{\varepsilon^2}{12}nI_k + \mathcal{O}(\varepsilon^4),$$

where $I_k = (\partial_i + \partial_i A + \partial_i B\cdot B)(\partial_i B_k - \partial_k B_i)$*. In particular,*

$$u = B + \mathcal{O}(\varepsilon^2). \tag{15}$$

P r o o f. We write

$$\begin{aligned} nu &= \int_{\mathbb{R}^d} \operatorname{Exp}\left(A+B\cdot p - \frac{|p|^2}{2}\right)(p-B)dp + \int_{\mathbb{R}^d} \operatorname{Exp}\left(A+B\cdot p-\frac{|p|^2}{2}\right)Bdp \\ &= \int_{\mathbb{R}^d} \operatorname{Exp}\left(A+B\cdot p - \frac{|p|^2}{2}\right)(p-B)dp + nB, \end{aligned}$$

and Lemmas 3.1 and 3.2 yield

$$\begin{aligned} &\int_{\mathbb{R}^d} \operatorname{Exp}\left(A+B\cdot p - \frac{|p|^2}{2}\right)(p_k-B_k)dp \\ &= \frac{\varepsilon^2}{12}(2\pi)^{d/2}e^{A+|B|^2/2}(\partial_i + \partial_i A + \partial_i B\cdot B)(\partial_i B_k - \partial_k B_i) + \mathcal{O}(\varepsilon^4) \\ &= \frac{\varepsilon^2}{12}n(\partial_i + \partial_i A + \partial_i B\cdot B)(\partial_i B_k - \partial_k B_i) + \mathcal{O}(\varepsilon^4). \end{aligned}$$

In the last step we have used the relation (14). □

Lemma 4.3 *It holds for* $k,\ell=1,\ldots,d$*:*

$$\begin{aligned} P_{k\ell} &= \int_{\mathbb{R}^d} \operatorname{Exp}\left(A(x)+B(x)\cdot p - \frac{|p|^2}{2}\right)p_k p_\ell dp \\ &= n\delta_{k\ell} + nu_k u_\ell - \frac{\varepsilon^2}{12}n\partial_{k\ell}(A+\tfrac{1}{2}|B|^2) + \frac{\varepsilon^2}{12}nJ_{k\ell} + \mathcal{O}(\varepsilon^4), \end{aligned}$$

where

$$J_{k\ell} = (\partial_i B_k - \partial_k B_i)(\partial_i B_\ell - \partial_\ell B_i). \tag{16}$$

P r o o f. Again, we write the integrand in terms of $p - B$:

$$\begin{aligned}
P_{k\ell} &= \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right)(p_k - B_k)(p_\ell - B_\ell)dp \\
&\quad + B_k \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right) p_\ell dp + B_\ell \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right) p_k dp \\
&\quad - B_k B_\ell \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right) dp \\
&= \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right)(p_k - B_k)(p_\ell - B_\ell)dp + B_k(nu_\ell) + B_\ell(nu_k) - B_k B_\ell n \qquad (17)\\
&= \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right)(p_k - B_k)(p_\ell - B_\ell)dp \qquad (18)\\
&\quad + n\left(u_k - \frac{\varepsilon^2}{12}I_k\right)u_\ell + n\left(u_\ell - \frac{\varepsilon^2}{12}I_\ell\right)u_k - n\left(u_k - \frac{\varepsilon^2}{12}I_k\right)\left(u_\ell - \frac{\varepsilon^2}{12}I_\ell\right) + \mathcal{O}(\varepsilon^4) \qquad (19)\\
&= \int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right)(p_k - B_k)(p_\ell - B_\ell)dp + nu_k u_\ell + \mathcal{O}(\varepsilon^4). \qquad (20)
\end{aligned}$$

Here, we have replaced B_i by $u_i - (\varepsilon^2/12)I_i + \mathcal{O}(\varepsilon^4)$ (see Lemma 4.2). Using Lemma 3.1, one computes

$$\begin{aligned}
&\int_{\mathbb{R}^d} \text{Exp}\left(A + B\cdot p - \frac{|p|^2}{2}\right)(p_k - B_k)(p_\ell - B_\ell)dp \\
&\quad = n\delta_{k\ell} - \frac{\varepsilon^2}{12}n\left[\partial_{k\ell}(A + \tfrac{1}{2}|B|^2) - (\partial_i B_k - \partial_k B_i)(\partial_i B_\ell - \partial_\ell B_i)\right] + \mathcal{O}(\varepsilon^4). \qquad (21)
\end{aligned}$$

Inserting (21) into (20) gives

$$P_{k\ell} = n\delta_{k\ell} + nu_k u_\ell - \frac{\varepsilon^2}{12}n\left[\partial_{k\ell}(A + \tfrac{1}{2}|B|^2) - (\partial_i B_k - \partial_k B_i)(\partial_i B_\ell - \partial_\ell B_i)\right] + \mathcal{O}(\varepsilon^4),$$

concluding the proof. □

Lemma 4.4 *It holds:*

$$\text{div}P = \nabla n + \text{div}(nu\otimes u) - \frac{\varepsilon^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) + \frac{\varepsilon^2}{12}\text{div}(nJ) + \mathcal{O}(\varepsilon^4),$$

where the tensor J is defined in (16).

P r o o f. First we observe, following [3], that (14) implies $\nabla n = n\nabla(A + \frac{1}{2}|B|^2) + \mathcal{O}(\varepsilon^2)$ and thus

$$|\nabla(A + \tfrac{1}{2}|B|^2)|^2 = \frac{|\nabla n|^2}{n^2} + \mathcal{O}(\varepsilon^2), \quad \Delta(A + \tfrac{1}{2}|B|^2) = \text{div}\left(\frac{\nabla n}{n}\right) + \mathcal{O}(\varepsilon^2) = \frac{\Delta n}{n} - \frac{|\nabla n|^2}{n^2} + \mathcal{O}(\varepsilon^2),$$

which yields

$$2\Delta(A + \tfrac{1}{2}|B|^2) + |\nabla(A + \tfrac{1}{2}|B|^2)|^2 = 2\frac{\Delta n}{n} - \frac{|\nabla n|^2}{n^2} + \mathcal{O}(\varepsilon^2) = 4\frac{\Delta\sqrt{n}}{\sqrt{n}} + \mathcal{O}(\varepsilon^2). \qquad (22)$$

Hence, in view of Lemma 4.3,

$$\begin{aligned}
(\text{div}P)_\ell &= \partial_k P_{k\ell} = \partial_\ell n + \partial_k(nu_k u_\ell) - \frac{\varepsilon^2}{12}\left[\partial_k n \partial_{k\ell}(A + \tfrac{1}{2}|B|^2) + n\partial_{kk\ell}(A + \tfrac{1}{2}|B|^2)\right] \\
&\quad + \frac{\varepsilon^2}{12}\partial_k(nJ_{k\ell}) + \mathcal{O}(\varepsilon^4).
\end{aligned}$$

Above we have shown that $\partial_k n = n\partial_k(A + \frac{1}{2}|B|^2) + \mathcal{O}(\varepsilon^2)$. Therefore, using (22),

$$\begin{aligned}
(\text{div}P)_\ell &= \partial_\ell n + \partial_k(nu_k u_\ell) - \frac{\varepsilon^2}{12}n\partial_\ell\left[\tfrac{1}{2}\partial_k(A + \tfrac{1}{2}|B|^2)\partial_k(A + \tfrac{1}{2}|B|^2) + \partial_{kk}(A + \tfrac{1}{2}|B|^2)\right] \\
&\quad + \frac{\varepsilon^2}{12}\partial_k(nJ_{k\ell}) + \mathcal{O}(\varepsilon^4) \\
&= \partial_\ell n + \partial_k(nu_k u_\ell) - \frac{\varepsilon^2}{12}n\partial_\ell\left[\Delta(A + \tfrac{1}{2}|B|^2) + \tfrac{1}{2}|\nabla(A + \tfrac{1}{2}|B|^2)|^2\right] + \frac{\varepsilon^2}{12}\partial_k(nJ_{k\ell}) + \mathcal{O}(\varepsilon^4) \\
&= \partial_\ell n + \partial_k(nu_k u_\ell) - \frac{\varepsilon^2}{6}n\partial_\ell\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) + \frac{\varepsilon^2}{12}\partial_k(nJ_{k\ell}) + \mathcal{O}(\varepsilon^4).
\end{aligned}$$

This shows the lemma. □

Now we are able to prove the main theorem.

Proof. (Theorem 2.1.) Performing formally the limit $\delta \to 0$ in the Wigner equation (7), we obtain for $w = \lim_{\delta\to 0} w_\delta$ the equation $M[w] - w = Q(w) = 0$ and thus, w equals the quantum Maxwellian $M[w]$. The moment equations for w_δ read

$$\partial_t\langle w_\delta\rangle + \mathrm{div}\langle w_\delta p\rangle = 0, \qquad \partial_t\langle w_\delta p\rangle + \mathrm{div}\langle w_\delta p\otimes p\rangle - \langle w_\delta\rangle\nabla V = 0.$$

Using the definitions $n = \langle M[w]\rangle$ and $nu = \langle M[w]p\rangle$, we obtain in the formal limit $\delta \to 0$:

$$\partial_t n + \mathrm{div}(nu) = 0, \qquad \partial_t(nu) + \mathrm{div}\langle M[w]p\otimes p\rangle - n\nabla V = 0.$$

Replacing $\mathrm{div}P = \mathrm{div}\langle M[w]p\otimes p\rangle$ by its expansion derived in Lemma 4.4, we infer the quantum hydrodynamic equations (5)-(6). □

5 Proof of Corollary 2.2

A computation shows that the velocity u formally solves

$$\partial_t u + (u\cdot\nabla)u + \nabla(\ln n - V) = \mathcal{O}(\varepsilon^2).$$

Therefore,

$$\partial_t(\mathrm{Curl}\,u)_{ij} + u\cdot\nabla(\mathrm{Curl}\,u)_{ij} + \partial_i u_k(\mathrm{Curl}\,u)_{kj} + \partial_j u_k(\mathrm{Curl}\,u)_{ik} = \mathcal{O}(\varepsilon^2). \tag{23}$$

Multiplying this equation by $(\mathrm{Curl}\,u)_{ij}$, integrating over $\mathbb{R}^d$ and summing over all i, j, yields

$$\begin{aligned}\frac{1}{2}\partial_t\|\mathrm{Curl}\,u\|^2_{L^2(\mathbb{R}^d)} &= -\frac{1}{2}\sum_{i,j=1}^d\int_{\mathbb{R}^d} u\cdot\nabla(\mathrm{Curl}\,u)^2_{ij}dx - \int_{\mathbb{R}^d}\partial_i u_k(\mathrm{Curl}\,u)_{kj}(\mathrm{Curl}\,u)_{ij}dx\\ &\quad - \int_{\mathbb{R}^d}\partial_j u_k(\mathrm{Curl}\,u)_{ik}(\mathrm{Curl}\,u)_{ij}dx + \mathcal{O}(\varepsilon^2).\end{aligned}$$

Since, by integration by parts,

$$-\int_{\mathbb{R}^d} u\cdot\nabla(\mathrm{Curl}\,u)^2_{ij}dx = \int_{\mathbb{R}^d}\mathrm{div}\,u(\mathrm{Curl}\,u)^2_{ij}dx,$$

we arrive after applying Hölder's inequality to

$$\frac{1}{2}\partial_t\|\mathrm{Curl}\,u\|^2_{L^2(\mathbb{R}^d)} \le c\|\mathrm{Curl}\,u\|^2_{L^2(\mathbb{R}^d)} + \mathcal{O}(\varepsilon^2),$$

where $c > 0$ is a constant which is independent of ε (since we assume that u and its derivatives are uniformly bounded in ε). Integration over $(0,t)$ and Gronwall's lemma give

$$\|\mathrm{Curl}\,u(t)\|^2_{L^2(\mathbb{R}^d)} \le e^{2ct}\|\mathrm{Curl}\,u(0)\|^2_{L^2(\mathbb{R}^d)} + \mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon^2).$$

Differentiating (23) with respect to x_k, multiplying by $\partial_k(\mathrm{Curl}\,u)_{ij}$, integrating over $\mathbb{R}^d$ and performing the same manipulations as above leads to

$$\|\partial_k\mathrm{Curl}\,u(t)\|^2_{L^2(\mathbb{R}^d)} = \mathcal{O}(\varepsilon^2), \qquad k = 1,\ldots,d.$$

This shows that $\|\mathrm{Curl}\,u(t)\|^2_{H^1(\mathbb{R}^d)} = \mathcal{O}(\varepsilon^2)$. Taking higher derivatives and proceeding as above yields (11).

Finally, writing (6) in a weak form, employing (11),

$$\begin{aligned}&\int_0^T\left\langle \partial_t(nu) + \mathrm{div}(nu\otimes u) + \nabla n - n\nabla V - \frac{\varepsilon^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right), \phi\right\rangle dt\\ &= \frac{\varepsilon^2}{2}\int_0^T\int_{\mathbb{R}^d} n(\mathrm{Curl}\,u)_{ji}(\mathrm{Curl}\,u)_{jk}\partial_i\phi_k\,dxdt\\ &\le c\varepsilon^2\|\mathrm{Curl}\,u\|^2_{L^\infty(0,T;L^\infty(\mathbb{R}^d))}\int_0^T\|\phi\|_{H^1(\mathbb{R}^d)}dt\\ &\le c\varepsilon^4\int_0^T\|\phi\|_{H^1(\mathbb{R}^d)}dt\end{aligned}$$

for all smooth test functions ϕ, where $\langle\cdot,\cdot\rangle$ is the duality product in the space of distributions, and $c > 0$ is a constant independent of ε. Hence, (12) follows.

Remark 5.1 The above derivation also holds true for more general collision operators. In fact, we only need the following properties of $Q(w)$:

(1) If $Q(w) = 0$ then $w = M[w]$; (2) $\langle Q(w)\rangle = 0$ and $\langle Q(w)p\rangle = 0$.

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