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Dissipative quantum fluid models

Abstract. Some macroscopic models for diffusive quantum systems are reviewed. The model equations are derived from Wigner-Boltzmann equations by a moment method. Depending on the properties of the collision operator and the scaling of the Wigner equation, three model classes are presented: the quantum drift-diffusion equations, inviscid and viscous quantum hydrodynamic equations, and quantum Navier-Stokes equations. For each of these models, the derivation is sketched and analytical results are reviewed.

Keywords. Quantum transport, Schrödinger equation, Wigner equation, Wigner-Fokker-Planck equation, quantum drift-diffusion equation, DLSS equation, quantum hydrodynamic equations, viscous quantum hydrodynamic equations, quantum Navier-Stokes equations.

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Contents

1 Introduction **2**

2 Quantum kinetic models **4**
2.1 Density-matrix formalism 4
2.2 Wigner equations 8
2.3 Quantum equilibrium 11
2.4 Wigner-Boltzmann equations 14
2.4.1 Wigner-BGK model 15
2.4.2 Wigner-Fokker-Planck model 15

3 Quantum drift-diffusion models **16**
3.1 Derivation 17
3.1.1 Nonlocal quantum drift-diffusion model 17
3.1.2 Local quantum drift-diffusion model 19
3.2 Analysis of the fourth-order equation 22
3.2.1 Existence of global solutions 22
3.2.2 Long-time behavior of solutions 26
3.2.3 The stationary equations 28
3.2.4 Asymptotic limits 29
3.3 Analysis of the sixth-order equation 31
3.4 Analysis of the nonlocal equation 33

4 Viscous quantum hydrodynamic models **35**
4.1 Derivation 35
4.1.1 Quantum hydrodynamics and the Schrödinger equation . 35
4.1.2 Quantum hydrodynamics and the Wigner equation 38
4.1.3 Viscous quantum hydrodynamics 43
4.2 Analysis 45
4.2.1 Thermal equilibrium 45
4.2.2 Stationary equations 46
4.2.3 Transient equations 49
4.2.4 Viscous equations 52

5 Quantum Navier-Stokes models **54**
5.1 Derivation 54
5.2 Analysis 56

References **59**

1 - Introduction

Quantum fluids have been studied experimentally for many years and have by now become very attractive due to novel experimental discoveries in Bose-Einstein condensation, the use of liquid helium for superconducting materials, and potential applications in quantum computing. Recently, disordered superfluids and, in particular, the interplay between superfluidity and the onset of dissipative processes have been investigated [28]. Typically, the dynamics of the condensate is modeled by a nonlinear Schrödinger equation involving dissipative terms [5]. Whereas diffusion has been extensively studied in classical physical systems, much less is known in quantum systems, and the theoretical understanding of quantum diffusion is difficult and not complete. The reason is that diffusion is an incoherent process, whereas quantum dynamics are typically very coherent.

In this paper, we review some approaches to include diffusive phenomena in quantum fluid models. The target reader is supposed to be mathematically

oriented since we present the mathematical modeling and analysis of the model equations only. For a more physical exposition, we refer to the book [91]. Semiconductor devices are modeled and analyzed in [125]. Furthermore, numerical schemes and simulations can be found, e.g., in [33, 68, 98, 100, 106, 107, 132, 134] and references therein.

A simple fluiddynamical model is obtained from the single-state Schrödinger equation via the Madelung transform [123]. In fact, by separating the imaginary and real part of the Schrödinger equation, we arrive at the pressureless Euler equations involving a third-order quantum correction with the so-called Bohm potential. However, these Madelung equations describe ballistic transport only. An alternative approach to derive quantum fluid models is to apply a moment method to the Wigner equation. It has the advantage that dissipation can be included in a rather natural way via collision operators on the right-hand side of the Wigner equation. Examples, used in semiconductor modeling, are the Caldeira-Leggett scattering operator, the Fokker-Planck operator, or BGK-type operators (named after Bhatnagar, Gross, and Krook [16]); see Section 2.4 for a detailed description.

Depending on the properties of the collision operator, various model equations can be derived. In this survey, we present three model classes (see Figure 1).

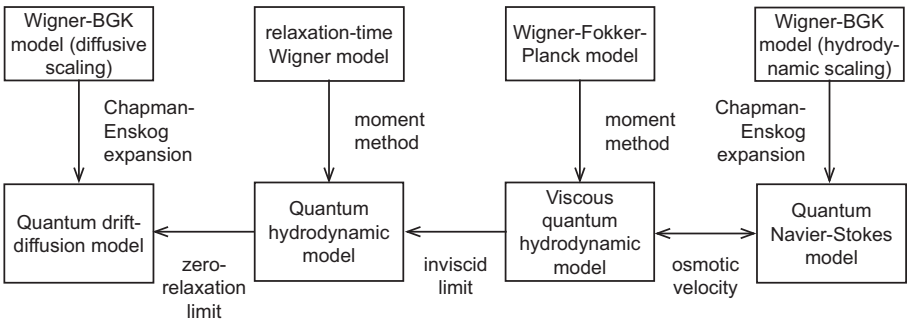

Figure 1: *Model hierarchy. The Wigner models are explained in Section 2.4.*

The first class, the *quantum drift-diffusion* equations, are derived from the Wigner equation, in the diffusive scaling, with a BGK-type collision operator which conserves mass [53]. The quantum drift-diffusion model consists of a nonlinear parabolic fourth-order equation for the particle density and the Poisson equation for the electric potential. The main difficulty of the analysis of this model is due to the fourth-order operator in the particle equation, which is highly nonlinear and prevents the use of maximum principles.

This technique has been also applied to spinorial systems by Barletti and Méhats in [12] obtaining quantum drift-diffusion systems for the spin-up and spin-down electron densities (also see [13, 64] for related macroscopic spin models).

The second model class are the *(viscous) quantum hydrodynamic equations.*

They consist of balance equations for the particle, current, and energy densities, self-consistently coupled to the Poisson equation. The equations are derived from the Wigner-Fokker-Planck equation using a moment method [78]. Compared to the Madelung equations, they contain a pressure function and spatially diffusive terms (Laplacians) in the macroscopic variables. Although the Laplacian operator makes the mass equation parabolic, the momentum equation still contains the nonlinear third-order Bohm-potential term whose mathematical treatment is challenging.

When a Chapman-Enskog expansion is applied to the Wigner-BGK model, diffusive corrections to the quantum equilibrium can be derived [24]. This leads to the third model class, the *quantum Navier-Stokes equations*. A characteristic feature is that the viscosity depends on the particle density. Surprisingly, there exists a connection between the quantum Navier-Stokes and viscous quantum hydrodynamic models. By introducing a new velocity variable, containing the so-called "osmotic velocity", both models are formally equivalent (see Section 5.2).

This review is organized as follows. In Section 2, three quantum view points—the density-matrix, Schrödinger, and Wigner formalism—and their relations are sketched. Furthermore, the quantum equilibrium is defined and examples for Wigner-Boltzmann equations are given. Section 3 is concerned with the derivation and analysis of local and nonlocal quantum drift-diffusion models. Quantum hydrodynamic equations, derived from the (mixed-state) Schrödinger, Wigner, or Wigner-Fokker-Planck equations, are introduced in Section 4. Moreover, some analytical results for the inviscid and viscous quantum equations are reviewed. Finally, the derivation and analysis of quantum Navier-Stokes equations is presented in Section 5.

We remark that the derivations of the models are purely formal, and a "proof" of a theorem on the model derivation is not a proof in the strict mathematical sense but rather signifies formal computations. The sections on the analysis of the equations contain theorems which are rigorous in the mathematical sense, but only the key ideas of their proofs are given.

2 - Quantum kinetic models

In this section, we present various formulations of the evolution of quantum systems: the density-matrix, the (mixed-state) Schrödinger, and the Wigner formalism. The Wigner equation is the starting point for deriving quantum fluid models in the subsequent sections.

2.1 - *Density-matrix formalism*

The quantum mechanical state of a system can be described by the Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi = H\psi \quad \text{in } \mathbb{R}^3,\ t>0, \quad \psi(\cdot,0)=\psi_I,$$

where $\varepsilon > 0$ is the scaled Planck constant and H is the quantum mechanical Hamiltonian, for instance, $H = -(\varepsilon^2/2)\Delta - V(x,t)$ with $V(x,t)$ being a potential. When we have an ensemble of many particles, like electrons, the Schrödinger equation needs to be solved in a very high-dimensional state space. Moreover, there exist systems which cannot be described by a single-state wave function since they are statistical mixtures. This leads to the concept of *density matrices*. We assume in the following that the quantum state is represented by a *density-matrix operator* $\widehat{\rho}$, whose evolution is governed by the *Liouville-von Neumann equation*

$$\mathrm{i}\varepsilon\partial_t\widehat{\rho} = [H,\widehat{\rho}], \quad t>0, \quad \widehat{\rho}(0) = \widehat{\rho}_I, \tag{1}$$

where $[H,\widehat{\rho}] = H\widehat{\rho} - \widehat{\rho}H$ is the commutator. In this section, we perform formal computations only, and we refer to the literature for the mathematical setting in functional spaces [1, 6].

The density-matrix operator $\widehat{\rho}$ is a positive, self-adjoint, and trace-class operator on $L^2(\mathbb{R}^3)$. A bounded linear operator $\widehat{\rho}$ is called *trace class* if it is compact and its trace $\mathrm{Tr}(\widehat{\rho}) = \sum_j((\widehat{\rho}^*\widehat{\rho})^{1/2}u_j,u_j)$ is finite, where $(\cdot,\cdot)$ is a scalar product and (u_j) is any complete orthonormal set of $L^2(\mathbb{R}^3)$. The self-adjointness and compactness of $\widehat{\rho}$ provide the existence of a complete orthonormal set (ψ_j) of eigenvectors with eigenvalues (λ_j). The positivity implies that the eigenvalues λ_j are nonnegative and hence, $\mathrm{Tr}(\widehat{\rho}) = \sum_j \lambda_j < \infty$. We assume that the initial operator $\widehat{\rho}_I$ is positive, self-adjoint, and trace class too, such that there exist orthonormal eigenvectors (ψ_j^0).

We claim that the wave functions $\psi_j(x,t)$ are solutions to the Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi_j = H\psi_j \quad \text{in } \mathbb{R}^3,\ t>0, \quad \psi_j(\cdot,0) = \psi_j^0.$$

More precisely, ψ_j describes a *pure state* of the quantum system, and the eigenvalue λ_j is the corresponding occupation probability. The sequence (ψ_j,λ_j) of eigenvectors-eigenvalues is called a *mixed state*. For a system of many particles, the mixed state describes a statistical mixture of states ψ_j with occupation probabilities $\lambda_j \ge 0$ ($j\in\mathbb{N}$). These numbers depend on the initial state of the system. Before we detail the connection between the Liouville-von Neumann equation and the Schrödinger equation, we need some properties of the density-matrix operator. We follow Section 10.1 in [91].

Each density-matrix operator has the unique integral representation

$$(\widehat{\rho}\psi)(x,t) = \int_{\mathbb{R}^3}\rho(x,y,t)\psi(y,t)dy, \quad t\ge 0, \tag{2}$$

for all $\psi\in L^2(\mathbb{R}^3)$, where ρ is the density matrix (function). The self-adjointness of $\widehat{\rho}$ implies the symmetry $\rho(x,y,t) = \rho(y,x,t)$. The "diagonal" of the density matrix is interpreted as the *particle density*

$$n(x,t) = \rho(x,x,t), \quad x\in\mathbb{R}^3,\ t>0.$$

Furthermore, the *particle current density* is defined by

$$J(x,t) = \varepsilon\mathrm{Im}\nabla_x\rho(x,x,t), \quad x\in\mathbb{R}^3,\ t>0,$$

where $\mathrm{Im}(z)$ denotes the imaginary part of $z \in \mathbb{C}$. The density matrix solves the Liouville-von Neumann equation in the "matrix" formulation

$$\mathrm{i}\varepsilon\partial_t\rho(x,y,t) = (H_x - H_y)\rho(x,y,t), \quad t > 0, \quad \rho(x,y,0) = \rho_I(x,y), \tag{3}$$

where $x,\ y \in \mathbb{R}^3$, H_x denotes the Hamiltonian acting only on the variable x and H_y only acts on y. This follows from the self-adjointness of H_y. Indeed, by integrating by parts, we find for any function $\psi(y,t)$:

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{i}\varepsilon\partial_t\rho(x,y,t)\psi(y,t)dy &= \mathrm{i}\varepsilon(\partial_t\widehat{\rho})\psi(x,t) = (H\widehat{\rho}\psi - \widehat{\rho}H\psi)(x,t)\\ &= \int_{\mathbb{R}^3}\big(H_x\rho(x,y,t)\psi(y,t) - \rho(x,y,t)H_y\psi(y,t)\big)dy\\ &= \int_{\mathbb{R}^3}\big(H_x\rho(x,y,t)\psi(y,t) - H_y\rho(x,y,t)\psi(y,t)\big)dy\\ &= \int_{\mathbb{R}^3}(H_x - H_y)\rho(x,y,t)\psi(y,t)dy.\end{aligned}$$

The initial datum ρ_I is computed from the representation

$$(\widehat{\rho}_I\psi)(x) = \int_{\mathbb{R}^3}\rho_I(x,y)\psi(y)dy, \quad x \in \mathbb{R}^3.$$

L e m m a 2.1. *The density matrix can be expanded in terms of the eigenfunctions ψ_j,*

$$\rho(x,y,t) = \sum_{j=1}^{\infty}\lambda_j\psi_j(x,t)\overline{\psi_j(y,t)}.$$

Here, $\overline{z}$ denotes the complex conjugate of $z \in \mathbb{C}$.

P r o o f. We employ the representation (2) for the eigenfunction $\psi = \psi_j$, multiply this equation by $\overline{\psi_\ell(x,t)}$ and integrate over $\mathbb{R}^3$. Then, in view of the orthonormality of (ψ_j),

$$\delta_{j\ell}\lambda_j = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\rho(x,y,t)\psi_j(y,t)\overline{\psi_\ell(x,t)}dx\,dy, \tag{4}$$

where $\delta_{j\ell}$ is the Kronecker delta. The set $(\psi_j(x,t)\overline{\psi_\ell(y,t)})$ is complete and orthonormal in $L^2(\mathbb{R}^3\times\mathbb{R}^3)$. Therefore, the density matrix can be expanded in this basis:

$$\rho(x,y,t) = \sum_{m,n=1}^{\infty}c_{mn}(t)\psi_m(x,t)\overline{\psi_n(y,t)}.$$

Inserting this expansion into (4) and employing again the orthonormality of (ψ_j), it follows that the coefficients $c_{\ell j}(t)$ equal $\delta_{j\ell}\lambda_j$ such that the lemma follows. □

The density-matrix operators $\widehat{\rho}_I$ and $\widehat{\rho}$ can be expanded in the form

$$\widehat{\rho}_I = \sum_{j=1}^{\infty}\lambda_j|\psi_j^0\rangle\langle\psi_j^0|, \quad \widehat{\rho} = \sum_{j=1}^{\infty}\lambda_j|\psi_j\rangle\langle\psi_j|, \tag{5}$$

where $|\psi_j\rangle$ denotes the function ψ_j and $\langle\psi_j|$ the projection on ψ_j (bra-ket notation).

The following theorem roughly states that the Liouville-von Neumann equation is equivalent to the mixed-state Schrödinger equations (see Theorem 10.2 in [91]).

T h e o r e m 2.1 (Mixed-state Schrödinger equations). *Let $\widehat{\rho}$ be a density-matrix operator, satisfying the Liouville-von Neumann equation* (1)*, with a complete orthonormal set of eigenfunctions (ψ_j) and eigenvalues (λ_j). The eigenfunctions of the initial-data operator $\widehat{\rho}_I$ are denoted by (ψ_j^0). Then ψ_j is the solution of the Schrödinger equation*

$$\mathrm{i}\varepsilon\partial_t\psi_j = H\psi_j, \quad t>0, \quad \psi_j(\cdot,0)=\psi_j^0 \quad \text{in } \mathbb{R}^3,\ j\in\mathbb{N}. \tag{6}$$

The particle density $n(x,t)$ can be written as

$$n(x,t) = \sum_{j=1}^\infty \lambda_j|\psi_j(x,t)|^2, \quad x\in\mathbb{R}^3,\ t>0. \tag{7}$$

Conversely, let (ψ_j,λ_j) be a solution of the Schrödinger equation (6) *with numbers $\lambda_j\ge 0$ satisfying $\sum_j\lambda_j<\infty$. Then the density matrix operator, defined by* (5)*, solves the Liouville-von Neumann equation* (1).

P r o o f. The proof is taken from Section 10.1 in [91]. Let $\widehat{\rho}$ be a solution of the Liouville-von Neumann equation (1), represented as in (5). The solution of the Liouville-von Neumann equation can be written *formally* as

$$\widehat{\rho}(t) = e^{-\mathrm{i}Ht/\varepsilon}\widehat{\rho}_I e^{\mathrm{i}Ht/\varepsilon}, \quad t\ge 0,$$

since

$$\partial_t\widehat{\rho} = -\frac{\mathrm{i}}{\varepsilon}He^{-\mathrm{i}Ht/\varepsilon}\widehat{\rho}_I e^{\mathrm{i}Ht/\varepsilon} + \frac{\mathrm{i}}{\varepsilon}e^{-\mathrm{i}Ht/\varepsilon}\widehat{\rho}_I He^{\mathrm{i}Ht/\varepsilon} = -\frac{\mathrm{i}}{\varepsilon}\big(H\widehat{\rho}-\widehat{\rho}H\big).$$

Here, we have used the fact that the Hamiltonian H and the operator $e^{\mathrm{i}Ht/\varepsilon}$ commute. Then, inserting the expansion (5) for $\widehat{\rho}_I$ in the above formula gives

$$\widehat{\rho}(t) = \sum_{j=1}^\infty \lambda_j|e^{-\mathrm{i}Ht/\varepsilon}\psi_j^0\rangle\langle e^{\mathrm{i}Ht/\varepsilon}\psi_j^0|.$$

Comparing this expression with the expansion (5) for $\widehat{\rho}$ shows that $\psi_j(\cdot,t) = e^{-\mathrm{i}Ht/\varepsilon}\ \psi_j^0$. Finally, differentiation with respect to time yields $\varepsilon\partial_t\psi_j = -\mathrm{i}H\psi_j$ which is equivalent to the Schrödinger equation (6).

Conversely, let ψ_j be the solution of the Schrödinger equation (6) and let $\widehat{\rho}$ be given by (5). Then

$$\begin{aligned}\partial_t\widehat{\rho} &= \sum_{j=1}^\infty \lambda_j\big(|\partial_t\psi_j\rangle\langle\psi_j| + |\psi_j\rangle\langle\partial_t\psi_j|\big)\\ &= \sum_{j=1}^\infty \lambda_j\Big(-\frac{\mathrm{i}}{\varepsilon}|H\psi_j\rangle\langle\psi_j| + \frac{\mathrm{i}}{\varepsilon}|\psi_j\rangle\langle H\psi_j|\Big) = -\frac{\mathrm{i}}{\varepsilon}(H\widehat{\rho}-\widehat{\rho}H).\end{aligned}$$

Thus, $\widehat{\rho}$ is a solution of the Liouville-von Neumann equation (1). $\square$

If the initial quantum state can be written as $\rho_I(x,y) = \psi_I(x)\overline{\psi_I(y)}$, the density matrix is given by $\rho(x,y,t) = \psi(x,t)\overline{\psi(y,t)}$, where ψ solves the Schrödinger equation (6). The particle density equals $n(x,t) = 2\rho(x,x,t) = 2|\psi(x,t)|^2$ and the particle current density

$$J = -\varepsilon \mathrm{Im}(\overline{\psi}\nabla_x \psi).$$

We refer to such a situation as a *single state* as the single wave function ψ completely describes the quantum state.

For the self-consistent modeling of charged-carrier systems (for instance, electrons), the Poisson equation for the electric potential is added to the Schrödinger equations (6). Let V be the sum of an external potential V_{ex}, modeling, for instance, semiconductor heterostructures, and the self-consistent potential V_{sc}, which is given by

$$\lambda_D^2 \Delta V_{\mathrm{sc}} = n - C(x), \quad x \in \mathbb{R}^3, \tag{8}$$

where λ_D is the scaled Debye length and $C(x)$ models fixed charged background ions (doping concentration). The electron density n is computed according to (7). The system of equations, consisting of the Schrödinger equations (6), the Poisson equation (8) with (7), is referred to as the *mixed-state Schrödinger-Poisson system*.

2.2 - *Wigner equations*

In the previous subsection, we have explained how the quantum mechanical motion of an electron ensemble can be described in the mixed-state Schrödinger or density-matrix formalism. There is an alternative description based on the quantum-kinetic Wigner formulation, which we present and discuss in this section. There are two main reasons for using this framework in applications (mostly for transient problems). First, the Wigner picture allows, in contrast to Schrödinger models, for a modeling of scattering phenomena in the form of a quantum Boltzmann equation. Second, when considering bounded domains modeling electronic devices, the quantum-kinetic framework makes it easier to formulate boundary conditions at the device contacts, which may be inspired from classical kinetic considerations [67].

We derive the Wigner equation (or quantum Liouville equation) from the Liouville-von Neumann equation (3). To this end, we recall the Fourier transform

$$(\mathcal{F}(f))(p) = \int_{\mathbb{R}^3} f(y) e^{-\mathrm{i}y\cdot p/\varepsilon} dy,$$

and its inverse,

$$(\mathcal{F}^{-1}(g))(y) = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} g(p) e^{\mathrm{i}y\cdot p/\varepsilon} dp,$$

for functions $f,\, g : \mathbb{R}^3 \to \mathbb{C}$.

For the kinetic formulation of the Liouville-von Neumann equation, we need the so-called *Wigner function* introduced by Wigner in 1932 [143]:

$$w(x,p,t) = W[\rho](x,p,t) = \int_{\mathbb{R}^3} \rho\Big(x + \frac{y}{2}, x - \frac{y}{2}, t\Big) e^{-\mathrm{i}y\cdot p/\varepsilon} dy. \tag{9}$$

Setting

$$u(x,y,t) = \rho\Big(x + \frac{y}{2}, x - \frac{y}{2}, t\Big), \tag{10}$$

the Wigner function can be written as the Fourier transform of u, $w = \mathcal{F}(u)$. Furthermore, $u = \mathcal{F}^{-1}(w)$. We notice that the operator $W[\rho]$ is called the *Wigner-Weyl transform*. Its inverse W^{-1}, also called Weyl quantization, is defined as an operator on $L^2(\mathbb{R}^3)$:

$$(W^{-1}[f]\phi)(x) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f\Big(\frac{x+y}{2}\Big)\phi(y) e^{\mathrm{i}p\cdot(x-y)/\varepsilon} \frac{dp\,dy}{(2\pi\varepsilon)^3}$$

for functions $\phi \in L^2(\mathbb{R}^3)$. The Wigner transform and the Weyl quantization are isometries between the space of operators $\widehat{\rho}$ such that $\widehat{\rho}\widehat{\rho}^*$ is trace class ($\widehat{\rho}^*$ denotes the adjoint of $\widehat{\rho}$) and the space $L^2(\mathbb{R}^6)$. Indeed, from Plancherel's formula follows that

$$\mathrm{Tr}(\widehat{\rho}_1\widehat{\rho}_2^*) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} W[\rho_1](x,p,t)\overline{W[\rho_2](x,p,t)}\frac{dp\,dx}{(2\pi\varepsilon)^3}, \tag{11}$$

where ρ_1 and ρ_2 are the corresponding density matrix functions.

The evolution equation for the Wigner function is obtained by transforming the Liouville-von Neumann equation to the (x,y) variables and applying the Fourier transformation. The result is expressed in the following proposition (Proposition 11.1 in [91]).

P r o p o s i t i o n 2.1 (Wigner equation). *Let ρ be a solution of the Liouville-von Neumann equation* (3)*. Then the Wigner function* (9) *is formally a solution of the* Wigner equation

$$\partial_t w + p\cdot\nabla_x w + \theta[V]w = 0, \quad t > 0, \quad w(x,p,0) = w_I(x,p) \tag{12}$$

for $x,\, p \in \mathbb{R}^3$, where the initial datum is given by

$$w_I(x,p) = \int_{\mathbb{R}^3} \rho_I\Big(x + \frac{y}{2}, x - \frac{y}{2}\Big) e^{-\mathrm{i}y\cdot p/\varepsilon} dy,$$

and $\theta[V]$ is a pseudo-differential operator, defined by

$$(\theta[V]w)(x,p,t) = \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3\times\mathbb{R}^3} (\delta V)(x,y,t) w(x,p',t) e^{\mathrm{i}y\cdot(p-p')/\varepsilon} dp'\,dy, \tag{13}$$

where

$$\delta V(x,y,t) = \frac{\mathrm{i}}{\varepsilon}\Big(V\Big(x + \frac{y}{2}, t\Big) - V\Big(x - \frac{y}{2}, t\Big)\Big).$$

P r o o f. The proof is taken from Section 11.1 of [91]. First, we derive the evolution equation for u, defined in (10), and then take the inverse Fourier transform. We compute, for $r = x + y/2$ and $s = x - y/2$,

$$\begin{aligned}\mathrm{div}_y(\nabla_x u)(x,y,t) &= \mathrm{div}_y(\nabla_r\rho + \nabla_s\rho)\Big(x+\frac{y}{2}, x-\frac{y}{2}, t\Big)\\ &= \frac{1}{2}(\Delta_r\rho - \Delta_s\rho)\Big(x+\frac{y}{2}, x-\frac{y}{2}, t\Big).\end{aligned}$$

Then the transformed Liouville-von Neumann equation for u becomes,

$$\begin{aligned}\partial_t u(x,y,t) = \partial_t\rho(r,s,t) &= -\frac{\mathrm{i}}{\varepsilon}\Big(-\frac{\varepsilon^2}{2}(\Delta_r - \Delta_s) - V(r,t) + V(s,t)\Big)\rho(r,s,t)\\ &= \mathrm{i}\varepsilon\,\mathrm{div}_y(\nabla_x u)(x,y,t) + \delta V(x,y,t)u(x,y,t)\end{aligned}$$

or

$$\partial_t u - \mathrm{i}\varepsilon\ \mathrm{div}_y(\nabla_x u) - (\delta V)u = 0, \quad x,y\in\mathbb{R}^3,\ t>0.$$

The Fourier transform gives

$$\partial_t\mathcal{F}(u) - \mathrm{i}\varepsilon\mathcal{F}(\mathrm{div}_y\,\nabla_x u) - \mathcal{F}((\delta V)u) = 0. \tag{14}$$

The second term on the left-hand side can be written, by integrating by parts, as

$$\begin{aligned}\mathcal{F}(\mathrm{div}_y\,\nabla_x u)(x,p,t) &= \int_{\mathbb{R}^3}\mathrm{div}_y(\nabla_x u)(x,y,t)e^{-\mathrm{i}y\cdot p/\varepsilon}dy\\ &= \frac{\mathrm{i}}{\varepsilon}\int_{\mathbb{R}^3} p\cdot\nabla_x u(x,y,t)e^{-\mathrm{i}y\cdot p/\varepsilon}dy\\ &= \frac{\mathrm{i}}{\varepsilon}p\cdot\nabla_x\mathcal{F}(u)(x,p,t) = \frac{\mathrm{i}}{\varepsilon}p\cdot\nabla_x w(x,v,t).\end{aligned}$$

The third-term on the left-hand side of (14) becomes, by (13),

$$\begin{aligned}\mathcal{F}((\delta V)u)(x,p,t) &= \int_{\mathbb{R}^3}(\delta V)(x,y,t)u(x,y,t)e^{-\mathrm{i}y\cdot p/\varepsilon}dy\\ &= (2\pi\varepsilon)^{-3}\int_{\mathbb{R}^3}(\delta V)(x,y,t)w(x,p',t)e^{\mathrm{i}y\cdot(p'-p)/\varepsilon}dp'\,dy\\ &= (2\pi\varepsilon)^{-3}\int_{\mathbb{R}^3}(\delta V)(x,-y,t)w(x,p',t)e^{\mathrm{i}y\cdot(p-p')/\varepsilon}dp'\,dy\\ &= -(\theta[V]w)(x,p,t).\end{aligned}$$

Therefore, (14) equals the Wigner equation (12). □

The local term $p\cdot\nabla_x w$ is the quantum analogue of the classical transport term of the Liouville equation (see Chapter 3 of [91]). The nonlocal term $\theta[V]w$ models the influence of the electric potential. The nonlocality has the effect

that the electron ensemble "feels" an upcoming potential barrier. The pseudo-differential operator can be written as, by slight abuse of notation and for $w = \mathcal{F}(u)$,

$$\begin{aligned}(\theta[V]w)(x,p,t) &= \int_{\mathbb{R}^3} (\delta V)(x,y,t)u(x,-y,t)e^{\mathrm{i}y\cdot p/\varepsilon}dy \\ &= \mathcal{F}\big((\delta V)(x,-y,t)u(x,y,t)\big).\end{aligned}$$

Therefore, it acts in the Fourier space essentially as a multiplication operator. The multiplicator δV is called the *symbol* of the operator $\theta[V]$. The symbol δV is a discrete directional derivative, since in the formal limit $\varepsilon \to 0$, we find that

$$\delta V(x,\varepsilon y,t) \to \mathrm{i}\nabla_x V(x,t)\cdot y.$$

We refer to [139] for a mathematical theory of pseudo-differential operators. In particular, the Wigner equation (12) is a linear pseudo-differential equation. For mathematical results on the Wigner equation, we refer to the review of Arnold [6].

2.3 - *Quantum equilibrium*

The thermal equilibrium of a gas can be defined in classical kinetic theory as the maximizer f^* of the fluid entropy (or, more precisely, free energy)

$$S_{\mathrm{cl}}(f) = -\int_{\mathbb{R}^3} \big(f(\log f - 1) + h(x,p)f\big)dp,$$

where p is the momentum and $h(x,p) = |p|^2/2 - V(x)$ the classical Hamiltonian. A simple calculation yields

$$f^*(x,p) = \exp\big(V(x) - \tfrac{1}{2}|p|^2\big), \quad x,p \in \mathbb{R}^3.$$

In quantum mechanics, the above local definition of entropy (as a function of the position) does not exist. In fact, the quantum entropy refers to the entire system whose statistical uncertainty is described by the density-matrix operator $\widehat{\rho}$. The quantum entropy as a measure of the uncertainty is expressed in terms of the eigenvalues μ_j of $\widehat{\rho}$:

$$S_{\mathrm{qu}}(\widehat{\rho}) = -\mathrm{Tr}(\widehat{\rho}(\log\widehat{\rho} - 1)) = -\sum_j \mu_j(\log\mu_j - 1).$$

The expression $\widehat{\rho}(\log\widehat{\rho} - 1)$ is defined by functional calculus applied to the function $f(x) = x(\log x - 1)$. Instead of the entropy S_{qu}, we consider the free energy

$$S(\widehat{\rho}) = -\mathrm{Tr}\big(\widehat{\rho}(\log\widehat{\rho} - 1) + H(\widehat{\rho})\big),$$

where $H = -(\varepsilon^2/2)\Delta - V(x)$ is the quantum Hamiltonian. Applying the Plancherel-type formula (11) and the identity $h = W[H]$, we can write for

$w = W[\widehat{\rho}]$, with a slight abuse of notation,

$$S(w) = -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big(w(\mathrm{Log}(w) - 1) + h(x,p)w\big)\frac{dp\,dx}{(2\pi\varepsilon)^3}.$$

Here, the *quantum logarithm* and *quantum exponential* have been introduced by Degond and Ringhofer [55]:

$$\mathrm{Log}(w) = W[\log W^{-1}[w]], \quad \mathrm{Exp}(w) = W[\exp W^{-1}[w]],$$

where log and exp are the operator logarithm and exponential, respectively, defined by their corresponding spectral decomposition.

In order to compute the (formal) maximizer of S, we compute first its derivative. For this, we notice that for any differentiable function g, the Gâteaux derivative of $\mathrm{Tr}(g(\widehat{\rho}))$ (if it exists) is given by

$$\Big(\frac{d}{d\widehat{\rho}}\mathrm{Tr}(g(\widehat{\rho}))\Big)\widehat{\sigma} = \mathrm{Tr}(g'(\widehat{\rho})\widehat{\sigma}),$$

where $\widehat{\rho}$ and $\widehat{\sigma}$ are density-matrix operators. For a proof, we refer to [55, Lemma 3.3]. Hence, with $g(\widehat{\rho}) = \widehat{\rho}(\log\widehat{\rho} - 1)$, we find that

$$\Big(\frac{dS}{d\widehat{\rho}}(\widehat{\rho})\Big)\widehat{\sigma} = -\mathrm{Tr}\big((\log(\widehat{\rho}) - H)\widehat{\sigma}\big) = -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}(W[\log\widehat{\rho}] + W[H])W[\widehat{\sigma}]\frac{dp\,dx}{(2\pi\varepsilon)^3}.$$

Thus, if $w = W[\widehat{\rho}]$ and $u = W[\widehat{\sigma}]$,

$$\Big(\frac{dS}{d\widehat{\rho}}(\widehat{\rho})\Big)\widehat{\sigma} = -\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\big(\mathrm{Log}(w) + h(x,p)\big)u\frac{dp\,dx}{(2\pi\varepsilon)^3}. \tag{15}$$

A necessary condition for extremality of S is that its Gâteaux derivative vanishes, which implies that $\mathrm{Log}(w_{\mathrm{eq}}) + h(x,p) = 0$ or

$$w_{\mathrm{eq}} = \mathrm{Exp}(-h(x,p)). \tag{16}$$

If there exists an operator $\widehat{\rho}_{\mathrm{eq}}$ such that $W[\widehat{\rho}_{\mathrm{eq}}] = w_{\mathrm{eq}}$, we find that the quantum equilibrium is given by

$$\widehat{\rho}_{\mathrm{eq}} = \exp(-H).$$

Inspired by the classical case, we may define equilibrium states which satisfy prescribed moments [55]. Given the weight function $\kappa(p)$, we call

$$m(x,t) = \langle\kappa(p)w\rangle := \int_{\mathbb{R}^3} w(x,p,t)\kappa(p)\frac{dp}{(2\pi\varepsilon)^3}$$

the *moment* of w. Physically relevant moments are the particle density n, particle current density $-nu$, and energy density ne, defined by, respectively,

$$\begin{pmatrix} n \\ nu \\ ne \end{pmatrix} = \int_{\mathbb{R}^3} w(x,p,t)\begin{pmatrix} 1 \\ p \\ \frac{1}{2}|p|^2 \end{pmatrix}\frac{dp}{(2\pi\varepsilon)^3}.$$

Given a Wigner function w, we define the quantum equilibrium as follows. We write the moments of w as

$$m_j(x,t) = \langle w(x,p,t)\kappa_j(p)\rangle = \int_{\mathbb{R}^3} w(x,p,t)\kappa_j(p)\frac{dp}{(2\pi\varepsilon)^3},$$

where $\kappa_0,\dots,\kappa_N$ are some weight functions. The constrained maximization problem reads as

$$\max\big\{S(w) : \langle w(x,p,t)\kappa_j(p)\rangle = m_j(x,t) \text{ for all } (x,t),\ j=0,\dots,N\big\}. \tag{17}$$

L e m m a 2.2. *The formal solution of the constrained maximization problem* (17)*, if it exists, is given by*

$$M[w](x,p,t) = \operatorname{Exp}\Big(\xi(x,t)\cdot\kappa(p) + V(x,t) - \frac{|p|^2}{2}\Big),$$

where $\xi(x,t)\in\mathbb{R}^{N+1}$ *are some Lagrange multipliers.*

P r o o f. The proof is taken from Section 21.1 in [91]. We define for $\xi=(\xi_0,\dots,\xi_N)$ and $m=(m_0,\dots,m_N)$ the Lagrange functional

$$F(w,\xi) = H(w) + \int_{\mathbb{R}^3}\xi(x)\cdot\big(m - \langle w(x,p,t)\kappa(p)\rangle\big)dx.$$

A necessary condition for extremality of F is that its Gâteaux derivative with respect to $\widehat{\rho}=W^{-1}[w]$ vanishes. In view of (15), this condition becomes

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\Big(\operatorname{Log}(w^*) + \frac{|p|^2}{2} - V - \xi^*(x)\cdot\kappa(p)\Big)u(x,p)dp\,dx = 0$$

for some functions $w^*(x,p)$ and $\xi^*(x)$ and for all functions $u(x,p)$, which implies that

$$\operatorname{Log}(w^*) + \frac{|p|^2}{2} - V(x,t) - \xi^*(x)\cdot\kappa(p) = 0$$

and finally,

$$w^* = \operatorname{Exp}\Big(\xi^*\cdot\kappa + V - \frac{|p|^2}{2}\Big),$$

finishing the proof. □

We call $M[w]$ the *quantum Maxwellian* of w. If we assume that $\kappa_0(p)=1$ and $\kappa_2(p)=\frac{1}{2}|p|^2$, setting $\lambda_0=\xi_0+V$, $\lambda_2=\xi_2-1$, and $\lambda_j=\xi_j$ otherwise, we can write the quantum Maxwellian more compactly as

$$M[w] = \operatorname{Exp}(\lambda\cdot\kappa(p)). \tag{18}$$

We give some examples of quantum Maxwellians which are used in the following sections. If only the electron density is prescribed, we obtain the quantum Maxwellian

$$M[w](x,p,t) = \operatorname{Exp}\Big(A(x,t) - \frac{|p|^2}{2}\Big),$$

where the Lagrange multiplier A is uniquely determined by the zeroth moment of w. This Maxwellian will be employed for the derivation of the quantum drift-diffusion model in Section 3. In the case of prescribed particle density, velocity, and energy density, we obtain the quantum Maxwellian

$$M[w] = \mathrm{Exp}\Big(A(x,t) - \frac{|p - v(x,t)|^2}{2T(x,t)}\Big), \tag{19}$$

where A, v, and T are determined by the moments of w. This Maxwellian is taken as the thermal equilibrium state in the quantum hydrodynamic equations (see Sections 4 and 5). Finally, prescribing zeroth- and second-order moments, one obtains the quantum Maxwellian $M[w] = \mathrm{Exp}(A - |p|^2/(2T))$, used in the derivation of the quantum energy-transport equations. Since this model is not well understood, we do not explain its derivation and refer to [52, 53, 91] for details. A simplified quantum energy-transport model was derived recently from the quantum hydrodynamic equations and analyzed in [102]. A quantum-corrected energy-transport model (using the quantum drift-diffusion approach) was numerically investigated in [40, 41].

The quantum Maxwellian is a nonlocal function on the phase space. It can be made more explicit when expanding it in terms of the scaled Planck constant ε, which appears in the definition of the Wigner transform. We state only a result for the quantum Maxwellian with prescribed particle density (see [98] for a proof).

L e m m a 2.3 (Expansion of the quantum Maxwellian). *The following expansions holds*

$$\mathrm{Exp}\left(A - \frac{|p|^2}{2}\right) = \exp\left(A - \frac{|p|^2}{2}\right)\Big[1 + \frac{\varepsilon^2}{8}\Big(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top \nabla^2 A p\Big)\Big] + O(\varepsilon^4),$$

where $\nabla^2 A$ denotes the Hessian of A.

This expansion corresponds to the equilibrium function found by Wigner [143]. We remark that in the classical limit $\varepsilon \to 0$, the above quantum equilibrium reduces to $f_{\mathrm{eq}} = \exp(A - |p|^2/2)$. In the unconstrained case, we find that $f_{\mathrm{eq}} = \exp(V - |p|^2/2)$, which is consistent with classical kinetic theory.

2.4 - *Wigner-Boltzmann equations*

In Section 2.2, we have considered ballistic and hence reversible quantum transport. When the characteristic length of the quantum system is larger than the mean free path of the particles, scattering effects have to be taken into account. Scattering may occur between the particles and between the particles and a background. For instance, in semiconductors, one may encounter electron-electron collisions, scattering of the electrons with the quantized vibrations of the semiconductor crystal (phonons) or with the doping atoms (ionized impurity

collisions). Inspired from classical kinetic theory, scattering may be modeled by an appropriate collision operator $Q(w)$, which is added to the Wigner equation, leading to the *Wigner-Boltzmann equation*

$$\partial_t w + p \cdot \nabla_x w + \theta[V]w = Q(w), \quad x, p \in \mathbb{R}^3,\ t > 0. \tag{20}$$

Although there does not exist a complete theory of quantum scattering, many approaches have been studied in the (physical) literature, see [17, 127] for references. In contrast to classical kinetic models, quantum collision operators are typically nonlocal in time. The Levinson equation at time t, for instance, includes an integral over the time interval $[0, t]$ [11, 113]. For simplicity, we present in the following *local* collision operators which are employed in numerical simulations of the Wigner equation.

2.4.1 - `Wigner-BGK model`

A simple phenomenological model for the particle-background or, in semiconductors, electron-phonon interactions is given by the relaxation-time BGK-type operator

$$Q(w) = \frac{1}{\tau}(w_{\rm eq} - w), \tag{21}$$

where $w_{\rm eq}$ is some equilibrium state and $\tau > 0$ is the relaxation time which may depend on the energy. It is reasonable to assume that the collision operator satifies some collisional invariants. For instance, we expect that collisions preserve the total mass of the system, $\langle Q(w)\rangle = 0$. More generally, let Q satisfy, for some weight functions $\kappa = (\kappa_0, \ldots, \kappa_N)$,

$$\langle \kappa_j(p) Q(w)\rangle = \int_{\mathbb{R}^3} \kappa_j(p) Q(w) \frac{dp}{(2\pi\varepsilon)^3} = 0.$$

By definition of $Q(w)$, this implies that $w_{\rm eq}$ and w have the same moments. In Section 2.3, we have introduced a quantum equilibrium state $M[w]$, which has the same moments as a given Wigner function w. Thus, we may set

$$w_{\rm eq} = M[w] = \mathrm{Exp}(\lambda \cdot \kappa).$$

Clearly, the BGK-type operator vanishes if and only if the Wigner function equals the quantum Maxwellian $M[w]$.

2.4.2 - `Wigner-Fokker-Planck model`

Considering an electron ensemble which interacts dissipatively with an idealized heat bath, consisting of an ensemble of harmonic oscillators, Caldeira and Leggett [30] and Diósi [57] derived the following collision operator

$$Q(w) = D_{pp}\Delta_p w + 2\gamma\, \mathrm{div}_p(pw),$$

where $D_{pp} > 0$ is some diffusion coefficient and $\gamma > 0$ is a friction parameter. The Wigner equation with the Caldeira-Leggett operator is also known under the name of *quantum Brownian motion* or *quantum Langevin equation* and it received large interest in the context of interaction between light and matter (see, e.g., [48]).

The Caldeira-Leggett scattering term does not satisfy the so-called Lindblad condition (see below) which is a generic condition for quantum systems to preserve complete positivity of the density matrix along the evolution (i.e. $\widehat{\rho}(0) \geq 0$ implies $\widehat{\rho}(t) \geq 0$ for all $t > 0$). Such a property has to be satisfied for a true quantum evolution. Thus the Wigner-Caldeira-Leggett equation is quantum mechanically not correct. The reason for this shortcoming comes from the inconsistency that the equation contains the temperature T, through its coefficients, but the $1/T \to 0$ limit was performed in [30] along the derivation of the model.

In [32], the approach of Caldeira and Leggett has been improved by deriving the following Fokker-Planck operator with finite temperature:

$$Q(w) = D_{pp}\Delta_p w + 2\gamma \operatorname{div}_p(pw) + D_{qq}\Delta_x w + 2D_{pq}\operatorname{div}_x(\nabla_p w), \tag{22}$$

where the nonnegative coefficients D_{pp}, D_{pq}, and D_{qq} constitute the phase-space diffusion matrix of the system, which is assumed to satisfy the Lindblad condition

$$D_{pp}D_{qq} - D_{pq}^2 \geq \frac{\gamma^2}{4}.$$

The coefficients D_{qq} and D_{pq} model quantum diffusion. The Wigner equation with this collision operator is called the *Wigner-Fokker-Planck equation* and it has been analyzed by Arnold, López, and co-workers in [7, 8, 31].

More generally, the interactions of the electron ensemble with the environment (called an open quantum system) can be described by the *Lindblad equation* or the *master equation in Lindblad form*

$$\mathrm{i}\varepsilon\partial_t\widehat{\rho} = \mathrm{i}J(\widehat{\rho}) := [H,\widehat{\rho}] + \mathrm{i}\sum_k \Big(L_k\widehat{\rho}L_k^* - \frac{1}{2}(L_k^*L_k\widehat{\rho} + \widehat{\rho}L_k^*L_k)\Big),$$

where H is some (quantum) Hamiltonian, L_k are (possibly countable many) so-called Lindblad operators, and L_k^* is the adjoint operator of L_k [6]. A solution $\widehat{\rho}$ is formally positivity preserving and the operator J is dissipative on the space of self-adjoint trace-class operators. Hence, the time evolution of $\widehat{\rho}$ is no longer reversible.

If all Lindblad operators vanish, we recover the Liouville-von Neumann equation (1). Setting $L_k = \alpha_k \cdot x + \beta_k \cdot \nabla_x$, the quantum Fokker-Planck term (22) can be written as a Lindblad equation [6].

3 - Quantum drift-diffusion models

In this section, we derive formally the nonlocal quantum drift-diffusion model. Expanding the quantum Maxwellian in terms of powers of ε^2, local model

equations are obtained. In the $O(\varepsilon^4)$ approximation (and neglecting pressure and electric force terms), we find the so-called *Derrida-Lebowitz-Speer-Spohn equation* [56], which is a parabolic equation with fourth-order derivatives. Furthermore, in the $O(\varepsilon^6)$ approximation, a sixth-order quantum diffusion equation is derived. These equations possess very interesting mathematical properties which we detail below.

3.1 - *Derivation*

The quantum drift-diffusion model is derived from the Wigner-Boltzmann equation (20) in the diffusion scaling with the BGK-type scattering operator (21). We follow here the derivation of Degond et al. in [53] (also see the reviews [54, 91]).

3.1.1 - `Nonlocal quantum drift-diffusion model`

Assuming that collisions conserve mass, the quantum Maxwellian in (21) reads as

$$w_{\rm eq} = M[w] = \mathrm{Exp}\Big(A - \frac{|p|^2}{2}\Big),$$

where the Lagrange multiplier A is determined through

$$\int_{\mathbb{R}^3} M[w]dp = \int_{\mathbb{R}^3} w dp.$$

We consider a diffusion scaling in the Wigner-Boltzmann equation (20), i. e., we replace the time t and $Q(w)$ by t/α and $Q(w)/\alpha$, respectively. Then (20) becomes

$$\alpha^2\partial_t w_\alpha + \alpha(p\cdot\nabla_x w_\alpha + \theta[V_\alpha]w_\alpha) = M[w_\alpha] - w_\alpha, \quad x,p\in\mathbb{R}^3,\ t>0, \tag{23}$$

with initial datum $w(\cdot,\cdot,0) = w_I$ in $\mathbb{R}^3\times\mathbb{R}^3$. The potential operator $\theta[V_\alpha]$ is defined in (13). The electric potential V_α is a solution of the Poisson equation (see (8))

$$\lambda_D^2\Delta V_\alpha = \langle w_\alpha\rangle - C(x) = \int_{\mathbb{R}^3}\frac{w dp}{(2\pi\varepsilon)^3} - C(x). \tag{24}$$

We wish to perform the formal limit $\alpha\to 0$. This limit is carried out in three steps, following [91, Section 12.2].

Step 1: limit in the Wigner-Boltzmann equation. The limit $\alpha\to 0$ in (23) leads to $M[w] = w$, where $w = \lim_{\alpha\to 0} w_\alpha$. The function $M[w]$ is the lowest-order approximation of w_α. In order to obtain more information for w_α, we make a Chapman-Enskog expansion.

Step 2: Chapman-Enskog expansion. We insert the expansion $w_\alpha = M[w_\alpha] + \alpha g_\alpha$ (which in fact defines the function g_α) into the collision operator. Then the

Wigner-Boltzmann equation (20) becomes

$$\alpha\partial_t w_\alpha + p\cdot\nabla_x w_\alpha + \theta[V]w_\alpha = \alpha^{-1}(M[w_\alpha]-w_\alpha) = -g_\alpha.$$

In the limit $\alpha\to 0$, this yields

$$g = -\big(p\cdot\nabla_x M[w] + \theta[V]M[w]\big). \tag{25}$$

Step 3: limit in the moment equation. The moment equations are generally obtained by multiplying the Wigner-Boltzmann equation by the weight functions and by integrating over the momentum space. In the present situation, the weight function is simply $\kappa(p)=1$, and the moment equation reads as

$$\partial_t\langle w_\alpha\rangle + \alpha^{-1}\operatorname{div}_x\langle pM[w_\alpha]\rangle + \operatorname{div}_x\langle pg_\alpha\rangle + \alpha^{-1}\langle\theta[V]w_\alpha\rangle = \alpha^{-2}\langle Q(w_\alpha)\rangle.$$

It can be verified that the function $p\mapsto pM[w_\alpha]$ is odd and hence, its integral over $\mathbb{R}^3$ vanishes. Furthermore, a computation shows that $\langle\theta[V]f\rangle = 0$ for all functions $f(p)$. Finally, by mass conservation, $\langle Q(w_\alpha)\rangle = 0$. Then the moment equation becomes

$$\partial_t\langle w_\alpha\rangle + \operatorname{div}_x\langle pg_\alpha\rangle = 0,$$

and the limit $\alpha\to 0$ gives, inserting (25),

$$\partial_t\langle w\rangle - \operatorname{div}_x\langle p(p\cdot\nabla_x w + \theta[V]w)\rangle = 0.$$

Since $\langle p\theta[V]w\rangle = -n\nabla_x V$, where $n=\langle w\rangle$, we infer that

$$\partial_t n - \operatorname{div}_x\big(\operatorname{div}_x\langle p\otimes pw\rangle - n\nabla_x V\big) = 0.$$

We have proved the following result.

T h e o r e m 3.1 (Nonlocal quantum drift-diffusion model). *Let (w_α, V_α) be a solution of the Wigner-Boltzmann-Poisson system* (23)-(24) *with initial datum $w_\alpha(\cdot,\cdot,0) = w_I$. Then, formally, $w_\alpha\to w$ and $V_\alpha\to V$ as $\alpha\to 0$, where $w(x,p,t) = \operatorname{Exp}(A(x,t)-|p|^2/2)$ and (A,V) is a solution of the* quantum drift-diffusion equations

$$\begin{aligned}&\partial_t n - \operatorname{div} J_n = 0,\quad J_n = \operatorname{div} P - n\nabla V,\quad \lambda_D^2\Delta V = n - C(x),\quad t>0,\\ &n(\cdot,0) = n_I \quad \text{in } \mathbb{R}^3,\end{aligned} \tag{26}$$

the particle density and quantum stress tensor are, respectively,

$$n = \int_{\mathbb{R}^3}\operatorname{Exp}\Big(A - \frac{|p|^2}{2}\Big)\frac{dp}{(2\pi\varepsilon)^3}, \tag{27}$$

$$P = \int_{\mathbb{R}^3} p\otimes p\operatorname{Exp}\Big(A - \frac{|p|^2}{2}\Big)\frac{dp}{(2\pi\varepsilon)^3}, \tag{28}$$

where the matrix $p\otimes p$ consists of the elements $(p\otimes p)_{j\ell} = p_j p_\ell$, and the initial datum is given by $n_I = \langle w_I\rangle$.

The quantum stress tensor is a nonlocal operator involving the Lagrange multiplier A which relates to the particle density n through (27). It is shown in [53] that $\nabla P = n\nabla A$ and hence, the quantum drift-diffusion model can be written equivalently as

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = n\nabla(A - V). \tag{29}$$

A local model is obtained by expanding the quantum Maxwellian up to terms of order $O(\varepsilon^{2n})$ for $n \in \mathbb{N}$. This is detailed in the following subsection.

3.1.2 - Local quantum drift-diffusion model

We derive local versions of the quantum drift-diffusion model from the previous subsection, in particular the $O(\varepsilon^4)$ and $O(\varepsilon^6)$ approximations.

T h e o r e m 3.2 (Local quantum drift-diffusion model). *Let (n, J_n, V) be a solution of the nonlocal quantum drift-diffusion equations* (26). *Then, formally, $J_n = J + O(\varepsilon^4)$ and (n, J, V) solves the (local)* quantum drift-diffusion equations

$$\partial_t n - \operatorname{div} J = 0, \quad J = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big), \tag{30}$$

$$\lambda_D^2 \Delta V = n - C(x), \quad n(\cdot, 0) = n_I \quad \text{in } \mathbb{R}^3,\ t > 0. \tag{31}$$

For the proof of this theorem, we need the following elementary integral identities:

$$\begin{aligned} \int_{\mathbb{R}^3} e^{-|p|^2/2} dp &= (2\pi)^{3/2}, \\ \int_{\mathbb{R}^3} p_j p_\ell e^{-|p|^2/2} dp &= (2\pi)^{3/2}\delta_{j\ell}, \\ \int_{\mathbb{R}^3} p_j p_\ell p_m p_n e^{-|p|^2/2} dp &= (2\pi)^{3/2}(\delta_{j\ell}\delta_{mn} + \delta_{jm}\delta_{\ell n} + \delta_{jn}\delta_{\ell m}), \end{aligned} \tag{32}$$

where $\delta_{j\ell}$ denotes the Kronecker delta. In the following, we only sketch the proof and refer to the proof of Theorem 12.11 in [91] for details of the computations.

P r o o f. *(of Theorem 3.2.)* We need to expand the electron density and the stress tensor in powers of ε^2. By Lemma 2.3, the $O(\varepsilon^4)$-expansion of the quantum Maxwellian is given by

$$\begin{aligned} \operatorname{Exp}\Big(A - \frac{|p|^2}{2}\Big) = \exp\Big(A - \frac{|p|^2}{2}\Big)\Big[1 + \frac{\varepsilon^2}{8}\Big(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top \nabla^2 A p\Big)\Big] \\ + O(\varepsilon^4). \end{aligned}$$

Thus, using (32), the electron density $n = \langle \operatorname{Exp}(A - |p|^2/2)\rangle$ can be expanded

as follows:

$$
\begin{aligned}
n &= e^A\Big(1+\frac{\varepsilon^2}{8}\Big(\Delta A+\frac{1}{3}|\nabla A|^2\Big)\Big)\langle e^{-|p|^2/2}\rangle \\
&\quad -\frac{\varepsilon^2}{24}e^A\sum_{j,\ell=1}^{3}\frac{\partial^2 A}{\partial x_j\partial x_\ell}\langle p_jp_\ell e^{-|p|^2/2}\rangle+O(\varepsilon^4) \\
&= (2\pi\varepsilon^2)^{-3/2}e^A\Big(1+\frac{\varepsilon^2}{12}\Big(\Delta A+\frac{1}{2}|\nabla A|^2\Big)\Big)+O(\varepsilon^4). \qquad (33)
\end{aligned}
$$

Next, we develop the quantum stress tensor P in powers of ε^2. By its definition (28) and by (32),

$$
\begin{aligned}
P_{j\ell} &= e^A\Big(1+\frac{\varepsilon^2}{8}\Big(\Delta A+\frac{1}{3}|\nabla A|^2\Big)\Big)\langle p_jp_\ell e^{-|p|^2/2}\rangle \\
&\quad -\frac{\varepsilon^2}{24}\sum_{m,n=1}^{3}\frac{\partial^2 A}{\partial x_m\partial x_n}\langle p_jp_\ell p_mp_n e^{-|p|^2/2}\rangle+O(\varepsilon^4) \\
&= (2\pi\varepsilon^2)^{-3/2}e^A\Big(1+\frac{\varepsilon^2}{12}\Big(\Delta A+\frac{1}{2}|\nabla A|^2\Big)\Big)\delta_{j\ell} \\
&\quad -\frac{\varepsilon^2}{12}\,\frac{e^A}{(2\pi\varepsilon^2)^{3/2}}\,\frac{\partial^2 A}{\partial x_j\partial x_\ell}+O(\varepsilon^4).
\end{aligned}
$$

The $O(\varepsilon^4)$-expansion (33) leads to

$$
P_{j\ell}=n\delta_{j\ell}-\frac{\varepsilon^2}{12}\,n\frac{\partial^2 A}{\partial x_j\partial x_\ell}+O(\varepsilon^4).
$$

Differentiating the $O(\varepsilon^2)$-expansion of n with respect to x, we arrive at $\nabla n = n\nabla A+O(\varepsilon^2)$. Hence, after some computations,

$$
(\operatorname{div}P)_j=\sum_{\ell=1}^{3}\frac{\partial P_{j\ell}}{\partial x_\ell}=\frac{\partial n}{\partial x_j}-\frac{\varepsilon^2}{12}\sum_{\ell=1}^{3}n\frac{\partial}{\partial x_j}\left(\frac{1}{2}\Big(\frac{\partial A}{\partial x_\ell}\Big)^2+\frac{\partial^2 A}{\partial x_\ell^2}\right)+O(\varepsilon^4).
$$

In vector form, this reads as

$$
\operatorname{div}P=\nabla n-\frac{\varepsilon^2}{12}n\nabla\Big(\Delta A+\frac{1}{2}|\nabla A|^2\Big)+O(\varepsilon^4).
$$

It remains to express A in terms of n. We already noticed that $\nabla A = \nabla n/n+O(\varepsilon^2)$ from which we conclude that

$$
\begin{aligned}
\Delta A+\frac{1}{2}|\nabla A|^2 &= \frac{\Delta n}{n}-\frac{|\nabla n|^2}{n^2}+\frac{1}{2}\Big|\frac{\nabla n}{n}\Big|^2+O(\varepsilon^2) \\
&= \frac{\Delta n}{n}-\frac{|\nabla n|^2}{2n^2}+O(\varepsilon^2)=2\,\frac{\Delta\sqrt{n}}{\sqrt{n}}+O(\varepsilon^2). \qquad (34)
\end{aligned}
$$

Therefore,

$$J_n = \operatorname{div} P - n\nabla V = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) + O(\varepsilon^4),$$

and the conclusion follows. □

Expanding the quantum Maxwellian up to order $O(\varepsilon^{2n})$, quantum diffusion equations of order $2n$ can be derived. Above we have treated the case $n = 2$. In [25], the case $n = 3$ was carried out. The crucial step is to determine an $O(\varepsilon^6)$ approximation of $\mathrm{Exp}(a)$ with $a(x, p; t) = A(x, t) - |p|^2/2$. To this end, we follow the strategy proposed in [53]. The idea is to define $F(z) = \mathrm{Exp}(za)$ and to expand $F(z)$ formally as a series in ε, i.e. $F(z) = \sum_{k=0}^{\infty} \varepsilon^k F_k(z)$. The functions $F_k(z)$ can be computed by pseudo-differential calculus. For odd indices k, we have $F_k(z) = 0$, and for even indices, we have to solve the differential equation

$$\frac{dF_k}{dz}(z) = a \circ_0 F_k(z) + a \circ_2 F_{k-2}(z) + \cdots + a \circ_k F_0(z), \quad z > 0, \tag{35}$$

with initial condition $F_k(0) = \delta_{k0}$. The multiplication $\circ_n$ is defined as a sum of partial derivatives of order n (see the appendix of [25]). The sixth-order quantum diffusion equation is obtained by solving (35) for $k = 4$. It turns out that $F_0(1) = e^a$ and that (35) can be written as

$$\frac{dF_k}{dz}(z) = aF_k(z) + e^{za} P_k(z, p, A), \quad F_k(0) = 0,$$

where $P_k(z, p, A)$ is a multivariate polynomial in z and p and contains spatial derivatives of A up to order k. This linear differential equation can be easily solved, and $F_k(1)$ $(k = 0, 2, 4)$ gives the $O(\varepsilon^{k+2})$ approximation of the quantum Maxwellian $\mathrm{Exp}(a)$.

It remains to represent the density n as a function of A. Inserting the expressions for $F_k(1)$, we obtain

$$n = \int_{\mathbb{R}^3} \mathrm{Exp}(a) \frac{dp}{(2\pi\varepsilon)^3} = \int_{\mathbb{R}^3} \big(F_0(1) + \varepsilon^2 F_2(1) + \varepsilon^4 F_4(1)\big) \frac{dp}{(2\pi\varepsilon)^3} + O(\varepsilon^6).$$

After integration, the density can be written as the sum $G_0(A) + \varepsilon^2 G_2(A) + \varepsilon^4 G_4(A) + O(\varepsilon^6)$. To derive an ε-approximation of A in terms of n, we insert the ansatz $A = A_0 + \varepsilon^2 A_2 + \varepsilon^4 A_4 + O(\varepsilon^6)$ in the above expression for n and equate equal powers of ε. The resulting system of equations can be solved for A_k leading to

$$A_0 = \log((2\pi)^{3/2} n), \quad A_2 = -\frac{1}{6} \frac{\Delta\sqrt{n}}{\sqrt{n}},$$
$$A_4 = \frac{1}{360}\Big(\frac{1}{2}|\nabla^2 \log n|^2 + \frac{1}{n}\nabla^2 : (n\nabla^2 \log n)\Big).$$

Here, ∇^2 denotes the Hessian matrix and the double points in $A : B$ signify summation over both indices of the matrices A and B. The sixth-order model is obtained by inserting the approximations A_k into the formulation (29),

$$\partial_t n - \operatorname{div}(n\nabla(A - V)) = 0,$$

which gives the following result [25, Appendix].

T h e o r e m 3.3 (Sixth-order local quantum drift-diffusion model). *In the $O(\varepsilon^6)$ approximation, the nonlocal quantum drift-diffusion equation* (26) *can be written as follows:*

$$\partial_t n = \operatorname{div}\left(\nabla n - \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) + \frac{\varepsilon^4}{360} n\nabla\Big(\frac{1}{2}|\nabla^2 \log n|^2 + \frac{1}{n}\nabla^2 : (n\nabla^2 \log n)\Big)\right),$$

where $|\nabla^2 \log n|$ is the matrix norm of the Hessian of $\log n$.

3.2 - *Analysis of the fourth-order equation*

In this subsection, we present some analytical results on the quantum drift-diffusion model (30)-(31) and related equations.

3.2.1 - `Existence of global solutions`

The main difficulty of the mathematical analysis of the initial-value problem (30)-(31) is due to the fourth-order differential term $\operatorname{div}(n\nabla(n^{-1/2}\Delta n^{1/2}))$. Indeed, there is generally no maximum principle available for fourth-order equation, which would allow one to conclude positivity preservation and a priori estimates. Consequently, one has to rely on suitable regularization techniques and energy-type a priori estimates. The latter, however, is difficult to obtain because of the highly nonlinear structure of the equation. We remark that similar difficulties appear in the study of the thin-film equation

$$\partial_t u + \operatorname{div}(u^\alpha \nabla\Delta u) = 0, \quad u(\cdot, t) = u_0 \geq 0,$$

for which preservation of positivity strongly depends on the exponent $\alpha > 0$; see [15] for details.

The first existence result for the simplified equation (obtained from (30) by neglecting the second-order diffusion and electric force and by setting $\varepsilon^2/6 = 1$)

$$\partial_t n + \operatorname{div}\left(n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\right) = 0, \quad n(\cdot, t) = n_0 \geq 0 \quad \text{in } \mathbb{T}^d,\ t > 0, \tag{36}$$

where $\mathbb{T}^d$ is the d-dimensional torus, is due to Bleher et al. [18]. This equation is called the Derrida-Lebowitz-Speer-Spohn or DLSS equation in [97] since it

has been first derived in [56] by these authors. The result of [18] provides the existence and uniqueness of local-in-time classical solutions of (36) for strictly positive initial data from $W^{1,p}(\mathbb{T}^d)$ with $p > d$. The proof is based on semigroup theory applied to the formulation

$$2\partial_t(\sqrt{n}) + \Delta^2\sqrt{n} - \frac{(\Delta\sqrt{n})^2}{\sqrt{n}} = 0,$$

which is equivalent to (36) as long as n remains bounded away from zero. Lacking suitable a priori estimates, existence was proven only locally in time. In one spatial dimension, global existence of solutions can be related to strict positivity: if a classical solution breaks down at $t = t^*$, then the limit profile $\lim_{t\to t^*_-} n(x,t)$ is an element of H^1 but vanishes at some point $x \in \mathbb{T}$.

This observation has motivated the study of nonnegative weak solutions instead of positive classical solutions. The first global existence result was proven in [105] and later generalized in [80]. The DLSS equation (36) was considered on the interval $(0,1) \subset \mathbb{R}$ with physically motivated boundary conditions

$$n(0,t) = n_1, \quad n(1,t) = n_2, \quad n_x(0,t) = m_1, \quad n_x(1,t) = m_2, \quad t > 0. \tag{37}$$

Global existence was proven in the class of functions with finite (generalized) entropy

$$E_0(n) = \int_0^1 (n - \log n)dx.$$

The following result corresponds to Theorem 1.2 in [80].

T h e o r e m 3.4 (Existence for the one-dimensional DLSS equation). *Let n_1, $n_2 > 0$ and m_1, $m_2 \in \mathbb{R}$. Let $n_0 \geq 0$ be an integrable function satisfying $E_0(n_0) < \infty$. Then there exists a weak solution n of (36)-(37) satisfying $n(x,t) \geq 0$ in $(0,1)\times(0,\infty)$ and*

$$n \in W^{1,10/9}_{\rm loc}(0,\infty;H^{-2}(0,1)) \cap L^{5/2}_{\rm loc}(0,\infty;W^{1,1}(0,1)),$$
$$\log n \in L^2_{\rm loc}(0,\infty;H^2(0,1)).$$

To explain the key ideas of the proof, we simplify by assuming $n_1 = n_2 = 1$, $m_1 = m_2 = 0$; see [80] for the general case. A formal computation shows that

$$\frac{dE_0}{dt} + \int_0^1 \Big((\log n)^2_{xx} + \frac{8}{3}\frac{n_x^4}{n^4}\Big)dx = 0. \tag{38}$$

This estimate as well as the equivalent formulation of (36),

$$\partial_t n + \frac{1}{2}(n(\log n)_{xx})_{xx} = 0,$$

motivates to employ $y = \log n$ as a new variable. Theorem 3.4 is proved by the following strategy. First, the equation $\partial_t(e^y) + \frac{1}{2}(e^y y_{xx})_{xx} = 0$ is discretized

in time by the backward Euler scheme with approximation parameter $\tau > 0$, which provides a sequence of elliptic equations. The Leray-Schauder fixed-point theorem yields the existence of a weak solution $y_\tau \in H^2(0,1)$. The compactness of the fixed-point operator follows from the uniform H^2 bounds obtained from a discrete variant of the entropy dissipation identity (38). This variant also provides estimates for y_τ independent of τ, and compactness (Aubin's lemma) allows one to extract a subsequence of $n_\tau = \exp(y_\tau)$ strongly converging to a weak solution to (36)-(37).

This technique was used by Chen et al. [45] to prove the global-in-time existence of weak solutions supposing Dirichlet boundary conditions on the particle density, quantum Fermi potential (see (47) below), and electric potential.

The restriction to one space dimension in Theorem 3.4 is essential since E_0 is seemingly not a Lyapunov functional in higher dimensions.

For the multidimensional equation (36) on a domain $\Omega \subset \mathbb{R}^d$, global existence of weak solutions was obtained only recently by two different methods [76, 97]. Whereas the framework of the first approach is that of mass transportation theory, the second approach extends the fixed-point argument used in the proof of Theorem 3.4. Both proofs, however, rely at a crucial point on a compactness argument, i.e., a consequence of the estimate

$$\frac{dE_1}{dt} + c\int_\Omega n|\nabla^2 \log n|^2 dx \le 0, \tag{39}$$

where $|\nabla^2 \log n|$ is the euclidean norm of the Hessian of $\log n$,

$$E_1(n) = \int_\Omega n(\log n - 1)dx \tag{40}$$

is the physical entropy and $c > 0$ is some constant. This inequality is shown for $\Omega = \mathbb{T}^d$ or $\Omega = \mathbb{R}^d$ since this avoids boundary integrals. It follows that E_1 is a Lyapunov functional but, lacking a lower bound on n, the above inequality does not yield an H^2 estimate for $\log n$. However, it is possible to show that

$$\int_\Omega n|\nabla^2 \log n|^2 dx \ge \kappa \int_\Omega |\nabla^2 \sqrt{n}|^2 dx, \tag{41}$$

where $\kappa = 4(4d-1)/(d(d+2))$ if $\Omega = \mathbb{T}^d$ [97]. The proof is based on the method of systematic integration by parts developed in [96] to one-dimensional functions and extended in [25] for radially symmetric functions. Inequality (41) leads to an H^2 bound for $\sqrt{n}$. This motivates to rewrite the nonlinearity in (36) in terms of $\sqrt{n}$ giving

$$\partial_t n + \nabla^2 : \big(\sqrt{n}\nabla^2\sqrt{n} - \nabla\sqrt{n}\otimes\nabla\sqrt{n}\big) = 0$$

or, more explicitly, with the notation $\partial_i = \partial/\partial x_i$ etc.,

$$\partial_t n + \sum_{i,j=1}^d \partial_{ij}^2\big(\sqrt{n}\partial_{ij}^2\sqrt{n} - \partial_i\sqrt{n}\partial_j\sqrt{n}\big) = 0. \tag{42}$$

The key idea in the paper [76] of Gianazza et al. is the observation that (36) constitutes the gradient flow of the so-called Fisher information

$$F(n) = \int_\Omega |\nabla \sqrt{n}|^2 dx$$

with respect to the Wasserstein metric. Then, the above estimates are used to prove that the subdifferential of the Fisher information is closed. Employing deep results from mass transportation theory [2], this eventually provides the existence of a global solution of (36) with the natural regularity $\sqrt{n} \in L^2_{\rm loc}(0,\infty;H^2(\Omega))$, where Ω may be the whole space $\mathbb{R}^d$ or a bounded domain equipped with variational boundary conditions.

The ideas in [97] are more elementary and straight-forward. As in the one-dimensional case, (36) is written in logarithmic form, discretized in time by the backward Euler scheme, and additionally regularized by a bi-Laplacian,

$$\partial_t^\tau n_\varepsilon + \frac{1}{2}\nabla^2 : \big(n_\varepsilon \nabla^2 \log n_\varepsilon\big) + \varepsilon(\Delta^2 \log n_\varepsilon + n_\varepsilon) = 0 \quad \text{in } \Omega = \mathbb{T}^d.$$

Here, ∂_t^h is the discrete time derivative with time step $\tau > 0$. The regularization is needed to ensure the existence of solutions of the linearized elliptic problem for $y_\varepsilon = \log n_\varepsilon$ in the space $H^2(\mathbb{T}^d)$ via the Lax-Milgram lemma. A variant of (39) together with (41) provides an a priori estimate for $\sqrt{n_\varepsilon}$ in $H^2(\mathbb{T}^d)$ uniform in ε and τ. Moreover, thanks to the elliptic regularization, we obtain an estimate for $\log n_\varepsilon$ in $H^2(\mathbb{T}^d)$ (*not* uniform in ε) and hence, by Sobolev embedding, in $L^\infty(\mathbb{T}^d)$ for $d \le 3$. This shows that n_ε is strictly positive in $\mathbb{T}^d$, which justifies all formal calculations. The uniform bounds allow one to apply compactness (Aubin's lemma) and to pass to the limits $\varepsilon \to 0$ and $\tau \to 0$, yielding the existence of a global solution of (42) on the torus $\mathbb{T}^d$. The precise result is as follows (see Theorem 1.1 in [97]).

T h e o r e m 3.5 (Existence for the multidimensional DLSS equation). *Let $d \le 3$ and let n_0 be a nonnegative measurable function on $\mathbb{T}^d$ with finite entropy $E_1(n_0) < \infty$ (see (40)). Then there exists a weak solution n of (42) satisfying $n(\cdot,t) \ge 0$ on $\mathbb{T}^d$ for $t \ge 0$,*

$$n \in W^{1,11/10}_{\rm loc}(0,\infty;H^{-2}(\mathbb{T}^d)), \quad \sqrt{n} \in L^2_{\rm loc}(0,\infty;H^2(\mathbb{T}^d)),$$

and the initial data is satisfied in the sense of $L^1_{\rm loc}(0,\infty;H^{-2}(\mathbb{T}^d))$.

The theorem is valid in the physically relevant dimensions $d \le 3$. This restriction is related to the lack of certain Sobolev embeddings in higher dimensions $d \ge 4$. Most prominently, the fixed-point argument exploits the continuous embedding $H^2(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ to conclude absolute boundedness of $y_\varepsilon = \log n_\varepsilon$ and hence strict positivity of $n_\varepsilon = \exp(y_\varepsilon)$. We have chosen periodic boundary conditions in order to avoid boundary integrals.

Based on the above ideas, Chen [42] proved the existence of global solutions of the quantum drift-diffusion system

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big), \tag{43}$$

$$\lambda_D^2 \Delta V = n - C(x), \quad n(\cdot,0) = n_0 \quad \text{in } \mathbb{T}^d,\ t > 0. \tag{44}$$

We recall that n is the electron density, J_n the electron current density, V the electric potential, $C(x)$ the given doping profile (see (8)), and the given parameters are the scaled Planck constant ε and the Debye length λ_D.

T h e o r e m 3.6 (Existence for the quantum drift-diffusion model). *Let $d \le 3$, $C \in L^\infty(\Omega)$, and let n_0 be a nonnegative measurable function such that*

$$E_1(n_0) < \infty \quad \textit{and} \quad \int_{\mathbb{T}^d} n_0 dx = \int_{\mathbb{T}^d} C(x)dx$$

(see (40) for the definition of E_1). Then there exists a weak solution (n, V) of (42) and (44) satisfying $n \ge 0$ and

$$n \in W^{1,8/7}_{\rm loc}(0,\infty; H^{-2}(\mathbb{T}^d)), \quad \sqrt{n} \in L^2_{\rm loc}(0,\infty; H^2(\mathbb{T}^d)),$$
$$V \in L^2_{\rm loc}(0,\infty; H^2(\mathbb{T}^d)), \quad \int_{\mathbb{T}^d} V dx = 0, \quad \int_{\mathbb{T}^d} n dx = \int_{\mathbb{T}^d} C(x)dx.$$

The proof uses the following identity:

$$\frac{dE_1}{dt} + \int_{\mathbb{T}^d} \Big(\frac{\varepsilon^2}{12} n|\nabla^2 \log n|^2 + 4|\nabla\sqrt{n}|^2\Big)dx = -\lambda_D^{-2}\int_{\mathbb{T}^d} n(n - C(x))dx. \tag{45}$$

Since the right-hand side is bounded and (41) holds, we obtain uniform H^2 bounds for $\sqrt{n}$ and uniform L^2 estimates for n. Then, the Poisson equation implies uniform H^2 bounds for V. These key estimates and the Gagliardo-Nirenberg inequality lead to further uniform estimates needed to achieve compactness results.

The paper [106] shows the stability and, in one space dimension, the convergence of a positivity-preserving semi-discrete scheme for the quantum drift-diffusion model.

3.2.2 - Long-time behavior of solutions

Several papers have been concerned with the analysis of the long-time behavior of solutions n of the DLSS equation (36) with unit mass. As an example, let us consider (36) on the torus. The essential tool to derive a priori estimates needed for the long-time decay are the so-called *relative entropies*, as introduced in [9],

$$E_\alpha(n_1|n_2) = \int_{\mathbb{T}^d} \phi_\alpha\Big(\frac{n_1}{n_2}\Big) n_2 dx,$$

where n_1 and n_2 are nonnegative functions on $\mathbb{T}^d$ with unit mean value, and ϕ_α is given by

$$\phi_\alpha(s) = \frac{1}{\alpha(\alpha-1)}\big(s^\alpha - \alpha s + \alpha - 1\big), \quad s \geq 0,$$

where $\alpha \neq 0, 1$. The natural continuation for $\alpha = 1$ is $\phi_1(s) = s(\log s - 1) + 1$; the functional E_1 corresponds to the physical entropy (40). The functional E_α is nonnegative and vanishes if and only if $n_1 = n_2$. To obtain a priori estimates (and decay rates), we consider entropies of solutions $n_1 = n$ relative to the spatial homogeneous steady state $n_2 = 1$:

$$E_\alpha(n) = \frac{1}{\alpha(\alpha-1)}\left(\int_{\mathbb{T}^d} n^\alpha dx - 1\right), \quad \alpha \geq 1.$$

Then a formal computation shows that

$$\frac{dE_\alpha}{dt} = -\frac{1}{\alpha - 1}\sum_{i,j=1}^d \int_{\mathbb{T}^d} n\partial_{ij}^2(\log n)\partial_{ij}^2(n^{\alpha-1})dx,$$

where $\partial_{ij}^2 = \partial^2/\partial x_i \partial x_j$. By an inequality similar to (41) (see Lemma 2.2 in [97]), we find that the right-hand side can be estimated, up to a factor, by the integral over $(\Delta n^{\alpha/2})^2$, which gives

$$\frac{dE_\alpha}{dt} + \kappa_\alpha \int_{\mathbb{T}^d} (\Delta n^{\alpha/2})^2 dx \leq 0,$$

for some constant $\kappa_\alpha > 0$. To conclude decay to equilibrium, we need to relate the entropy production $\int_{\mathbb{T}^d}(\Delta n^{\alpha/2})^2 dx$ to the entropy E_α. This is done by applying the generalized convex Sobolev inequality [97, Lemma 2.5]

$$\frac{p}{p-1}\left(\int_{\mathbb{T}^d} f^2 dx - \left(\int_{\mathbb{T}^d} f^{2/p} dx\right)^p\right) \leq \frac{1}{8\pi^4}\int_{\mathbb{T}^d} (\Delta f)^2 dx, \tag{46}$$

valid for all nonnegative functions $f \in H^2(\mathbb{T}^d)$ and $1 < p \leq 2$, to $f = n^{\alpha/2}$ and $p = \alpha$. Then, taking into account that n has unit mass, we find that

$$\frac{dE_\alpha}{dt} + 8\pi^4\alpha^2\kappa_\alpha E_\alpha \leq 0,$$

and Gronwall's lemma implies that $t \mapsto E_\alpha(n(\cdot,t))$ decays exponentially with rate $8\pi^4\alpha^2\kappa_\alpha$. By the Csiszár-Kullback inequality [49, 112], the solution decays exponentially in the L^1 norm with half rate:

$$\|n(\cdot,t) - 1\|_{L^1(\mathbb{T}^d)} \leq (2E_1(n_0))^{1/2} e^{-4\pi^2\kappa_1 t}, \quad t \geq 0.$$

Notice that, as remarked in [58] for the one-dimensional equation, this global decay rate for E_1 coincides with the decay rate of the linearized equation and thus, it is optimal.

Decay rates were also shown for the functionals

$$F_\alpha(n) = \int_{\mathbb{T}^d} |\nabla n^{\alpha/2}|^2 dx, \quad F_0(n) = \int_{\mathbb{T}^d} |\nabla \log n|^2 dx, \quad \alpha > 0.$$

The first decay result is due to [29], where exponential decay of F_0 was shown under a smallness condition of F_0. Exponential convergence of the Fisher information F_1 along weak solutions was obtained in [58]. It was observed in [96] that actually all functionals F_α with $\frac{2}{53}(25 - 6\sqrt{10}) < \alpha < \frac{2}{53}(25 + 6\sqrt{10})$ are nonincreasing along smooth solutions. This observation was rigorously proven for weak solutions in [109].

The long-time decay of solutions of the one-dimensional DLSS equation with homogeneous Neumann boundary data and constant Dirichlet data was shown in [105] without rate and in [108] with exponential rate. For nonconstant boundary conditions, the steady state n_∞ is no longer spatially homogeneous. It was proved in [80] that this steady state is exponentially attracting in terms of the relative entropy under the additional assumption that $\log n_\infty$ is concave. In several space dimensions, a very general result on the long-time behavior of the DLSS equation was proved in [76].

The asymptotic behavior of solutions of the quantum drift-diffusion model can be analyzed similarly as for the DLSS equation by combining the results for the DLSS equation and the drift-diffusion model. For instance, for the one-dimensional system with constant doping profile, Chen et al. [46] showed, by using the methods of [58], that the electron density converges exponentially fast to the constant steady state. The multidimensional case was considered in [47].

3.2.3 - The stationary equations

The stationary quantum drift-diffusion model corresponding to (43)-(44) has been studied by Ben Abadallah and Unterreiter [14]. They considered the system of equations on a bounded domain and imposed physically relevant mixed Dirichlet-Neumann boundary conditions. The equations are written in terms of the generalized Fermi potential

$$F = V + \log n - \frac{\varepsilon^2}{6} \frac{\Delta\sqrt{n}}{\sqrt{n}}, \tag{47}$$

which can be interpreted as an elliptic second-order equation for $\sqrt{n}$, coupled to the divergence equation

$$0 = \operatorname{div} J_n = \operatorname{div}(n\nabla F).$$

The advantage of this formulation is that the maximum principle can be applied to the last equation, yielding L^∞ bounds for F. Then, using fixed-point arguments and a minimization procedure of the free energy functional, the existence of bounded weak solutions was proved in [14]. The authors also tackled the case of vanishing particle density at the Dirichlet boundary. Interestingly, the

density is positive in the whole domain although it may vanish at the boundary. Chen and Guan [39] used the techniques of [14] to simplify the step proceeding from the minimizer property to the Euler-Lagrange property of weak solution.

The question of the uniqueness of solutions was left open in [14] and has been answered in [136]. More precisely, it has been shown that the solution is unique for sufficiently small applied biasing voltages. This is in analogy to the results for the classical drift-diffusion equations for which it is known that there may exist multiple steady states.

The stationary quantum drift-diffusion model was employed to simulate strong inversion layers near the gate of MOS (metal-oxide-semiconductor) transistors [3] (also see the discussion in [10]). Scientists developed Gummel-type iteration schemes [27, 50, 51, 136], finite-element approximations [134, 135], finite-volume discretizations [33, 131], and high-resolution slope-limiter schemes [132]. A hybrid quantum drift-diffusion Schrödinger-Poisson model was numerically solved in [63]. The model has been also used to calculate current-voltage characteristics of resonant tunneling diodes, which have the characteristic feature that the current density may decrease with increasing applied voltage in a certain region (the so-called region of negative resistance). This feature allows for the construction of ultrafast oscillators. It seems, however, that the quantum drift-diffusion model is less suited for that application since negative resistance effects occur numerically at very low lattice temperature and for modified effective masses only. Finally, we notice that an optimal control problem was analyzed in [142] to optimize the shape of the quantum barriers in the diode.

3.2.4 - Asymptotic limits

In the quantum drift-diffusion model (43)-(44),

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n \nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big), \tag{48}$$

$$\lambda_D^2 \Delta V = n - C(x), \quad n(\cdot,0) = n_0 \quad \text{in } \Omega,\ t > 0, \tag{49}$$

there are two scaled parameters, the Planck constant ε and the Debye length λ_D. In certain physical regimes, these parameters may be very small compared to one, and one may ask if the limits $\varepsilon \to 0$ or $\lambda_D \to 0$ can be performed rigorously, leading to simpler models. In fact, when we perform formally the *semiclassical limit* $\varepsilon \to 0$, we obtain the semiclassical drift-diffusion model

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V, \quad \text{in } \Omega,\ t > 0, \tag{50}$$

with the Poisson equation and initial condition (49). The limit $\lambda_D \to 0$ in (44) would lead to the equation $n - C(x) = 0$ which is less interesting. The so-called *quasineutral limit* $\lambda_D \to 0$ makes more sense in the bipolar model, in which a quantum drift-diffusion equation for the hole density p is added,

$$\partial_t p - \operatorname{div} J_p = 0, \quad J_p = \nabla p + p\nabla V - \frac{\varepsilon^2}{6} p \nabla\Big(\frac{\Delta\sqrt{p}}{\sqrt{p}}\Big), \tag{51}$$

and the Poisson equation is replaced by

$$\lambda_D^2 \Delta V = n - p - C(x). \tag{52}$$

If $C(x) = 0$, the limit $\lambda_D \to 0$ gives formally $n = p$ and hence, by adding the equations for n and p, the drift terms vanish:

$$\partial_t n + \operatorname{div}\left(\frac{\varepsilon^2}{6} n \nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) - \nabla n\right) = 0.$$

We first review some results on the semiclassical limit. The entropy estimate (45) provides an H^1 bound for $\sqrt{n}$ which is independent of the scaled Planck constant ε. This observation was used by Chen [42] to prove the semiclassical limit $\varepsilon \to 0$ for the solutions $(n_\varepsilon, V_\varepsilon)$ of (43)-(44). In fact, this bound is essential to apply the Aubin lemma showing that (n_ε) converges strongly to n in some Lebesgue space and that (V_ε) converges strongly to V in some space. Moreover, using the Gagliardo-Nirenberg inequality, Chen showed that the uniform gradient bound on $\sqrt{n_\varepsilon}$ implies that $\varepsilon^{7/4} n_\varepsilon \nabla^2 \log n_\varepsilon$ is uniformly bounded in $L^{8/7}(0,T;L^2(\mathbb{T}^d))$, for any $T > 0$. Since $7/4 < 2$, we infer that

$$\varepsilon^2 n_\varepsilon \nabla^2 \log n_\varepsilon \to 0 \quad \text{strongly in } L^{8/7}(0,T;L^2(\mathbb{T}^d)).$$

The limit function (n, V) satisfies the drift-diffusion model (50) in $\Omega = \mathbb{T}^d$.

The semiclassical limit has been studied in the literature for several variants of the model, considering the bipolar model, replacing the pressure term ∇n by an isentropic pressure $\nabla(n^\beta)$ with $\beta > 1$, or imposing homogeneous Neumann boundary conditions. The proofs, however, are based on the above described ideas, and we refer to [37, 38, 43, 86, 87, 88] for details.

The quasineutral limit $\lambda_D \to 0$ in (48), (51), and (52) was performed rigorously in [110] for the one-dimensional equations in the interval $x \in (0,1)$ with the boundary data

$$n = p = 1, \quad n_x = p_x = 0, \quad V = V_D \quad \text{for } x \in \{0,1\},\ t > 0.$$

The idea of the proof is to employ the entropy $E_0(n) = \int_0^1 (n - \log n) dx$, which provides λ_D-uniform bounds for $\log n$ and $\log p$ in $L^2(0,T;H^2(0,1))$ for any $T > 0$ (compare to (38)). The physical entropy $E_1(n,p) = \int_0^1 (n(\log n - 1) + p(\log p - 1)) dx$ gives the additional bounds

$$\|n - p\|_{L^2(\Omega\times(0,T))} \le c\lambda_D, \quad \|V_x\|_{L^2(\Omega\times(0,T))} \le c\lambda_D^{-1},$$

where $c > 0$ is some constant independent of λ_D. This shows that $n - p$ converges to zero, as expected. However, the estimates are not sufficient to pass to the limit $\lambda_D \to 0$ since we cannot control the drift term $(n-p)V_x$, which is uniformly bounded in $L^2(\Omega \times (0,T))$ but does not converge to zero. The key idea is to derive the estimates

$$\|\sqrt{n} - \sqrt{p}\|_{L^2(\Omega\times(0,T))} \le c\lambda_D, \quad \|(\sqrt{n} + \sqrt{p})V_x\|_{L^2(\Omega\times(0,T))} \le c\lambda^{-8/9}.$$

The first bound is a consequence of the estimate using the entropy E_0. The proof of the second bound is more delicate. It follows from an estimate of the electric energy $\lambda_D^2\int_0^1(V-W)_x^2dx$, where W satisfies the boundary data of V up to first order, i.e., $W=V$ and $W_x=V_x$ for $x\in\{0,1\}$. The exponent $8/9$ is related to the exponents of the Gagliardo-Nirenberg inequality.

The quasineutral limit in the multidimensional model was studied by Chen and Chen [44]. They impose a fast-time scaling and analyze the initial-time layer problem. The limit equations are the bipolar drift equations without diffusion.

3.3 - *Analysis of the sixth-order equation*

The analysis of the sixth-order equation from Theorem 3.3 in the d-dimensional torus,

$$\partial_t n = \operatorname{div}\left(n\nabla\Big(\frac{1}{2}|\nabla^2\log n|^2+\frac{1}{n}\nabla^2:(n\nabla^2\log n)\Big)\right), \quad x\in\mathbb{T}^d,\ t>0, \tag{53}$$

$$n(\cdot,0)=n_0\ge 0, \quad x\in\mathbb{T}^d, \tag{54}$$

is very involved due to the highly nonlinear structure of the sixth-order operator. (Notice that we have neglected the second- and fourth-order diffusions from the model in Theorem 3.3 and that we have set $\varepsilon^2/360=1$. These simplifications are not essential but simplify the presentation.) Moreover, it is not clear how to prove the nonnegativity of the particle density, which is expected physically.

These difficulties can be overcome by extending the tools employed in the analysis of the fourth-order DLSS equation. The first tool is to employ exponential and power variables $n=u^4=e^y$ and to write equation (53) first in terms of y:

$$\partial_t(e^y)=\nabla^3:(e^y\nabla^3 y)+2\nabla^2:(e^y(\nabla^2 y)^2), \tag{55}$$

where $\nabla^3 y$ is the tensor of all third-order derivatives of y and $A:B$ means summation over all indices of the tensors A and B. The advantage of this formulation is that it provides a symmetric structure in the sixth-order differential operator for the variable y, which is useful to apply the Lax-Milgram lemma to the linearization in the fixed-point argument. Moreover, when $y\in H^3(\mathbb{T}^d)\hookrightarrow L^\infty(\mathbb{T}^d)$ $(d<6)$ is a weak solution to (55), the particle density $n=e^y$ becomes strictly positive. This overcomes the lack of the maximum principle.

The second tool is based on entropy estimates from the physical entropy $E_1(n)=\int_{\mathbb{T}^d}n(\log n-1)dx$ (see (40)):

$$\frac{dE_1}{dt}+\int_{\mathbb{T}^d}n\big(|\nabla^3\log n|^2-2(\nabla^2\log n)^2:\nabla^2\log n\big)dx=0.$$

Extending the method of systematic integration by parts [96], we are able to prove that the entropy production is bounded from below by positive expressions

involving derivatives of n:

$$-\frac{dE_1}{dt} = \int_{\mathbb{T}^d} n\big(|\nabla^3 \log n|^2 - 2(\nabla^2 \log n)^2 : \nabla^2 \log n\big)dx$$
$$\geq c\int_{\mathbb{T}^d} \big(|\nabla^3\sqrt{n}|^2 + |\nabla^2\sqrt[4]{n}\nabla\sqrt[4]{n}|^2 + |\nabla\sqrt[6]{n}|^6\big)dx, \tag{56}$$

for some constant $c > 0$ which only depends on the dimension d. The proof of the above inequality is rather technical; see [25] for details. Similar as for the DLSS equation, this motivates us to write the nonlinearity in terms of $u = \sqrt[4]{n}$, giving

$$\begin{aligned}\partial_t n = {}& 8\nabla^3 : \big(\sqrt{n}\nabla^3\sqrt{n} + 4\sqrt[4]{n}\nabla\sqrt[4]{n}\otimes\nabla\sqrt[4]{n}\otimes\nabla\sqrt[4]{n}\big) - 6\Delta\nabla^2 : (\sqrt{n}\nabla^2\sqrt{n})\\ &+ 8\nabla^2 : \big((\nabla^2\sqrt{n})^2 - 8\nabla^2\sqrt{n}(\nabla\sqrt[4]{n}\otimes\nabla\sqrt[4]{n})\\ &+ 16|\nabla\sqrt[4]{n}|^2\nabla\sqrt[4]{n}\otimes\nabla\sqrt[4]{n}\big).\end{aligned} \tag{57}$$

With these tools, the steps of the existence proof are as follows. First, we semi-discretize (55) in time by the backward Euler scheme, regularized by a tri-Laplacian,

$$\begin{aligned}\partial_t^\tau n_\varepsilon = {}& \nabla^3 : (n_\varepsilon\nabla^3 y_\varepsilon) + 32\nabla^2 : \big(\sqrt{n_\varepsilon}(\nabla^2\sqrt{n_\varepsilon})^2\\ &- 2\sqrt[4]{n_\varepsilon}\nabla^2\sqrt[4]{n_\varepsilon}(\nabla\sqrt[4]{n_\varepsilon}\otimes\nabla\sqrt[4]{n_\varepsilon}) + |\nabla\sqrt[4]{n_\varepsilon}|^2\nabla\sqrt[4]{n_\varepsilon}\otimes\nabla\sqrt[4]{n_\varepsilon}\big)\\ &+ \varepsilon(\Delta^3 y_\varepsilon - y_\varepsilon) \quad \text{in } \mathbb{T}^d,\end{aligned}$$

where $n_\varepsilon = \exp(y_\varepsilon)$, $\varepsilon > 0$, and ∂_t^τ is the discrete time derivative with time step $\tau > 0$. The regularization is needed to guarantee coercivity of the right-hand side with respect to y_ε. The existence of solutions y_ε is obtained from the Leray-Schauder fixed-point theorem. Compactness of the fixed-point operator is a consequence of a variant of the entropy estimate (56) with additional ε-dependent bounds for y_ε in $H^3(\mathbb{T}^d)$. Since the entropy estimates for $\sqrt{n_\varepsilon}$ and $\sqrt[4]{n_\varepsilon}$ are independent of ε and τ, we can pass to the limit $\varepsilon\to 0$ and then $\tau\to 0$, yielding the existence of a global solution of (53) on the torus.

There is a technical difficulty in the limit $\varepsilon\to 0$ (and similarly, $\tau\to 0$). Since (n_ε) is bounded in $H^3(\mathbb{T}^d)$ and $W^{1,6}(\mathbb{T}^d)$, we infer by compactness that, as $\varepsilon\to 0$, up to subsequences,

$$\sqrt{n_\varepsilon}\to\sqrt{n} \quad \text{strongly in } H^2(\mathbb{T}^d), \quad \sqrt[6]{n_\varepsilon}\rightharpoonup\sqrt[6]{n} \quad \text{weakly in } W^{1,6}(\mathbb{T}^d).$$

The difficulty now is to pass to the limit in, for instance, the sequence $\sqrt[4]{n_\varepsilon}\nabla\sqrt[4]{n_\varepsilon}\otimes\nabla\sqrt[4]{n_\varepsilon}\otimes\nabla\sqrt[4]{n_\varepsilon}$ and to identify its (weak) limit. This is done by applying the following result, which is a consequence of Theorem 5.4.4 in [2], proved in [101, Appendix]: Let (u_ε) be a sequence of positive functions such that

$$u_\varepsilon^\alpha\to u^\alpha \quad \text{strongly in } W^{1,p}(\mathbb{T}^d), \quad (u_\varepsilon^\beta) \text{ is bounded in } W^{1,q}(\mathbb{T}^d).$$

Then, if $0<\beta<\gamma<\alpha<\infty$, $1<p,q,r<\infty$, and $\alpha p=\beta q=\gamma r$,

$$u_\varepsilon^\gamma\to u^\gamma \quad \text{strongly in } W^{1,r}(\mathbb{T}^d).$$

The assumptions are satisfied for $u_\varepsilon = \sqrt[4]{n_\varepsilon}$, $\alpha = 2$, $\beta = 2/3$, $\gamma = 1$, and $p = 2$, $q = 6$, $r = 4$, and we conclude that

$$\nabla \sqrt[4]{n_\varepsilon} \to \nabla \sqrt[4]{n} \quad \text{strongly in } L^4(\mathbb{T}^d).$$

This implies that

$$\sqrt[4]{n_\varepsilon} \nabla \sqrt[4]{n_\varepsilon} \otimes \nabla \sqrt[4]{n_\varepsilon} \otimes \nabla \sqrt[4]{n_\varepsilon} \to \sqrt[4]{n} \nabla \sqrt[4]{n} \otimes \nabla \sqrt[4]{n} \otimes \nabla \sqrt[4]{n}$$

strongly in $L^1(\mathbb{T}^d)$. The existence result reads as follows (see Theorem 2 in [26]).

T h e o r e m 3.7 (Existence for the sixth-order equation). *Let $d \le 3$ and let n_0 be a nonnegative measurable function with finite entropy $E_1(n_0) < \infty$. Then there exists a weak solution $n \ge 0$ of (54) and (57) satisfying*

$$n \in W^{1,6/5}_{\rm loc}(0,\infty; H^{-3}(\mathbb{T}^d)), \quad \sqrt{n} \in L^2_{\rm loc}(0,\infty; H^3(\mathbb{T}^d)),$$
$$\sqrt[4]{n} \in L^4_{\rm loc}(0,\infty; W^{1,4}(\mathbb{T}^d)), \quad \sqrt[6]{n} \in L^6_{\rm loc}(0,\infty; W^{1,6}(\mathbb{T}^d)).$$

Equations (54) and (57) are satisfied in the sense of $L^{6/5}_{\rm loc}(0,\infty; H^{-3}(\mathbb{T}^d))$.

We notice that in [26] also the exponential decay of weak solutions was shown. Indeed, by an extension of the convex Sobolev inequality (46), we can relate the entropy production $\int_{\mathbb{T}^d} |\nabla^3 \sqrt{n}|^2 dx$ by the entropy $E_1(n)$, and we infer from (56) an inequality of the type $dE_1/dt + \kappa E_1 \le 0$ for some $\kappa > 0$. Then, Gronwall's lemma implies that $E_1(n(\cdot,t)) \le E_1(n_0)\exp(-\kappa t)$ for $t > 0$.

3.4 - *Analysis of the nonlocal equation*

While the existence theory for the fourth-order and sixth-order quantum diffusion equations is rather well developed, there are up to now no complete existence results for the nonlocal quantum drift-diffusion equation (26). In this subsection, we review a partial result due to Gallego and Méhats [68] who proved that the time-discretized model with no-flux boundary conditions possesses a solution.

According to (29), the nonlocal quantum model can be written as

$$\partial_t n = \operatorname{div}(n\nabla(A - V)), \quad \lambda_D^2 \Delta V = n,$$
$$n = \int_\Omega \operatorname{Exp}\Big(A - \frac{|p|^2}{2}\Big)\frac{dp}{(2\pi\varepsilon)^3} \quad \text{in } \Omega,\ t > 0,$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary. The equations are complemented by initial and no-flux boundary conditions

$$\nabla(A - V)\cdot\nu = 0, \quad V = 0 \quad \text{on } \partial\Omega,\ t > 0, \quad n(\cdot,0) = n_0 \quad \text{in } \Omega, \tag{58}$$

where ν denotes the exterior normal unit vector to the boundary $\partial\Omega$.

The relation between the electron density n and the chemical potential A can be formulated in a weak sense as [68, (2.4)]

$$\int_\Omega n\phi dx = \mathrm{Tr}(\exp(-H)\phi),$$

where "Tr" is the trace of an operator and $H = -(\varepsilon^2/2)\Delta + A$ is the Hamiltonian with domain $D(H) = \{\psi \in H^2(\Omega) : \nabla\psi\cdot\nu = 0 \text{ on } \partial\Omega\}$. Hence, if A belongs to, say, $L^2(\Omega)$, there exists an orthogonal basis of eigenfunctions $(\psi_p) = (\psi_p[A])$ with eigenvalues $\lambda_p = \lambda_p[A]$, and the nonlocal relation between $n = n[A]$ and A takes the more explicit form

$$n[A] = \sum_{p=1}^\infty e^{-\lambda_p[A]}|\psi_p[A]|^2.$$

It is proved in [68, Lemma 2.3] that the mapping $H^1(\Omega)\to\mathbb{R}$, $A\mapsto\int_\Omega n[A]dx$ is Fréchet differentiable and strictly convex.

The existence result holds for the semi-discrete model

$$\frac{1}{\tau}(n^{k+1}-n^k) = \mathrm{div}(n^k\nabla(A^{k+1}-V^{k+1})), \quad \lambda_D^2\Delta V^{k+1} = n^{k+1}, \tag{59}$$

$$n^{k+1} = \sum_{p=1}^\infty \exp(-\lambda_p[A^{k+1}])|\psi_p[A^{k+1}]|^2 \quad \text{in } \Omega \tag{60}$$

subject to the boundary conditions in (58), where n^k is a given function. The main result is as follows (Theorem 3.1 in [68]).

T h e o r e m 3.8 (Existence for the semi-dicrete nonlocal equation). *Let n_0 be continuous and positive on $\overline{\Omega}$. Then there exists a unique solution $(n^k, A^k, V^k) \in C^0(\overline{\Omega})\times H^2(\Omega)\times H^2(\Omega)$ of (58)-(60). Moreover, the total charge is conserved,*

$$\int_\Omega n^k dx = \int_\Omega n_0 dx \quad \textit{for all } k\in\mathbb{N},$$

and the free energy

$$S^k = \int_\Omega \Big(- n^k(A^k+1) + \frac{\lambda_D^2}{2}|\nabla V|^2\Big)dx$$

is nonincreasing in k.

The proof is inspired by the variational arguments of Nier [128, 129]. First, for given positive and continuous n^k, the variational arguments lead to a solution (A^{k+1}, V^{k+1}) to the elliptic system (59) with no-flux boundary conditions. By the above result on the mapping $A\mapsto n[A]$, we can define $n^{k+1} = n[A^{k+1}]$, and (60) is satisfied. The choice of the Neumann boundary conditions for the eigenfunctions ψ_p ensures that ψ_1^{k+1} does not vanish on $\overline{\Omega}$. Consequently, n^{k+1} is strictly positive (and continuous). Thus, the sequence (n^k, A^k, V^k) can be constructed by induction.

The limit of vanishing time steps $\tau \to 0$ is an open problem. One of the difficulties is to find a positive lower bound for the particle density. Furthermore, for a practical use of the model, boundary conditions which allow for a current flow through the boundary would be desirable, but it is not clear how to handle more physical boundary conditions in the existence analysis.

4 - Viscous quantum hydrodynamic models

In this section, we derive quantum hydrodynamic equations from the Schrödinger or Wigner equation. Viscous quantum hydrodynamic models are obtained from the Wigner-Fokker-Planck equation by the moment method. We sketch the derivations and summarize some analytical results for these equations.

4.1 - *Derivation*

We consider first the derivation starting from the Schrödinger equation via the so-called Madelung transform and then, we present the derivation from the Wigner equation.

4.1.1 - `Quantum hydrodynamics and the Schrödinger equation`

Quantum hydrodynamic models are well known since the early years of quantum mechanics. In fact, Madelung [123] showed already in 1927 that there exists a hydrodynamic formulation of the Schrödinger equation. More precisely, let ψ be a solution of the initial-value problem

$$\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi - V(x,t)\psi, \quad t>0, \quad \psi(\cdot,0) = \sqrt{n_0}\exp(\mathrm{i}S_0/\varepsilon) \quad \text{in } \mathbb{R}^3,$$

where the potential $V(x,t)$ is assumed to be given. Then $n = |\psi|^2$ and $J_n = -\varepsilon\mathrm{Im}(\overline{\psi}\nabla\psi)$ solves the *zero-temperature quantum hydrodynamic* or *Madelung equations*

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t J_n - \operatorname{div}\Big(\frac{J_n\otimes J_n}{n}\Big) + n\nabla V + \frac{\varepsilon^2}{2}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = 0, \tag{61}$$

$$n(\cdot,0) = n_0, \quad J_n(\cdot,0) = J_0 \quad \text{in } \mathbb{R}^3, \tag{62}$$

where the initial data is given by $n_0 = |\psi_0|^2$ and $J_0 = -n_0\nabla S_0$, as long as $n>0$ in $\mathbb{R}^3$. Here, "$\mathrm{Im}\, z$" denotes the imaginary part of a complex number z and $\overline{z}$ is its complex conjugate. This result can be shown by decomposing the wave function ψ as $\psi = \sqrt{n}\exp(\mathrm{i}S/\varepsilon)$, which is possible as long as $|\psi|>0$, by inserting this decomposition into the Schrödinger equation and taking the real and imaginary parts.

The above system is the quantum analogue of the classical pressureless Euler equations of fluid dynamics. The expression $\Delta\sqrt{n}/\sqrt{n}$ in the momentum equation in (61) can be interpreted as a quantum self-potential or *Bohm potential*. The quantum hydrodynamic equations are employed in Bohmian mechanics [144] and in the modeling of superfluids and Bose-Einstein condensates [28].

There is clearly a problem with the above decomposition if vacuum occurs, i.e. if $|\psi| = 0$ locally. In this situation, the phase S is not well defined which manifests in the fact that the Bohm potential may become singular at vacuum points. A study of these vacuum points in the quantum hydrodynamic equations was performed in El et al. [62]. The problem can be circumvented by using the polar decomposition of an arbitrary wave function ψ into its amplitude $\sqrt{n} = |\psi|$ and its unitary factor ϕ such that $\psi = \sqrt{n}\phi$ in the spirit of Brenier [19]. This idea has been exploited by Antonelli and Marcati [4] to analyze the quantum hydrodynamic equations (see Section 4.2.3).

The above model is derived for a single particle and therefore, it does not contain pressure or temperature terms. In order to include such terms, we consider an electron ensemble representing a mixed quantum state (see Theorem 2.1). In the following, we proceed as in [91, Chapter 14]. We recall that a mixed state is a sequence of occupation probabilities $\lambda_k \geq 0$ ($k \in \mathbb{N}$) for the k-th state ψ_k which is described by the single-state Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi_k = -\frac{\varepsilon^2}{2}\Delta\psi_k - V(x,t)\psi_k, \quad t > 0, \quad \psi_k(\cdot,0) = \psi_k^0 \quad \text{in } \mathbb{R}^3. \tag{63}$$

The single-state particle and current densities of the k-th state are defined as above by

$$n_k = |\psi_k|^2, \quad J_k = -\varepsilon\mathrm{Im}(\overline{\psi}_k\nabla\psi_k), \quad k \in \mathbb{N}.$$

Then the following result holds (see [75] or Theorem 14.2 in [91]).

T h e o r e m 4.1 (Quantum hydrodynamic equations). *Let ψ_k be a single-state solution of the Schrödinger equation* (63) *with occupation number λ_k of the k-th quantum state. Then (n, J), defined by*

$$n = \sum_{k=1}^\infty \lambda_k|\psi_k|^2, \quad J = \sum_{k=1}^\infty \lambda_k J_k,$$

is a solution of the quantum hydrodynamic equations

$$\partial_t n - \operatorname{div} J = 0,$$
$$\partial_t J - \operatorname{div}\Big(\frac{J\otimes J}{n} + n\theta\Big) + n\nabla V + \frac{\varepsilon^2}{2}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = 0,$$

where $x \in \mathbb{R}^3$ and $t > 0$, with initial conditions

$$n(\cdot,0) = \sum_{k=1}^\infty \lambda_k|\psi_k^0|^2, \quad J(\cdot,0) = -\varepsilon\sum_{k=1}^\infty \lambda_k\,\mathrm{Im}(\overline{\psi}_k^0\nabla\psi_k^0) \quad \text{in } \mathbb{R}^3.$$

The temperature tensor θ is defined by $\theta = \theta_{\rm cu} + \theta_{\rm os}$, where the "current temperature" and "osmotic temperature" are given by, respectively,

$$\theta_{\rm cu} = \sum_{k=1}^\infty \lambda_k \frac{n_k}{n}(u_{{\rm cu},k} - u_{\rm cu}) \otimes (u_{{\rm cu},k} - u_{\rm cu}),$$
$$\theta_{\rm os} = \sum_{k=1}^\infty \lambda_k \frac{n_k}{n}(u_{{\rm os},k} - u_{\rm os}) \otimes (u_{{\rm os},k} - u_{\rm os}),$$

and the variables

$$u_{{\rm cu},k} = -\frac{J_k}{n_k}, \quad u_{\rm cu} = -\frac{J}{n}, \quad u_{{\rm os},k} = \frac{\varepsilon}{2}\nabla \log n_k, \quad u_{\rm os} = \frac{\varepsilon}{2}\nabla \log n$$

are called the "current velocities" and "osmotic velocities", respectively.

The notion "osmotic" comes from the fact that the quantum term can be written as the divergence of the quantum stress tensor [75] $P = (\varepsilon^2/4)n\nabla^2 \log n$ since

$$\frac{\varepsilon^2}{2} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = \frac{\varepsilon^2}{4}\,{\rm div}(n\nabla^2 \log n).$$

Often, the above system is self-consistently coupled to the Poisson equation

$$\lambda_D^2 \Delta V = n - C(x) \quad \text{in } \mathbb{R}^3. \tag{64}$$

P r o o f. We follow the proof given in [91, Section 14.2]. The pair (n_k, J_k) solves the Madelung equations (61) with initial conditions

$$n_k(\cdot,0) = |\psi_k^0|^2, \quad J_k(\cdot,0) = -\varepsilon\,{\rm Im}(\overline{\psi}_k^0 \nabla\psi_k^0).$$

Multiplication of (61) by λ_k and summation over k yields

$$\partial_t n - {\rm div}\, J = 0,$$
$$\partial_t J - \sum_{k=1}^\infty \lambda_k\,{\rm div}\Big(\frac{J_k \otimes J_k}{n_k}\Big) + n\nabla V + \frac{\varepsilon^2}{2}\sum_{k=1}^\infty \lambda_k n_k \nabla\Big(\frac{\Delta\sqrt{n_k}}{\sqrt{n_k}}\Big) = 0. \tag{65}$$

We rewrite the second and fourth term of the second equation. With the definitions of the "current temperature" and "current velocity", we obtain

$$\begin{aligned}
\sum_{k=1}^\infty \lambda_k\,{\rm div}\Big(\frac{J_k \otimes J_k}{n_k}\Big) &= \sum_{k=1}^\infty \lambda_k\,{\rm div}(n_k u_{{\rm cu},k} \otimes u_{{\rm cu},k}) \\
&= \sum_{k=1}^\infty \lambda_k\,{\rm div}\big(n_k(u_{{\rm cu},k} - u_{\rm cu}) \otimes (u_{{\rm cu},k} - u_{\rm cu}) + 2n_k u_{{\rm cu},k} \otimes u_{\rm cu}\big) \\
&\quad - {\rm div}(nu_{\rm cu} \otimes u_{\rm cu}) \\
&= {\rm div}(n\theta_{\rm cu}) + 2\sum_{k=1}^\infty {\rm div}\Big(\lambda_k J_k \otimes \frac{J}{n}\Big) - {\rm div}\Big(\frac{J \otimes J}{n}\Big) \\
&= {\rm div}(n\theta_{\rm cu}) + {\rm div}\Big(\frac{J \otimes J}{n}\Big).
\end{aligned}$$

Furthermore, employing the definitions of the "osmotic temperature" and "osmotic velocity", we compute

$$\begin{aligned}
\frac{\varepsilon^2}{2}\sum_{k=1}^{\infty}\lambda_k n_k\nabla\Big(\frac{\Delta\sqrt{n_k}}{\sqrt{n_k}}\Big) &= \frac{\varepsilon^2}{4}\sum_{k=1}^{\infty}\lambda_k\,\mathrm{div}\,\Big(\nabla^2 n_k - \frac{\nabla n_k\otimes\nabla n_k}{n_k}\Big)\\
&= \frac{\varepsilon^2}{4}\sum_{k=1}^{\infty}\lambda_k\,\mathrm{div}\,\Big(\nabla^2 n_k + \frac{n_k}{n}\,\frac{\nabla n\otimes\nabla n}{n} - 2\frac{\nabla n\otimes\nabla n_k}{n}\\
&\quad - n_k\Big(\frac{\nabla n_k}{n_k}-\frac{\nabla n}{n}\Big)\otimes\Big(\frac{\nabla n_k}{n_k}-\frac{\nabla n}{n}\Big)\Big)\\
&= \frac{\varepsilon^2}{4}\,\mathrm{div}\,\Big(\nabla^2 n - \frac{\nabla n\otimes\nabla n}{n}\Big) - \mathrm{div}(n\theta_{\mathrm{os}})\\
&= \frac{\varepsilon^2}{2}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) - \mathrm{div}(n\theta_{\mathrm{os}}).
\end{aligned}$$

Inserting these expressions into (65) finishes the proof. □

The temperature tensor θ cannot be expressed in terms of the total particle and current densities without further assumptions. This is called a closure problem. Motivated by closure conditions in classical kinetic theory, one may assume that the temperature tensor is diagonal with equal entries on the diagonal, $\theta = T\,\mathbb{I}$, where $\mathbb{I}$ is the identity matrix. Then we obtain $\mathrm{div}(n\theta) = \nabla(nT)$ which corresponds to the pressure term in classical gas dynamics. We notice that this so-called isothermal model was first proposed by Grubin and Kreskovsky in the context of semiconductor modeling [77]. Furthermore, motivated by isentropic fluid dynamics where the temperature depends on the particle density, one may employ the closure $\theta = T(n)\,\mathbb{I}$ with $T(n) = n^{\beta-1}$ $(\beta > 1)$ leading to the pressure force $\mathrm{div}(n\theta) = \nabla(n^\beta)$. Another assumption to close the above quantum hydrodynamic system was proposed by Grasser et al. using small temperature and small scaled Planck constant asymptotics [74].

4.1.2 - `Quantum hydrodynamics and the Wigner equation`

The quantum hydrodynamic models of the previous section do not include collisional phenomena. In order to allow for such effects and to derive diffusive quantum fluid models, an alternative approach to derive macroscopic equations is to apply the moment model to a collisional Wigner equation:

$$\partial_t w + p\cdot\nabla_x w + \theta[V]w = Q(w), \quad (x,p)\in\mathbb{R}^6,\ t>0,$$

with the initial conditions $w(x,p,0) = w_0(x,p)$. We refer to Section 2.4 for a discussion of Wigner-Boltzmann models. The following presentation is based on [55] and [98] (also see Section 14.3 of [91]).

We assume that the collision operator $Q(w)$ is the sum of two operators, Q_0 and Q_1. We suppose that collisions modeled by Q_0 conserve mass, momentum,

and energy,

$$\langle Q_0(w)\rangle := \int_{\mathbb{R}^3} Q_0(w)\kappa(p)\frac{dp}{(2\pi\varepsilon)^3} = 0, \quad \kappa(p) = \{1, p, \tfrac{1}{2}|p|^2\}, \tag{66}$$

while the operator Q_1 conserves mass only, $\langle Q_1(w)\rangle = 0$. Furthermore, we suppose that $Q_0(w) = 0$ implies that w equals the quantum Maxwellian which has the same mass, momentum, and energy as w, i.e. $w = M[w]$ and $M[w]$ is given by (19), $M[w] = \mathrm{Exp}(A - |p - v|^2/2T)$ for some Lagrange multipliers A, v, and T coming from the constrained entropy maximization (see Section 2.3). Let $\alpha > 0$ be the ratio of the mean free paths corresponding to Q_0 and Q_1, respectively. We assume that collisions described by Q_0 occur more frequently than those modeled by Q_1 such that $\alpha \ll 1$.

A slightly different strategy was employed by Romano in [137]. He supposes that the zeroth-order part of the collision operator is the same as the classical one and that the first-order contribution is in relaxation form which is of order $O(\varepsilon^2)$. The quantum equilibrium is obtained by unconstrained entropy maximization.

We employ a hydrodynamic scaling in the Wigner-Boltzmann equation, i.e. we replace x by x/α and t by t/α. Then the Wigner-Boltzmann equation becomes

$$\alpha\partial_t w + \alpha\big(p\cdot\nabla_x w + \theta[V]w\big) = Q_0(w) + \alpha Q_1(w). \tag{67}$$

The derivation of the quantum hydrodynamic equations is performed in two steps. Let w_α be a solution to (67) with initial datum $w_\alpha(\cdot,\cdot,0) = w_0$.

Step 1: limit in the Wigner-Boltzmann equation. The limit $\alpha \to 0$ in (67) leads to $Q_0(w) = 0$, where $w = \lim_{\alpha\to 0} w_\alpha$. The conditions on Q_0 imply that $w = M[w] = \mathrm{Exp}(A - |p - v|^2/2T)$.

Step 2: limit in the moment equations. Multiplying (67) by the weight functions $\kappa(p)$, integrating over $p \in \mathbb{R}^3$, and employing (66) yields the moment equations

$$\partial_t\langle\kappa(p)w_\alpha\rangle + \mathrm{div}_x\langle p\kappa(p)w_\alpha\rangle + \langle\kappa(p)\theta[V]w_\alpha\rangle = \langle\kappa(p)Q_1(w_\alpha)\rangle.$$

The formal limit $\alpha \to 0$ gives

$$\partial_t\langle\kappa(p)M[w]\rangle + \mathrm{div}_x\langle p\kappa(p)M[w]\rangle + \langle\kappa(p)\theta[V]M[w]\rangle = \langle\kappa(p)Q_1(M[w])\rangle.$$

The moments of the potential operator can be computed explicitly (see (13.6) and Lemma 13.2 in [91]):

$$\langle\theta[V]f\rangle = 0, \quad \langle p\theta[V]f\rangle = -\langle f\rangle\nabla_x V, \quad \langle\tfrac{1}{2}|p|^2\theta[V]f\rangle = -\langle pf\rangle\cdot\nabla_x V \tag{68}$$

for all functions $f(p)$. Defining the particle density n, current density J_n, and energy density ne, respectively, by

$$n = \langle M[w]\rangle, \quad J_n = -\langle pM[w]\rangle, \quad ne = \langle\tfrac{1}{2}|p|^2M[w]\rangle,$$

the moment equations can be written as

$$\begin{aligned}\partial_t n - \operatorname{div} J_n &= 0,\\ \partial_t J_n - \operatorname{div}\langle p\otimes pM[w]\rangle + n\nabla V &= -\langle pQ_1(M[w])\rangle,\\ \partial_t(ne) + \operatorname{div}\langle \tfrac{1}{2}|p|^2 pM[w]\rangle + J_n\cdot\nabla V &= \langle \tfrac{1}{2}|p|^2 Q_1(M[w])\rangle.\end{aligned}$$

The second-order and third-order moments can be reformulated by introducing the quantum stress tensor P and the quantum heat flux q by

$$P = \langle (p-u)\otimes(p-u)M[w]\rangle, \quad q = \langle \tfrac{1}{2}(p-u)|p-u|^2 M[w]\rangle, \tag{69}$$

where $u = -J_n/n$ is the mean velocity. Then we obtain

$$\langle p\otimes pM[w]\rangle = P + \frac{J_n\otimes J_n}{n}, \quad \langle \tfrac{1}{2}p|p|^2 M[w]\rangle = -(P+ne\,\mathbb{I})\frac{J_n}{n} + q, \tag{70}$$

where $\mathbb{I}$ is the identity matrix in $\mathbb{R}^{3\times 3}$. The result is summarized in the following theorem (see Theorem 14.3 in [91]).

T h e o r e m 4.2 (Nonlocal quantum hydrodynamic model). *Let the collision operator satisfy the above assumptions. Let w_α be a solution of the Wigner-Boltzmann equation* (67). *Then, formally, as $\alpha\to 0$, $w_\alpha\to w$ where $w = \operatorname{Exp}(A - |p-v|^2/2T)$, and (A,v,T) is a solution of the* quantum hydrodynamic equations

$$\partial_t n - \operatorname{div} J_n = 0, \tag{71}$$

$$\partial_t J_n - \operatorname{div}\Big(\frac{J_n\otimes J_n}{n} + P\Big) + n\nabla V = -\langle pQ_1(w)\rangle, \tag{72}$$

$$\partial_t(ne) - \operatorname{div}\big((P+ne\,\mathbb{I})J_n - q\big) + J_n\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle \tag{73}$$

in $\mathbb{R}^3$, $t>0$, where the quantum stress tensor P and quantum heat flux q are defined in (69). *The initial data are given by*

$$n(\cdot,0) = \langle w_0\rangle, \quad J_n(\cdot,0) = -\langle pw_0\rangle, \quad (ne)(\cdot,0) = \langle \tfrac{1}{2}|p|^2 w_0\rangle,$$

and the Lagrange multipliers (A,v,T) are determined by

$$\begin{pmatrix} n\\ nu\\ ne\end{pmatrix} = \int_{\mathbb{R}^3} \operatorname{Exp}\Big(A - \frac{|p-v|^2}{2T}\Big)\begin{pmatrix}1\\ p\\ \frac{1}{2}|p|^2\end{pmatrix}\frac{dp}{(2\pi\varepsilon)^3},$$

where $J_n = -nu$ is the current density.

Similar as in Section 3.1.1, we obtain local versions of the quantum hydrodynamic system by expanding the quantum Maxwellian in terms up to order $O(\varepsilon^4)$. If only one moment is prescribed, an expansion is presented in Lemma 2.3. In the present situation, the expansion is computationally much more laborious, and we refer to Lemmas 3.2 and 3.3 in [98] for details. Inserting the

expansion into the definition of the moments and assuming that the vorticity $\nabla u - \nabla u^\top$ and the temperature variations are of order $O(\varepsilon^2)$, i.e.

$$\nabla u - \nabla u^\top = O(\varepsilon^2) \quad \text{and} \quad \nabla \log T = O(\varepsilon^2), \tag{74}$$

we arrive at

$$\begin{aligned} n &= 2(2\pi\varepsilon^2)^{-3/2} e^A + \frac{\varepsilon^2}{12T}(2\pi\varepsilon^2)^{-3/2} e^A (2\Delta A + |\nabla A|^2) + O(\varepsilon^4), \\ ne &= \frac{3}{2} nT + \frac{1}{2} n|u|^2 - \frac{\varepsilon^2}{24} n\Delta \log n + O(\varepsilon^4). \end{aligned}$$

The quantum stress tensor and quantum heat flux can be expanded as follows (see [98, Lemma 3.5] and Section 2.2 in [103]):

$$\begin{aligned} P &= nT\,\mathbb{I} - \frac{\varepsilon^2}{12} n\nabla^2 \log n + O(\varepsilon^4), \\ q &= -\frac{\varepsilon^2}{24} n(\Delta u + 2\nabla \operatorname{div} u) + O(\varepsilon^4). \end{aligned}$$

This leads to the following local version of the quantum hydrodynamic equations (see Theorem 14.4 in [91]).

T h e o r e m 4.3 (Local quantum hydrodynamic model). *Let the assumptions of Theorem 4.2 and let* (74) *hold. Then the moments* (n, J_n, ne) *of the limit quantum Maxwellian solve the* quantum hydrodynamic equations *up to order* $O(\varepsilon^4)$,

$$\partial_t n - \operatorname{div} J_n = 0, \tag{75}$$

$$\partial_t J_n - \operatorname{div}\Big(\frac{J_n \otimes J_n}{n}\Big) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = W_p, \tag{76}$$

$$\partial_t(ne) - \operatorname{div}\big((P + ne\,\mathbb{I})u\big) - \frac{\varepsilon^2}{24}\operatorname{div}\big(n(\Delta u + 2\nabla \operatorname{div} u)\big) + J_n \cdot \nabla V = W_e, \tag{77}$$

where $x \in \mathbb{R}^3$, $t > 0$, $W_p = -\langle pQ_1(w)\rangle$, $W_e = \langle \frac{1}{2}|p|^2 Q_1(w)\rangle$, *and the energy density* ne *and the quantum stress tensor* P *are given by*

$$P = nT\,\mathbb{I} - \frac{\varepsilon^2}{12} n\nabla^2 \log n, \quad ne = \frac{3}{2} nT + \frac{1}{2} n|u|^2 - \frac{\varepsilon^2}{24} n\Delta \log n. \tag{78}$$

The initial conditions for n, J_n, *and* ne *are as in Theorem 4.2.*

The quantum stress tensor is the sum of the classical pressure and a quantum stress tensor. The energy is the sum of the thermal, kinetic, and quantum energy. In the classical limit $\varepsilon \to 0$, we recover the classical Euler equations. Notice that the coefficient in front of the Bohm potential term in the momentum equation (76) equals $\varepsilon^2/6$ instead of $\varepsilon^2/2$ as in the momentum equation derived

in Theorem 4.1 from the mixed-state Schrödinger equations. The factor 1/3 is independent of the space dimension.

For constant temperature, we obtain the isothermal quantum hydrodynamic model which equals the model of Theorem 4.1 when the temperature tensor is a scalar and the factor $\varepsilon^2/2$ is changed to $\varepsilon^2/6$. Nonconstant temperatures in quantum hydrodynamics were first considered by Ferry and Zhou [66], who derived the model from the Bloch equation for the density matrix. A derivation from the Wigner equation was proposed by Gardner [72]. He obtained the same equations as in Theorem 4.3 except the dispersive velocity term coming from div q. The origin of this difference lies in the different choice of the quantum equilibrium. In order to explain this difference, let w_{eq} be the quantum equilibrium derived from the *unconstrained* entropy maximization process, given by (16),

$$w_{\mathrm{eq}}(x,p) = \mathrm{Exp}\Big(V(x) - \frac{|p|^2}{2}\Big) = e^{V(x)-|p|^2/2}\big(1+\varepsilon^2 g_1(x,p)\big) + O(\varepsilon^4),$$

where g_1 is an appropriate function which we do not specify here. Gardner mimicks the momentum-shift of the equilibrium in the classical situation and employs in his derivation the "shifted" quantum Maxwellian

$$\widetilde{w}_{\mathrm{eq}}(x,p) = \exp\Big((V(x) - \frac{|p-v(x)|^2}{2T(x)}\Big)\big(1+\varepsilon^2 g_1(x,p-v(x))\big) + O(\varepsilon^4).$$

On the other hand, the derivation of the quantum system in Theorem 4.3 employs the *constrained* thermal equilibrium (19),

$$\begin{aligned} M[w] &= \mathrm{Exp}\Big(A(x) - \frac{|p-v(x)|^2}{2T(x)}\Big) \\ &= \exp\Big(A(x) - \frac{|p-v(x)|^2}{2T(x)}\Big)\big(1+\varepsilon^2 g_2(x,p-v(x))\big) + O(\varepsilon^4). \end{aligned}$$

If only one moment is prescribed, both approaches coincide in the following sense. We write Gardner's momentum-shifted quantum Maxwellian more explicitly as [98, Section 3.5]

$$\widetilde{w}_{\mathrm{eq}}(x,p) = e^{V/T-|p|^2/2T}\left(1+\frac{\varepsilon^2}{8T}\Big(\Delta V + \frac{1}{3T}|\nabla V|^2 - \frac{1}{3T}p^\top(\nabla^2 V)p\Big)\right) + O(\varepsilon^4).$$

The quantum Maxwellian $M[w]$ obtained from entropy maximization with given particle density becomes

$$M[w] = e^{A/T-|p|^2/2T}\left(1+\frac{\varepsilon^2}{8T}\Big(\Delta A + \frac{1}{3T}|\nabla A|^2 - \frac{1}{3T}p^\top(\nabla^2 A)p\Big)\right) + O(\varepsilon^4),$$

where A is a Lagrange multiplier, and we see that both approximations coincide up to exchanging A and V.

4.1.3 - `Viscous quantum hydrodynamics`

In the local quantum hydrodynamic model (76)-(77), the averaged collision terms W_p and W_e are unspecified. In this section, we make explicit these terms by choosing the Caldeira-Leggett or Fokker-Planck operators discussed in Section (2.4.2).

The Caldeira-Leggett operator

$$Q_1(w) = \frac{1}{\tau}\big(\Delta_p w + \mathrm{div}_p(pw)\big), \quad \tau > 0,$$

conserves mass, $\langle Q_1(w)\rangle = 0$, and satisfies the assumption imposed in the previous subsection. Integrating by parts, we find that

$$\begin{aligned}
-\langle pQ_1(M[w])\rangle &= \frac{1}{\tau}\int_{\mathbb{R}^3}(\nabla_p M[w] + pM[w])\frac{dp}{(2\pi\varepsilon)^3} = -\frac{J_n}{\tau},\\
\langle \tfrac{1}{2}|p|^2 Q_1(M[w])\rangle &= -\frac{1}{\tau}\int_{\mathbb{R}^3} p\cdot(\nabla_p M[w] + pM[w])\frac{dp}{(2\pi\varepsilon)^3}\\
&= \frac{1}{\tau}\int_{\mathbb{R}^3}(3M[w] - |p|^2 M[w])\frac{dp}{(2\pi\varepsilon)^3} = -\frac{2}{\tau}\Big(ne - \frac{3}{2}n\Big).
\end{aligned}$$

These expressions are referred to as relaxation-time terms, and $\tau > 0$ is called the relaxation time.

Another choice is the Fokker-Planck operator (22),

$$Q_1(w) = D_{pp}\Delta_p w + 2\gamma\,\mathrm{div}_p(pw) + D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_p w),$$

with positive diffusion coefficients D_{pp}, D_{pq}, D_{qq} and the friction parameter $\gamma > 0$. This operator does not conserve mass:

$$\langle Q_1(w)\rangle = D_{qq}\Delta_x n,$$

and the mass equation becomes

$$\partial_t n - \mathrm{div}\ J_n = D_{qq}\Delta n.$$

However, introducing the effective current density $J_{\mathrm{eff}} = J_n + D_{qq}\nabla n$, this equation can be written in conservative form:

$$\partial_t n - \mathrm{div}\ J_{\mathrm{eff}} = 0.$$

The other moments become, for $w = M[w]$,

$$\begin{aligned}
-\langle pQ_1(w)\rangle &= 2(2\pi\varepsilon)^{-3}\int_{\mathbb{R}^3}(\gamma pw + D_{pq}\nabla_x w)dp - D_{qq}(2\pi\varepsilon)^{-3}\Delta_x\int_{\mathbb{R}^3} pw dp\\
&= -2\gamma J_n + 2D_{pq}\nabla_x n + D_{qq}\Delta_x J_n,\\
\langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle &= -(2\pi\varepsilon)^{-3}\int_{\mathbb{R}^3}\big(D_{pp}p\cdot\nabla_p w + 2\gamma|p|^2 w + 2D_{pq}p\cdot\nabla_x w\big)dp\\
&\quad + D_{qq}(2\pi\varepsilon)^{-3}\Delta_x\int_{\mathbb{R}^3}\tfrac{1}{2}|p|^2 w dp\\
&= -2\Big(2\gamma ne - \frac{3}{2}D_{pp}n\Big) + 2D_{pq}\,\mathrm{div}_x\, J_n + D_{qq}\Delta_x(ne).
\end{aligned}$$

The spatial second-order expressions $\Delta_x n$, $\Delta_x J_n$, and $\Delta_x(ne)$ can be interpreted as viscous terms. We choose $D_{qq} = \nu$, $D_{pp} = 1/(2\tau)$, $D_{pq} = 0$, and $2\gamma = 1/(2\tau)$. Then the Lindblad condition (see Section 2.4.2) $D_{pp}D_{qq} - D_{pq}^2 \geq \gamma^2/4$ is satisfied if $\nu \geq 1/(32\tau)$. We obtain the *viscous quantum hydrodynamic equations*, which have been first proposed in [78]:

$$\partial_t n - \operatorname{div} J_n = \nu\Delta n, \tag{79}$$

$$\partial_t J_n - \operatorname{div}\Big(\frac{J_n \otimes J_n}{n}\Big) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)$$

$$= -\frac{J_n}{\tau} + \nu\Delta J_n, \tag{80}$$

$$\partial_t(ne) - \operatorname{div}\big((P + ne\mathbb{I})u\big) - \frac{\varepsilon^2}{24}\operatorname{div}\big(n(\Delta u + 2\nabla \operatorname{div} u)\big) + J_n \cdot \nabla V$$

$$= -\frac{1}{\tau}\Big(ne - \frac{3}{2}n\Big) + \nu\Delta(ne). \tag{81}$$

The following result shows that the energy is dissipated (compare to Proposition 14.5 in [91]).

P r o p o s i t i o n 4.1 (Energy dissipation). *Let (n, J_n, ne, V) be a solution to the viscous system* (79)-(81) *and the Poisson equation* (64). *Define the energy*

$$E(t) = \int_{\mathbb{R}^3}\Big(ne + \frac{\lambda_D^2}{2}|\nabla V|^2\Big)dx,$$

where ne is defined in (78). *Then we can write the energy as the sum of thermal, kinetic, electric, and quantum energy,*

$$E(t) = \int_{\mathbb{R}^3}\Big(\frac{3}{2}nT + \frac{1}{2}n|u|^2 + \frac{\lambda_D^2}{2}|\nabla V|^2 + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2\Big)dx, \tag{82}$$

and the energy dissipation relation reads as

$$\frac{dE}{dt} = -\frac{1}{\tau}\int_{\mathbb{R}^3}\Big(\frac{3}{2}n(T-1) + \frac{1}{2}n|u|^2 + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2\Big)dx.$$

P r o o f. We differentiate the energy formally with respect to time and employ the energy equation (81) and the Poisson equation (64):

$$\begin{aligned}\frac{dE}{dt} &= \int_{\mathbb{R}^3}\big(\partial_t(ne) + \lambda_D^2\nabla V\cdot\nabla\partial_t V\big)dx \\ &= \int_{\mathbb{R}^3}\Big(-J_n\cdot\nabla V - \frac{1}{\tau}\Big(ne - \frac{3}{2}n\Big) - \lambda_D^2 V\partial_t\Delta V\Big) \\ &= \int_{\mathbb{R}^3}\Big((\operatorname{div} J_n)V - \frac{1}{\tau}\Big(ne - \frac{3}{2}n\Big) - \lambda_D^2 V\partial_t n\Big)dx \\ &= -\frac{1}{\tau}\int_{\mathbb{R}^3}\Big(ne - \frac{3}{2}n\Big)dx.\end{aligned}$$

Finally, formula (82) is obtained by integrating by parts. □

4.2 - *Analysis*

The mathematical analysis of the quantum hydrodynamic equations is very challenging due to the interplay between dispersion (coming from the third-order quantum term) and dissipation (originating from the relaxation-time or viscous terms). Therefore, there are only a few results in the literature. First, we review analytical results on the relaxation-time model with constant or isentropic temperature:

$$\partial_t n - \operatorname{div} J_n = 0, \tag{83}$$

$$\partial_t J_n - \operatorname{div}\Big(\frac{J_n\otimes J_n}{n}\Big) - \nabla(Tn) + n\nabla V + \frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = -\frac{J_n}{\tau}, \tag{84}$$

$$\lambda_D^2\Delta V = n - C(x) \quad \text{in } \Omega\subset\mathbb{R}^d,\ t>0, \tag{85}$$

with the initial conditions

$$n(\cdot,0) = n_0, \quad J_n(\cdot,0) = J_0 \quad \text{in } \Omega,\ t>0,$$

and appropriate boundary conditions. Here, T is either a positive constant (isothermal model) or related to the particle density via $T(n) = n^{\beta-1}$ with $\beta > 1$ (isentropic model).

4.2.1 - `Thermal equilibrium`

First results in the literature have been concerned with the thermal equilibrium state, i.e. $J_n = 0$. Then the isothermal model (83)-(85) with $T = 1$ reduces to

$$-\nabla n + n\nabla V + \frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = 0, \quad \lambda_D^2\Delta V = n - C(x). \tag{86}$$

If $n > 0$, we can divide the first equation by n. Integrating over Ω, we arrive at

$$F = \log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}}, \quad \lambda_D^2\Delta V = n - C(x). \tag{87}$$

The integration constant F can be interpreted as a quantum Fermi potential and it is determined by the boundary conditions. Thus, by integrating the third-order equation, we arrive to a second-order elliptic system in the variables (n, V). The first analytical result is due to Pacard and Unterreiter [133]. They prove the existence of weak solutions to

$$\nabla\Big(\log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = 0, \quad \lambda_D^2\Delta V = n - C(x)$$

with the mixed boundary conditions

$$V = V_D \quad \text{on } \Gamma_D, \quad \nabla V\cdot\nu = 0 \quad \text{on } \Gamma_N, \quad \int_\Omega n dx = N,$$

where Γ_D is the union of contacts, the remaining set $\Gamma_N = \partial\Omega\backslash\Gamma_D$ represents the insulating boundary segments, and $N > 0$ is the given particle number. The proof consists in minimizing the total energy

$$E(n) = \int_\Omega \Big(\frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 + n(\log n - 1) + \frac{\lambda_D^2}{2}|\nabla V|^2\Big)dx$$

in the set $\{n \in L^1(\Omega) : n \geq 0, \int_\Omega n dx = N, \sqrt{n} \in H^1(\Omega)\}$. The result has been generalized to the bipolar situation in [140].

The authors of [73] have imposed Dirichlet boundary conditions and proved the existence and, for sufficiently large $\varepsilon > 0$, the uniqueness of weak solutions of (87) with $n = n_D$ and $V = V_D$ on $\partial\Omega$ for some functions n_D and V_D. This result was generalized to mixed Dirichlet-Neumann boundary conditions in [59].

Another approach is to differentiate the third-order equation which yields a fourth-order problem. This idea has been first employed by Brezzi et al. [23] in the one-dimensional setting $\Omega = (0,1)$. Indeed, dividing the first equation in (86) by n, taking the derivative, observing that

$$n\Big(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\Big)_x = \frac{1}{2}\big(n(\log n)_{xx}\big)_x, \tag{88}$$

and finally using the Poisson equation in (86), we infer that

$$-\frac{\varepsilon^2}{12}\Big((\log n)_{xx}^2 + \frac{1}{2}(\log n)_x^2\Big)_{xx} + (\log n)_{xx} - \frac{1}{\lambda_D^2}(n - C(x)) = 0. \tag{89}$$

Brezzi et al. prescribe Dirichlet and homogeneous Neumann boundary conditions at $x \in \{0,1\}$:

$$n = n_D, \quad n_x = 0 \quad \text{for } x \in \{0,1\}. \tag{90}$$

The electric potential V can be computed from the first equation in (86) after having solved (89)-(90). Using a fixed-point argument, the following result was shown in [23, Theorem 2.1].

T h e o r e m 4.4 (Existence for the thermal equilibrium problem). *Let n_D be defined for $x \in \{0,1\}$ and let $C \in L^\infty(0,1)$. Then there exists a weak solution $n \in H^2(0,1)$ of (89)-(90) satisfying $n > 0$ in $(0,1)$. Moreover, for sufficiently small $\varepsilon > 0$, the solution is unique.*

Further results in the literature were concerned with the semiclassical limit $\varepsilon \to 0$ [23, 73, 140] and the quasi-neutral limit $\lambda_D \to 0$ [140, 141]. For the existence of solutions for the whole-space problem, we refer to [147].

4.2.2 - `Stationary equations`

The above ideas of the treatment of the third-order quantum term can be applied to the stationary equations: either integrating the momentum equation

to obtain a second-order equation or differentiating this equation to arrive to a fourth-order equation (also see [90]). In the one-dimensional setting, the ideas of the paper of Brezzi et al. [23] have been extended in [81]. Indeed, in the one-dimensional case, the current density J_n is constant, by the mass equation (83), and the momentum equation (84) can be formulated as

$$J_n^2\frac{n_x}{n^2} - Tn_x + nV_x + \frac{\varepsilon^2}{12}\big(n(\log n)_{xx}\big)_x = -\frac{J_n}{\tau},$$

where we have used (88) and introduced the temperature constant $T > 0$. Then, dividing this equation by n, differentiating, and setting $y = \log n$, we arrive at

$$\frac{\varepsilon^2}{12}\Big(y_{xx} + \frac{1}{2}y_x^2\Big)_{xx} + J_n^2(e^{-2y}y_x)_x - Ty_{xx} + \frac{1}{\lambda_D^2}(e^y - C(x)) = -\frac{J_n}{\tau}(e^{-y})_x, \tag{91}$$

for $x \in (0,1)$ with the boundary conditions (compare to (90))

$$y(0) = y_0, \quad y(1) = y_1, \quad y_x(0) = y_x(1) = 0. \tag{92}$$

The main problem is the treatment of the convective part $J_n^2(e^{-2y}y_x)_x$. In fact, for $\varepsilon = 0$, the quantum model reduces to the Euler (or hydrodynamic) equations which may change type: if the velocity is sufficiently small, the hydrodynamic system is elliptic (subsonic flow), whereas it is generally hyperbolic (supersonic flow), and the equations may exhibit discontinuous solutions. The quantum term acts like a dispersive regularization of the hydrodynamic equations; however, it appears to be difficult to exploit this fact. The approach to solve (91)-(92) is to consider small velocities (or current densities). Due to the analogy to the Euler equations, it is not surprising that under this assumption, equation (91) can be solved using elliptic methods. Multiplying (91) by y and integrating by parts, we infer that (if $y_0 = y_1 = 0$ to simplify)

$$\int_0^1 \Big(\frac{\varepsilon^2}{12}y_{xx}^2 + Ty_x^2\Big)dx = -\frac{1}{\lambda_D^2}\int_0^1 (e^y - C(x))ydx + J_n^2\int_0^1 e^{-2y}y_x^2dx.$$

The first integral on the right-hand side is bounded from above, while the second integral needs to be estimated by the left-hand side:

$$\frac{\varepsilon^2}{12}\int_0^1 y_{xx}^2dx + \int_0^1 (T - J_n^2e^{-2y})y_x^2dx \le c.$$

Hence, if the mean velocity $J_n/n = J_ne^{-y}$ is smaller than the sound speed $\sqrt{T}$ (i.e., the flow is "subsonic"), we find that $T - J_n^2e^{-2y} \le 0$, yielding an H^2 estimate for y. This is the key idea for the following theorem which is shown by the Leray-Schauder fixed-point theorem [81, Theorem 2.5].

T h e o r e m 4.5 (Existence for the one-dimensional model). *Let y_0, $y_1 \in \mathbb{R}$, $C \in L^2(0,1)$, and let*

$$0 < J_n \le e^{-K}\sqrt{T + \varepsilon^2/6},$$

where $K > 0$ depends on the given data. Then there exists a weak solution $y \in H^2(0,1)$ of (91)-(92) satisfying $\|y\|_{L^\infty(\Omega)} \le K$. Moreover, if $\varepsilon > 0$ and $J_n > 0$ are sufficiently small, the solution is unique.

This result was generalized in [93] for general pressure functions $p(n)$ instead of the isothermal pressure $p(n) = Tn$. Assuming that the electric potential and field are prescribed at the left boundary point (instead of the homogeneous Neumann conditions for n), the *non-existence* of weak solutions to the quantum hydrodynamic model can be shown if the current density is sufficiently large and the pressure $p(n) = Tn$ is replaced by $p(n) = n^\alpha$ with $\alpha > 2$ [69].

The second idea is to integrate the quantum hydrodynamic equations and to obtain a system of elliptic second-order equations. For this, we consider a potential flow, i.e., we assume that the current density can be written as $J_n = n\nabla F$, where F is the quantum Fermi potential. This condition means that the velocity $-J_n/n = -\nabla F$ is irrotational. Since $\operatorname{div}(J_n \otimes J_n/n) = \frac{1}{2}n\nabla|\nabla F|^2$, we can write the stationary variant of (84) as

$$n\nabla\Big(\frac{1}{2}|\nabla F|^2 + T\log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = -\frac{n}{\tau}\nabla F \quad \text{in } \Omega,$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain. If $n > 0$ in Ω, we can divide by n and integrate:

$$\frac{1}{2}|\nabla F|^2 + T\log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}} + \frac{F}{\tau} = 0.$$

The integration constant can be assumed to be zero by choosing a reference point for the electric potential. Now, the stationary quantum hydrodynamic system can be written in the potential-flow formulation as

$$\frac{\varepsilon^2}{6}\Delta\sqrt{n} = \sqrt{n}\Big(\frac{1}{2}|\nabla F|^2 + T\log n - V + \frac{F}{\tau}\Big), \tag{93}$$

$$\operatorname{div}(n\nabla F) = 0, \quad \lambda_D^2\Delta V = n - C(x) \quad \text{in } \Omega. \tag{94}$$

The boundary conditions are

$$n = n_D, \quad F = F_D, \quad V = V_D \quad \text{on } \partial\Omega. \tag{95}$$

The difficulties to solve this elliptic system are the squared gradient of F in (93) and the degenerated diffusion coefficient $n \geq 0$ in the first equation in (94). By using Stampacchia's truncation method, elliptic regularity, and fixed-point arguments, the existence of a weak solution was shown in [89] under the condition that F_D is sufficiently small in some Hölder space. Since F_D is related to the applied potential, this assumption means that the applied voltage has to be chosen sufficiently small. Since we expect that small applied voltages imply small current densities and small velocities, this is a kind of "subsonic" assumption. The following result was proven in [89, Theorem 2.1].

T h e o r e m 4.6 (Existence for the potential-flow model). *Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be a bounded domain with $\partial\Omega \in C^{1,1}$, $C \in L^\infty(\Omega)$, and let n_D, F_D, V_D be smooth functions satisfying $\inf_{\partial\Omega} n_D > 0$. Then there exists $\delta > 0$ such that if*

$$\|F_D\|_{C^{1,\gamma}(\overline{\Omega})} \leq \delta,$$

there exists a solution (n, F, V) *satisfying* $\inf_\Omega n > 0$ *and*

$$\sqrt{n} \in W^{2,p}(\Omega), \quad F \in C^{1,\gamma}(\overline{\Omega}), \quad V \in L^\infty(\Omega) \cap H^2(\Omega),$$

where $p > d/2$ *and* $\gamma = 2 - d/p > 0$. *The solution is unique if* ε *is sufficiently large.*

The positivity of n is needed for the first equation in (94) to be uniformly elliptic. It is shown in [89] that the positivity of n is related to the regularity of F: the density n is strictly positive if and only if $F \in W^{1,\infty}(\Omega)$.

Asymptotic limits such as the semiclassical limit $\varepsilon \to 0$ and the quasineutral limit $\lambda_D \to 0$ were studied too; we refer to [70, 81, 124] for details.

4.2.3 - `Transient equations`

First results for the time-dependent quantum hydrodynamic equations (83)-(85) were concerned with the local-in-time existence of solutions or the global-in-time existence for solutions with initial data close to thermal equilibrium.

One of the first results is contained in the paper [99]. Assuming a potential flow, the quantum hydrodynamic system can be written as (see Section 4.2.2)

$$\partial_t n - \operatorname{div}(n\nabla F) = 0, \quad \lambda_D^2 \Delta V = n - C(x),$$
$$\partial_t F - \frac{1}{2}|\nabla F|^2 - \log n + V + \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}} = -\frac{F}{\tau}.$$

Setting $\psi = \sqrt{n}\exp(\mathrm{i}F/\varepsilon)$, the first and last equations are formally equivalent to a nonlinear Schrödinger equation,

$$\mathrm{i}\delta\partial_t\psi = -\frac{\delta^2}{2}\Delta\psi - V\psi + \log(|\psi|^2)\psi + \frac{1}{\tau}F\psi,$$

where $\delta^2 = \varepsilon^2/3$. The phase (or velocity potential) F satisfies an equation of the type $\Delta F = f(\psi, \nabla\psi, \Delta\psi)$ for some nonlinear function f. Using semigroup theory and the Banach fixed-point theorem, the existence of mild solutions to the system, consisting of the above nonlinear Schrödinger equation, the elliptic equation for F, and the Poisson equation, is proved. The solutions are local in time with a bound for the time which comes from the contractivity argument of the fixed-point operator.

Later, the global-in-time existence of solutions of the one-dimensional model was proven [94]. More precisely, let $(n_\infty, J_\infty, V_\infty)$ be a solution of the stationary problem with boundary conditions $n = n_D$, $n_x = 0$, and $V = V_D$ on $\partial\Omega$. Then, if the differences between the stationary solution and the initial data $\sqrt{n_\infty} - \sqrt{n_0}$ and $J_\infty - J_0$ are sufficiently small in some Sobolev norm, there exists a global solution (n, J_n, V) of (83)-(85) and the solution decays exponentially fast to the steady-state solution,

$$\|\sqrt{n} - \sqrt{n_\infty}\|_{H^6(\Omega)} + \|J_n - J_\infty\|_{H^5(\Omega)} + \|V - V_\infty\|_{H^4(\Omega)} \le ce^{-\lambda t}, \ t > 0,$$

where c, $\lambda > 0$ are some constants. The proof is based on a formulation of the momentum equation as a nonlinear fourth-order wave equation. In fact, differentiating the mass equation $n_t - (J_n)_x = 0$ with respect to t and the momentum equation (84) with respect to x, we can eliminate $(J_n)_{xt}$, and dividing the resulting equation by $2\sqrt{n}$, we arrive at

$$(\sqrt{n})_{tt} + \frac{1}{\tau}(\sqrt{n})_t + \frac{1}{2\sqrt{n}}(\sqrt{n})_t^2 - \frac{1}{2\sqrt{n}}\Big(\frac{J_n^2}{n} + n\Big)_{xx} + \frac{1}{2\sqrt{n}}(nV_x)_x + \frac{\varepsilon^2}{12}\Big((\sqrt{n})_{xxxx} - \frac{(\sqrt{n})_{xx}^2}{\sqrt{n}}\Big) = 0.$$

This idea was extended to the whole line $\mathbb{R}$ in [83] and to the whole space $\mathbb{R}^3$ in [117, 118]. The long-time behavior is typically obtained as a by-product, also see [84].

The first general global existence result (in the whole-space $\mathbb{R}^3$ setting) was proved by Antonelli and Marcati [4]. They use the fact that, without relaxation processes, the quantum hydrodynamic equations are formally equivalent to a Schrödinger equation. Let (n, J_n, V) be a solution of (83)-(85) with the pressure $p(n) = Tn$ replaced by $p(n) = \frac{\beta-1}{\beta+1}n^\beta$ with $\beta > 1$. Then the evolution problem can be decomposed into two parts, the relaxation-free quantum hydrodynamic problem and a relaxation problem without quantum hydrodynamics. More precisely, let the initial data be given by $n_0 = |\psi_0|^2$, $J_0 = -\varepsilon\mathrm{Im}(\overline{\psi}_0\nabla\psi_0)$, where ψ_0 is a given wave function. At the first step $k = 0$, we solve the Cauchy problem for the Schrödinger-Poisson system

$$\mathrm{i}\delta\partial_t\psi = -\frac{\delta^2}{2}\Delta\psi + |\psi|^{\beta-1}\psi - V\psi, \quad \lambda_D^2\Delta V = |\psi|^2, \quad \psi(\cdot,0) = \psi_0 \quad \text{in } \mathbb{R}^3$$

on the time interval $(t_{k-1}, t_k]$, where $t_k = k\triangle t$. The solution defines the particle and current densities $n := |\psi|^2$ and $J_n := -\varepsilon\mathrm{Im}(\overline{\psi}\nabla\psi)$. Then we solve the differential equation

$$\partial_t J_n = -\frac{J_n}{\tau}, \quad t > t_k, \quad J_n(t_k) \text{ given.}$$

The function J_n is employed to update ψ, defined on $(t_{k-1}, t_k]$, and to close the loop. This procedure requires to decompose the wave function into its amplitude and phase which may be undefined if the amplitude vanishes. Antonelli and Marcati utilize the polar decomposition method developed by Brenier [19]. They prove that for given $\psi \in H^1(\mathbb{R}^3)$, there exists $\phi \in L^\infty(\mathbb{R}^3)$ such that $\psi = \sqrt{n}\phi$, where $\sqrt{n} = |\psi|^2 \in H^1(\mathbb{R}^3)$. Moreover $\Lambda := -\varepsilon\mathrm{Im}(\overline{\phi}\nabla\phi)$ is an element of $L^2(\mathbb{R}^3)$. The weak solution of the quantum hydrodynamic system is defined via (n, Λ) instead of (n, J_n). For smooth solutions, we have the relation $J_n = \sqrt{n}\Lambda$. The main result reads as follows (Theorem 4 in [4]).

T h e o r e m 4.7 (Existence for the transient model). *Let $T > 0$, $C(x) = 0$, $\psi_0 \in H^1(\mathbb{R}^3)$, and $n_0 = |\psi_0|^2$, $J_0 = -\varepsilon\mathrm{Im}(\overline{\psi}_0\nabla\psi_0)$. Then there exists a*

weak solution (n,Λ,V) *of the quantum hydrodynamic equations* (83)-(85) *in* $\mathbb{R}^3\times(0,T)$ *such that*

$$\sqrt{n}\in L^2_{\rm loc}(0,T;H^1_{\rm loc}(\mathbb{R}^3)),\quad \Lambda\in L^2_{\rm loc}(0,T;L^2_{\rm loc}(\mathbb{R}^3)),$$

and the energy is finite for almost every $t>0$,

$$\int_{\mathbb{R}^3}\Big(\frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2+\frac{1}{2}|\Lambda|^2+\frac{2}{\beta+1}n^{(\beta+1)/2}+\frac{\lambda_D^2}{2}|\nabla V|^2\Big)dx<\infty.$$

The current density is defined by $J_n=\sqrt{n}\Lambda$.

The quantum hydrodynamic model is related to the drift-diffusion equations studied in Section 3. Indeed, when we replace t by t/τ and J_n by τJ_n in (83)-(84), where τ is the momentum relaxation time, we have

$$\tau\partial_t n-\tau\,\mathrm{div}\,J_n=0,$$
$$\tau^2\partial_t J_n-\tau^2\,\mathrm{div}\Big(\frac{J_n\otimes J_n}{n}\Big)-T\nabla n+n\nabla V+\frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)=-J_n.$$

In the formal limit $\tau\to 0$, the limiting model becomes

$$\partial_t n-\mathrm{div}\,J_n=0,\quad J_n=-\frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)+T\nabla n-n\nabla V,$$

which equals the quantum drift-diffusion model. This limit was made rigorous (with initial data close to the equilibrium) in [95].

In the semiclassical limit $\varepsilon\to 0$, the quantum hydrodynamic model reduces to the hydrodynamic (or Euler) equations, see [130] for a result for the one-dimensional initial-boundary value problem. The combined semiclassical and zero-relaxation limit was studied in one space dimension [120] and in three dimensions [119]. The limits can also be performed independently, see [146]. Finally, we mention the result for the quasineutral limit $\lambda_D\to 0$ achieved in [116].

The numerical approximation of the quantum hydrodynamic equations is challenging due to the strong nonlinearity and dispersive effects in the quantum term. Up to our knowledge, all available numerical schemes in the literature treat the one-dimensional equations only. Gardner [72] employed the second-upwind finite-difference scheme originally designed for hyperbolic conservation laws. It was shown in [100] that this scheme introduces a numerical viscosity whose order is even larger than the order of the grid size. Kendrick [111] introduced artificial viscosity in his scheme to avoid numerical instabilities due to large Bohm forces. Xin and Tang [145] observed a deviation of the asymptotic transient solution from the stationary one, using a central finite-difference scheme. Another strategy was employed by Lin et al. [122]. They constructed a third-order modified Osher-Chakravarthy (MOC) upwind-centered finite-volume scheme for the conservation law to evaluate the convective terms and a second-order central finite-volume scheme to map the quantum potential field. Furthermore, a mixed/discontinuous Galerkin finite-element scheme was developed by Michowski et al. [126] for applications in quantum chemistry.

4.2.4 - Viscous equations

The first existence result for the viscous quantum hydrodynamic model

$$\partial_t n - \operatorname{div} J_n = \nu\Delta n, \tag{96}$$

$$\partial_t J_n - \operatorname{div}\Big(\frac{J_n\otimes J_n}{n}\Big) - \nabla p(n) + n\nabla V + \frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)$$

$$= -\frac{J_n}{\tau} + \nu\Delta J_n, \tag{97}$$

$$\lambda_D^2\Delta V = n - C(x), \tag{98}$$

where $p(n) = Tn^\beta$ ($\beta \geq 1$, $T > 0$) is the pressure function, was proved in [78]. In this work, the one-dimensional stationary equations with $\beta = 1$ were considered in the interval $(0,1)$ with boundary conditions for n, n_x at $x \in \{0,1\}$ and V and J_n at $x = 0$. Notice that the current density is prescribed at one boundary point but *not* the applied voltage $V(1) - V(0)$. Given $J(0)$, the applied voltage can be computed from the solution to the above boundary-value problem. The idea of the existence analysis is to differentiate the momentum equation such that we obtain a nonlinear fourth-order equation. This strategy requires, as in the stationary quantum hydrodynamic model (see Section 4.2.2), a "subsonic"-type condition on the mean velocity. Due to the regularizing viscous terms, this condition appears to be weaker than in the inviscid case $\nu = 0$: if

$$0 < J(0) \leq e^{-K}\sqrt{T + \frac{\varepsilon^2}{6} + \frac{\nu}{\tau}},$$

then there exists a weak solution (n, J_n, V) to (96)-(98) satisfying $n \geq e^{-K} > 0$ in $(0,1)$. Furthermore, if $J(0)$ and $\nu^2 + \varepsilon^2$ are sufficiently small, there exists a unique solution. Later, the smallness condition on $J(0)$ could be removed, and existence of stationary solutions for all $J(0)$ was shown in [100] (with different boundary conditions than above).

Later, the transient model was examined by Chen and Dreher [34]. They prove the local-in-time existence of solutions in the multidimensional torus and the global-in-time existence of solutions in the one-dimensional torus $\mathbb{T}$, with $\beta = 1$. The latter result holds if the initial energy

$$E = \int_{\mathbb{T}}\Big(\frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 + \frac{|J_n|^2}{2n} + Tn(\log n - 1) + \frac{\lambda_D^2}{2}|\nabla V|^2\Big)dx$$

is sufficiently small. The proof is based on a regularization of the momentum equation, by adding the bi-Laplacian $\Delta^2 J_n$, and energy estimates. Indeed, it holds formally that

$$\frac{dE}{dt} + \frac{\nu\varepsilon^2}{3}\int_{\mathbb{T}} n|\nabla^2\log n|^2 dx \leq 0, \tag{99}$$

and the inequality (41) provides H^2 estimates for $\sqrt{n}$. Related results, but with different boundary conditions, were shown in [61]. By showing that the principal

part of the viscous quantum system constitutes a parameter-elliptic operator in the sense of Douglis-Nirenberg-Volevich, provided that the boundary conditions satisfy the Shapiro-Lopatinskii criterion, the local-in-time well-posedness was achieved in [35]. This paper, as well as the review [36], gives some insight into the properties of the operator associated to the viscous quantum hydrodynamic system.

Two years later, Gamba et al. [71] were able to eliminate the smallness condition on the initial energy. They proved the global existence of weak solutions on the one-dimensional torus $\mathbb{T}$, which satisfy the momentum equation (97) in a "renormalized solution" sense, i.e., the test functions are $n^{3/2}\phi$ instead of ϕ. This allows one to avoid possible vacuum regions $n = 0$. The proof exploits the fact that the mass equation

$$\partial_t n + \operatorname{div}(nu) = \nu\Delta n,$$

where $nu = -J_n$, is parabolic in n. Thus, if the mean velocity satisfies $u \in L^2_{\rm loc}(0,\infty;H^1(\mathbb{T}))$, by the maximum principle, the particle density is strictly positive if it is strictly positive initially. The problem is that there is no gradient estimate for the velocity guaranteeing the $L^2_{\rm loc}(0,\infty;H^1(\mathbb{T}))$ regularity. In [71], therefore, a Faedo-Galerkin method is employed yielding smooth velocities and positive particle densities. Since this method uses the embedding $H^1(\mathbb{T}) \hookrightarrow L^\infty(\mathbb{T})$, it is restricted to the case of one space dimension only.

The global-in-time existence of the multidimensional problem on the torus $\mathbb{T}^d$ was recently proved in [92]. As in the one-dimensional case, the H^2 estimate for $\sqrt{n}$ (see (99)) is essential for the analysis. The existence proof employs the Faedo-Galerkin method, following [71], together with a second regularization, i.e. adding the term $\delta(\Delta u - u)$ to the momentum equation, where $u = -J_n/n$ is the mean velocity. This yields gradient estimates for u. By applying the results of Feireisl [65], we conclude the positivity of the particle density. In order to pass to the limit of vanishing approximation parameters, we prove compactness of the sequence of approximate solutions by the energy estimate. The very technical limit can be made rigorous only if we use $n^2\phi$ as test functions. The result reads as follows (see Theorem 1.1 in [92]).

T h e o r e m 4.8 (Existence for the viscous quantum hydrodynamic model). *Let $d \le 3$, $V \in L^\infty(0,\infty;L^\infty(\mathbb{T}^d))$, $p(n) = n^\beta$ with $\beta > 3$ if $d = 3$ and $\beta \ge 1$ if $d \le 2$, and let the initial energy be finite. Then there exists a weak solution to* (96)-(97) *satisfying $n \ge 0$ in $\mathbb{T}^d$ and*

$$\sqrt{n} \in L^\infty_{\rm loc}(0,\infty;H^1(\mathbb{T}^d)) \cap L^2_{\rm loc}(0,\infty;H^2(\mathbb{T}^d)),$$
$$nu \in L^2_{\rm loc}(0,\infty;W^{1,3/2}(\mathbb{T}^d)), \quad n|\nabla u| \in L^2_{\rm loc}(0,\infty;L^2(\mathbb{T}^d)).$$

The restriction $\beta > 3$ is needed to improve the uniform L^3 bound for n (obtained from the H^1 bound for $\sqrt{n}$) to an L^β bound. This property helps us in the limit of vanishing approximation parameter $\delta \to 0$ to achieve a suitable weak convergence result (see [92] for details).

In the literature, some asymptotic limits were studied. In [78], the semiclassical limit $\varepsilon \to 0$ and the inviscid limit $\nu \to 0$ were proved in the one-dimensional stationary problem. The quasineutral limit $\lambda_D \to 0$ in the multidimensional transient model was performed in [114] using modulated energy estimates. The long-time behavior of solutions was analyzed in [34, 35, 79]. A related result can be found in [121]; in this work, however, the third-order quantum term is replaced by its linear main part $\nabla\Delta n$. Numerical results for the one-dimensional equations were presented in [100] for the stationary equations and in [107] for the transient equations.

5 - Quantum Navier-Stokes models

This section is devoted to the derivation of Navier-Stokes equations for quantum fluids, starting from a Wigner-BGK equation. Compared to the previous section, the Chapman-Enskog expansion yields diffusive corrections to the macroscopic equations.

5.1 - *Derivation*

The hydrodynamic equations can be derived from the kinetic Boltzmann equation by a moment method, similar as in the quantum kinetic context of Section 4.1. It is well known that the next order expansion, the so-called Chapman-Enskog expansion, of the Boltzmann distribution function leads to the Navier-Stokes equations. This idea was extended by Brull and Méhats [24] to the quantum case with the aim to derive a quantum analogue of the Navier-Stokes equations with constant temperature. Quantum Navier-Stokes equations including the energy equation were derived in [103]. In the physical literature, quantum Navier-Stokes systems are typically motivated from the classical Navier-Stokes model by using a chemical potential obtained from the Thomas-Fermi-Dirac-Weizsäcker density functional theory (see, e.g., [138]).

We consider, following [103, 104], the Wigner-BGK equation in the hydrodynamic scaling

$$\alpha\partial_t w + \alpha(p\cdot\nabla_x w + \theta[V]w) = M[w] - w, \quad (x,p)\in\mathbb{R}^3\times\mathbb{R}^3,\ t>0, \tag{100}$$

where $w(x,p,t)$ is the Wigner function in the phase-space variables (x,p) and time $t>0$, and $\alpha>0$ is the scaled mean free path (see Section 2.2). The right-hand side of (100) describes a relaxation process towards the quantum Maxwellian $M[w]$ defined in Section 2.3. When scattering conserves mass, momentum, and energy, the quantum equilibrium is given by (see (19))

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

where A, v, and T are some Lagrange multipliers. The moment equations are derived as in Section 4.1.2: we multiply (100) by 1, p, and $|p|^2/2$, respectively,

which leads to

$$\begin{aligned}\partial_t\langle w\rangle + \operatorname{div}_x\langle pw\rangle + \langle\theta[V]w\rangle &= 0,\\ \partial_t\langle pw\rangle + \operatorname{div}_x\langle p\otimes pw\rangle + \langle p\theta[V]w\rangle &= 0,\\ \partial_t\langle \tfrac12|p|^2w\rangle + \operatorname{div}_x\langle \tfrac12 p|p|^2w\rangle + \langle \tfrac12|p|^2\theta[V]w\rangle &= 0,\end{aligned}$$

where $n=\langle w\rangle$ is the particle density, $J_n=-\langle pw\rangle$ the current density, and $ne=\langle\frac12|p|^2w\rangle$ is the energy density. The integrals involving the potential operator can be computed using (68). It remains to compute the higher-order moments $\langle p\otimes pw\rangle$ and $\langle\frac12 p|p|^2w\rangle$.

The idea in Section 4.1.2 is to replace these moments by $\langle p\otimes pM[w]\rangle$ and $\langle\frac12 p|p|^2M[w]\rangle$, which can be justified (formally) by a zero mean-free-path limit $\alpha\to 0$, and by expanding the integrals in powers of ε^2. Here, we follow a different strategy. We introduce the Chapman-Enskog expansion

$$w = M[w] + \alpha g$$

(this equation defines the function g), and we do *not* pass to the limit $\alpha\to 0$ but let $\alpha>0$ fixed. Furthermore, introducing as in Section 4.1.2 the quantum stress tensor P and the quantum heat flux q by

$$P=\langle (p-u)\otimes(p-u)M[w]\rangle,\quad q=\langle\tfrac12(p-u)|p-u|^2M[w]\rangle,$$

where $u=-J_n/n$ is the mean velocity, and employing the identities (68) and (70), the above moment equations can be written as

$$\begin{aligned}\partial_t n + \operatorname{div}_x(nu) &= 0,\\ \partial_t(nu) + \operatorname{div}_x(P+nu\otimes u) - n\nabla_x V &= -\alpha\operatorname{div}_x\langle p\otimes pg\rangle,\\ \partial_t(ne) + \operatorname{div}_x\big((P+ne\mathbb{I})u\big) + \operatorname{div}_x q - nu\cdot\nabla_x V &= -\alpha\operatorname{div}_x\langle\tfrac12 p|p|^2g\rangle,\end{aligned}$$

where $\mathbb{I}$ is the unit matrix in $\mathbb{R}^{3\times3}$. In order to calculate the moments of g, we take advantage of the simple structure of the collision operator, allowing us to specify g explicitly. Indeed, inserting the Wigner equation and Chapman–Enskog expansion, we find that

$$\begin{aligned}g &= -(M[w]-w)/\alpha = -w_t - p\cdot\nabla_x w - \theta[V]w\\ &= -(M[w]+\alpha g)_t - p\cdot\nabla_x(M[w]+\alpha g) - \theta[V](M[w]+\alpha g)\\ &= -M[w]_t - p\cdot\nabla_x M[w] - \theta[V]M[w] + O(\alpha),\end{aligned}$$

where $O(\alpha)$ contains terms of order α.

More explicit expressions are obtained by expanding the moments of $M[w]$ in powers of the squared scaled Planck constant ε^2. The quantum stress tensor and heat flux are expanded according to (78), assuming that the temperature variations and vorticity are of order $O(\varepsilon^4)$. Moreover, a tedious computation, detailed in [103], shows that

$$-\alpha\operatorname{div}_x\langle p\otimes pg\rangle = \alpha\operatorname{div}_x S,\quad -\alpha\operatorname{div}_x\langle\tfrac12 p|p|^2g\rangle = \alpha\operatorname{div}_x(Su)+\frac52 nT\nabla_x T,$$

where $S = 2nTD(u) - \frac{2}{3}nT\,\mathrm{div}_x\,u\,\mathbb{I} + O(\varepsilon^2+\alpha)$ can be interpreted as a viscous stress tensor. Here, $D(u) = (\nabla_x u + \nabla_x u^\top)/2$. The term $\frac{5}{2}nT\nabla_x T$ is the Fourier heat term, and it adds to the quantum heat flux. This shows the following result [103].

T h e o r e m 5.1 (Quantum Navier-Stokes model). *Assume that* $(\nabla u - \nabla u^\top)/2 = O(\varepsilon^2)$ *and* $\nabla \log T = O(\varepsilon^2)$. *Then, up to terms of order* $O(\alpha^2 + \alpha\varepsilon^2 + \varepsilon^4)$, *the moment equations of the Wigner equation read as*

$$\partial_t n + \mathrm{div}(nu) = 0, \tag{101}$$

$$\partial_t(nu) + \mathrm{div}(nu\otimes u) + \nabla(nT) - \frac{\varepsilon^2}{12}\,\mathrm{div}(n\nabla^2\log n) - n\nabla V = \alpha\,\mathrm{div}\,S, \tag{102}$$

$$(ne)_t + \mathrm{div}\big((ne+nT)u\big) - \frac{\varepsilon^2}{12}\,\mathrm{div}\big(n(\nabla^2\log n)u\big) + \mathrm{div}\;q - nu\cdot\nabla V = \alpha\,\mathrm{div}(Su),$$

where the quantum heat flux and viscous stress tensor are given by, respectively,

$$q = \frac{\varepsilon^2}{24}n(\Delta u + 2\nabla\,\mathrm{div}\,u) + \frac{5}{2}nT\nabla T, \quad S = 2nTD(u) - \frac{2}{3}nT\,\mathrm{div}\,u\,\mathbb{I}.$$

The energy density ne *is given by* (78).

When the collisions conserve mass and momentum only, the quantum equilibrium becomes $M[w] = \mathrm{Exp}(A - |p-v|^2/2)$. In this situation, a Chapman-Enskog expansion has been carried out by Brull and Méhats [24]. They obtain equations (101)-(102) with $T = 1$ and $S = 2nD(u)$.

5.2 - *Analysis*

System (101)-(102) with constant temperature $T = 1$ possesses a surprising property which has been exploited in [92] to prove the existence of global weak solutions. More precisely, we consider the system

$$\partial_t n + \mathrm{div}(nu) = 0, \quad x\in\mathbb{T}^d,\ t>0, \tag{103}$$

$$\partial_t(nu) + \mathrm{div}(nu\otimes u) + \nabla p(n) - \frac{\varepsilon^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) - n\nabla V = 2\alpha\,\mathrm{div}(nD(u)), \tag{104}$$

$$n(\cdot,0) = n_0, \quad (nu)(\cdot,0) = n_0u_0 \quad \text{in } \mathbb{T}^d, \tag{105}$$

where $\mathbb{T}^d$ is the d-dimensional torus ($d\le 3$). The function $p(n) = n^\beta$ with $\beta > 1$ is the pressure. Compared to (102), the quantum term is reformulated using the multidimensional analogue of (88),

$$\mathrm{div}(n\nabla^2\log n) = 2n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big).$$

In the treatment of (103)-(105), we need to overcome several mathematical difficulties. Besides the lack of maximum principle due to the third-order differential term, another problem is the density-dependent viscosity $\mu(n) = \alpha n$ which degenerates at vacuum. In fact, most results for the Navier-Stokes equations in the literature are valid for constant viscosities $\mu(n) = \alpha$ only, since this enables one to derive H^1 estimates for the velocity. Recently, some works were concerned with density-dependent viscosities, see, e.g., [21, 115] and references therein.

A third problem is the lack of suitable a priori estimates. Indeed, let us define the energy of (103)-(104) by the sum of the kinetic, internal, and quantum energy (compare to (82), which also includes the electric energy)

$$E_{\varepsilon^2}(n,u) = \int_{\mathbb{T}^d} \Big(\frac{n}{2}|u|^2 + H(n) + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2\Big)dx, \tag{106}$$

where $H(n) = n^\beta/(\beta-1)$ if $\beta > 1$ and $H(n) = n(\log n - 1)$ if $\beta = 1$. A formal computation shows that, without electric field $\nabla V = 0$,

$$\frac{dE_{\varepsilon^2}}{dt}(n,u) + \alpha\int_{\mathbb{T}^d} n|D(u)|^2 dx = 0.$$

This provides an H^1 estimate for $\sqrt{n}$, but this seems to be insufficient to obtain compactness for (an approximate sequence of) $\nabla\sqrt{n}$ needed to define the quantum term in a weak or distributional sense.

Our main idea to solve these problems is to transform the quantum Navier-Stokes system by means of the so-called *"osmotic velocity"*

$$w = u + \alpha\nabla\log n, \tag{107}$$

The term $\alpha\nabla\log n$ has been called in [82] the "kinematical quasivelocity". It also appears in the derivation of the quantum hydrodynamic model from the mixed-state Schrödinger system; see Theorem 4.1. A computation shows [92] that the system (103)-(105) can be equivalently written as the viscous quantum hydrodynamic equations

$$\partial_t n + \operatorname{div}(nw) = \alpha\Delta n, \tag{108}$$

$$\partial_t(nw) + \operatorname{div}(nw\otimes w) + \nabla p(n) - \frac{\varepsilon_0}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) - n\nabla V = \alpha\Delta(nw), \tag{109}$$

$$n(\cdot,0) = n_0, \quad (nw)(\cdot,0) = n_0 w_0 \quad \text{in } \mathbb{T}^d, \tag{110}$$

where $w_0 = u_0 + \alpha\nabla\log n_0$ and $\varepsilon_0 = \varepsilon^2 - 12\alpha^2$. This formulation has two advantages. The first advantage is that it allows for an additional energy estimate if $\varepsilon^2 > 12\alpha^2$. Indeed, if $\nabla V = 0$, we compute

$$\frac{dE_{\varepsilon_0}}{dt}(n,w) + \alpha\int_{\mathbb{T}^d}\Big(n|\nabla w|^2 + H'(n)|\nabla n|^2 + \frac{\varepsilon_0}{12}n|\nabla^2\log n|^2\Big)dx = 0. \tag{111}$$

Inequality (41) provides an $L^2_{\mathrm{loc}}(0,\infty;H^2(\mathbb{T}^d))$ bound for $\sqrt{n}$. This estimate is the key argument of the global existence analysis. The second advantage is that

we can apply the maximum principle to the parabolic equation (108) to deduce strict positivity of the density n if n_0 is strictly positive and the velocity w is smooth.

Interestingly, the "osmotic velocity" (107) has been used in related models. First, Bresch and Desjardins employed it to derive new entropy estimates for viscous Korteweg-type and shallow-water equations [22]. Brenner [20] suggested the modified Navier-Stokes model

$$\partial_t n + \operatorname{div}(nw) = 0, \quad \partial_t(nu) + \operatorname{div}(nu \otimes w) + \nabla p(n) = \operatorname{div} S.$$

The variables u and w are interpreted as the volume and mass velocities, respectively, and they are related by the constitutive equation $u - w = \alpha \nabla \log n$ with a phenomenological constant $\alpha > 0$. The variable $nw = nu + \alpha \nabla n$ was employed in [100] to prove the existence of solutions of the one-dimensional stationary viscous quantum Euler problem with physical boundary conditions (see Section 4.2.4).

According to the above equivalence, the existence of solutions of the quantum Navier-Stokes equations (103)-(104) is a consequence of the existence analysis for the viscous quantum hydrodynamic system presented in Section 4.2.4. The result reads as follows (see Corollary 1.2 in [92]).

T h e o r e m 5.2 (Existence for the quantum Navier-Stokes model). *Let $d \le 3$, $p(n) = n^\beta$ with $\beta > 3$ if $d = 3$ and $\beta \ge 1$ if $d \le 2$, $\nabla V \in L^\infty(0,\infty; L^\infty(\mathbb{T}^d))$, and (n_0, u_0) is such that $n_0 \ge 0$ and $E_{\varepsilon^2}(n_0, u_0 + \alpha \nabla \log n_0)$ is finite. Then there exists a weak solution (n, u) of (103)-(105) with the regularity*

$$\sqrt{n} \in L^\infty_{\rm loc}(0,\infty; H^1(\mathbb{T}^d)) \cap L^2_{\rm loc}(0,\infty; H^2(\mathbb{T}^d)), \quad n \ge 0 \text{ in } \mathbb{T}^d,$$
$$nu \in L^2_{\rm loc}(0,\infty; W^{1,3/2}(\mathbb{T}^d)), \quad n|\nabla u| \in L^2_{\rm loc}(0,\infty; L^2(\mathbb{T}^d)).$$

The weak formulation of the momentum equation (104) is defined similarly as for the viscous model using test functions $n^2\phi$ instead of ϕ. Theorem 5.2 is proved in [92] for the case $\varepsilon^2 > 12\alpha^2$ or, equivalently, $\varepsilon_0 > 0$. This condition is necessary to obtain H^2 bounds for $\sqrt{n}$ via the viscous quantum Euler model from the new energy estimate (111). In the case $\varepsilon^2 \le 12\alpha^2$, we loose the H^2 control on $\sqrt{n}$.

The limiting case $\varepsilon^2 = 12\alpha^2$ has been treated recently by Dong [60]. Indeed, using (an approximation of) the test function $\Delta\sqrt{n}/\sqrt{n}$ in (108) leads to

$$\frac{d}{dt}\int_{\mathbb{T}^d} |\nabla\sqrt{n}|^2 dx + \frac{\alpha}{4}\int_{\mathbb{T}^3} n|\nabla^2 \log n|^2 dx \le \frac{1}{4\alpha}\int_{\mathbb{T}^3} n|\nabla w|^2 dx. \tag{112}$$

In view of the energy inequality (111), the right-hand side is uniformly bounded. By (41), this shows the desired H^2 bound for $\sqrt{n}$. Jiang and Jiang [85] have combined the inequalities (111) and (112) to treat the remaining case $\varepsilon^2 < 12\alpha^2$. Let $\varepsilon_0 = \varepsilon^2 - 12\alpha^2 < 0$ and define

$$F(n,w) = \int_{\mathbb{T}^d} \Big(\frac{n}{2}|w|^2 + H(n) - \frac{\varepsilon_0}{6}|\nabla\sqrt{n}|^2\Big) dx \ge 0.$$

Then we use (111) and (112) to conclude

$$\begin{aligned}\frac{dF}{dt} &= \frac{dE_{\varepsilon_0}}{dt} - \frac{\varepsilon_0}{3}\frac{d}{dt}\int_{\mathbb{T}^d}|\nabla\sqrt{n}|^2dx \\ &\le -\alpha\int_{\mathbb{T}^d}\Big(\frac{1}{12\alpha^2}(12\alpha^2+\varepsilon_0)n|\nabla w|^2 + H'(n)|\nabla n|^2\Big)dx \le 0.\end{aligned}$$

Since $12\alpha^2+\varepsilon_0=\varepsilon^2>0$, we obtain an L^2 estimate for $\sqrt{n}|\nabla w|$. Going back to (112), we see that the right-hand side is bounded, which provides an L^2 bound for $\sqrt{n}|\nabla^2\log n|$ and hence, by (41), the desired H^2 bound for $\sqrt{n}$.

Finally, we remark that numerical results for the isothermal quantum Navier-Stokes model (103)-(104) or the full quantum Navier-Stokes model (101)-(102) have been presented in [103].

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