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Quantum Navier-Stokes Equations

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Quantum Navier–Stokes equations

Ansgar Jüngel and Josipa-Pina Milišić

Abstract Compressible Navier–Stokes models for quantum fluids are reviewed. They are derived from a collisional Wigner equation by a moment method and a Chapman–Enskog expansion around the quantum equilibrium. Introducing a new velocity variable, the barotropic quantum Navier-Stokes model can be reformulated as a viscous quantum Euler system, which possesses a new Lyapunov (energy) functional. This functional provides a priori estimates which are exploited to prove the global-in-time existence of weak solutions for general initial data. Furthermore, new numerical results for the isothermal model are presented.

1 Introduction

Quantum fluid modeling has become very attractive due to novel experimental discoveries in Bose–Einstein condensation. Recently, disordered superfluids and, in particular, the interplay between superfluidity and the onset of dissipative processes has been investigated [10]. Typically, the dynamics of the condensate is modeled by a nonlinear Schrödinger equation involving dissipative terms [3]. The normal component of the Bose–Einstein gas at low temperature may be described by using kinetic equations, such as the Wigner equation [1]. This approach 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-

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type operators (named after Bhatnagar, Gross, and Krook); see [22] for a detailed description.

The hydrodynamic dynamics of a superfluid may be modeled by the Madelung equations, which are derived from the Schrödinger equation via the Madelung transform [30]. The model consists of the Euler equations for a potential flow involving the quantum Bohm potential as a third-order derivative. The quantum Euler or quantum hydrodynamic equations have been also used to describe the carrier transport in open quantum systems such as semiconductor heterostructures and tunneling diodes [16, 22]. An alternative derivation is based on the Wigner equation by employing the moment method and the maximum entropy principle [13]. Quantum hydrodynamic models have the advantages that they allow for an efficient numerical discretization and that macroscopic boundary conditions in open systems may be imposed.

In this review, we summarize recent progress in the derivation and mathematical analysis of certain dissipative quantum hydrodynamic equations, namely *quantum Navier–Stokes models*. Such systems have been already proposed in the 1960s [19]. The first derivation from a Wigner–BGK equation has been performed by Brull and Méhats [9] for constant temperature. In [27], the full quantum Navier–Stokes system, including the energy equation, has been derived and numerically solved. The existence of weak solutions to the barotropic model has been shown in [14, 20, 23] (see Theorem 2 below).

In the physical literature, quantum Navier–Stokes systems are typically motivated from the classical model by using a chemical potential obtained from the Thomas–Fermi–Dirac–Weizsäcker density functional theory (see, e.g., [32]). Clearly, in this situation, the viscous correction is equal to the classical one and often, constant viscosity coefficients are assumed. The derivation from the Wigner–BGK equation leads to *nonconstant* viscosity coefficients depending on the particle density and temperature (see Theorem 1 below). Density-dependent viscosities may generate vacuum, which leads to mathematical difficulties in the analysis of the equations (see, e.g., [5, 29]).

This review is organized as follows. In Section 2, following [27], the derivation of the quantum Navier–Stokes system from a Wigner–BGK equation using a Chapman–Enskog expansion of the Wigner function around the quantum equilibrium is sketched. Section 3 is concerned with the analysis of the compressible barotropic model (density-dependent pressure function). The existence analysis is based on the formulation of the model as a viscous quantum Euler system via a new variable, the so-called effective velocity, first used in viscous Korteweg models [6]. Finally, in Section 4, the isothermal equations (constant temperature) are numerically discretized by central finite differences in one space dimension, and new numerical simulations for a tunneling diode are presented.

2 Derivation

The quantum Navier–Stokes equations are derived from a Wigner–BGK model using the moment method and a Chapman–Enskog expansion. Degond et al. [12] have proposed the Wigner–BGK equation

$$w_t + p\cdot\nabla_x w + \theta[V]w = \frac{1}{\alpha}(M[w]-w), \quad (x,p)\in\mathbb{R}^3\times\mathbb{R}^3,\ t>0, \tag{1}$$

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. The potential operator $\theta[V]$ is a pseudo-differential operator modeling the influence of the electric potential $V=V(x,t)$; see [22] for a definition. The kernel of the potential operator is of quantum mechanical nature and contains the scaled Planck constant ε. The right-hand side of (1) describes a relaxation process towards the quantum equilibrium $M[w]$. The equilibrium is defined as the formal maximizer of the von-Neumann entropy (or quantum free energy) under the constraint that its moments, i.e. the integrals $\int_{\mathbb{R}^3} M[w]\kappa(p)dp$ for some vector-valued function $\kappa(p)$, are the same as those for the given function w. This concept has been introduced by Degond and Ringhofer [13]. Denoting the Lagrange multipliers by $\lambda(x,t)$, the quantum equilibrium reads as

$$M[w](x,p,t) = \mathrm{Exp}(\lambda(x,t)\cdot\kappa(p)),$$

where the so-called quantum exponential is given by $\mathrm{Exp}(w)=W(\exp W^{-1}(w))$, W is the Wigner transform, W^{-1} its inverse, and exp is the operator exponential. When the collision operator $Q(w)=(M[w]-w)/\alpha$ conserves mass, we prescribe the local particle density, and the quantum equilibrium becomes $M[w]=\mathrm{Exp}(A(x,t)-|p|^2/2)$ for some Lagrange multiplier $A(x,t)$. The existence and uniqueness of this maximizer has been proved in [31] in a one-dimensional setting. When scattering conserves mass, momentum, and energy (thus, we take $\kappa(p)=(1,p,|p|^2/2)$), we have

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

where now A, v, and T are Lagrange multipliers. The expressions for the equilibrium distributions look similar to the corresponding classical Maxwell distributions [28]. However, $M[w]$ is a *nonlocal* operator, which expresses the nonlocal nature of quantum mechanics, and the Lagrange multipliers do *not* correspond to the moments as in the classical model. For instance, v equals the mean velocity only up to terms of order $O(\varepsilon^2)$. We derive macroscopic equations by multiplying the Wigner equation (1) by the weight vector $\kappa(p)=(1,p,\frac{1}{2}|p|^2)$. To simplify the notation, we introduce the notation $\langle f(p)\rangle = (2\pi\varepsilon)^{-3}\int_{\mathbb{R}^3} f(p)dp$, where $f(p)$ is a function. The collisions are assumed to conserve mass, momentum, and energy, $\langle (M[w]-w)\kappa(p)\rangle = 0$. Then the moment equations become

$$\partial_t\langle w\rangle + \mathrm{div}_x\langle pw\rangle + \langle\theta[V]w\rangle = 0,$$
$$\partial_t\langle pw\rangle + \mathrm{div}_x\langle p\otimes pw\rangle + \langle p\theta[V]w\rangle = 0,$$
$$\partial_t\langle \tfrac{1}{2}|p|^2w\rangle + \mathrm{div}_x\langle \tfrac{1}{2}p|p|^2w\rangle + \langle \tfrac{1}{2}|p|^2\theta[V]w\rangle = 0,$$

where $p\otimes p$ denotes a matrix with components p_jp_k $(j,k=1,2,3)$, governing the evolution of the particle density n, the momentum nu, and the energy density ne, defined by

$$n = \langle w\rangle, \quad nu = \langle pw\rangle, \quad ne = \langle \tfrac{1}{2}|p|^2w\rangle.$$

The variable $u=(nu)/n$ is the macroscopic velocity and $e=(ne)/n$ the macroscopic energy. The integrals involving the potential can be expressed in terms of the moments n, nu, and ne (see [27] for details). It remains to compute the higher-order moments $\langle p\otimes pw\rangle$ and $\langle \frac{1}{2}p|p|^2w\rangle$. For this, we employ the Chapman–Enskog expansion $w=M[w]+\alpha g$.

Introducing the quantum stress tensor $P=\langle (p-u)\otimes(p-u)M[w]\rangle$ and the quantum heat flux $q=\langle \frac{1}{2}(p-u)|p-u|^2M[w]\rangle$, a straight-forward computation leads to the following moment equations:

$$n_t + \mathrm{div}_x(nu) = 0,$$
$$(nu)_t + \mathrm{div}_x(P+nu\otimes u) - n\nabla_xV = -\alpha\mathrm{div}_x\langle p\otimes pg\rangle,$$
$$(ne)_t + \mathrm{div}_x\big((P+ne\mathbb{I})u\big) + \mathrm{div}_xq - nu\cdot\nabla_xV = -\alpha\mathrm{div}_x\langle \tfrac{1}{2}p|p|^2g\rangle,$$

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 $g=-(M[w]-w)/\alpha=-M[w]_t-p\cdot\nabla_xM[w]-\theta[V]M[w]+O(\alpha)$, 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 heat flux becomes $q=-\frac{\varepsilon^2}{24}n(\Delta_xu+2\nabla_x\mathrm{div}_xu)+O(\varepsilon^4)$, and the quantum stress tensor expands according to $P=nT\,\mathbb{I}-\frac{\varepsilon^2}{12}n\nabla_x^2\log n+O(\varepsilon^4)$, where $\nabla_x^2\log n$ is the Hessian of $\log n$, Furthermore, a tedious computation shows that (see [27])

$$-\alpha\mathrm{div}_x\langle p\otimes pg\rangle = \alpha\mathrm{div}_xS, \quad -\alpha\mathrm{div}_x\langle \tfrac{1}{2}p|p|^2g\rangle = \alpha\mathrm{div}_x(Su) + \frac{5}{2}nT\nabla_xT,$$

where $S=2nTD(u)-\frac{2}{3}nT\mathrm{div}_xu\,\mathbb{I}+O(\varepsilon^2+\alpha)$ can be interpreted as a viscous stress tensor. Here, $D(u)=(\nabla_xu+\nabla_xu^\top)/2$. The term $\frac{5}{2}nT\nabla_xT$ is the Fourier heat term, and it adds to the quantum heat flux. This shows the following result [27].

Theorem 1. *Assume that $A(u)=(\nabla u-\nabla u^\top)/2=O(\varepsilon^2)$ 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*

$$n_t + \operatorname{div}(nu) = 0, \tag{2}$$

$$(nu)_t + \operatorname{div}(nu\otimes u) + \nabla(nT) - \frac{\varepsilon^2}{12}\operatorname{div}(n\nabla^2\log n) - n\nabla V = \alpha\operatorname{div} S, \tag{3}$$

$$(ne)_t + \operatorname{div}\big((ne+nT)u\big) - \frac{\varepsilon^2}{12}\operatorname{div}\big(n(\nabla^2\log n)u\big) + \operatorname{div} q_0 - nu\cdot\nabla V = \alpha\operatorname{div}(Su),$$

where $q_0 = q + \frac{5}{2}nT\nabla T$ is the total heat flux and $S = 2nTD(u) - \frac{2}{3}nT\operatorname{div}_x u\,\mathbb{I}$ is the viscous stress tensor.

For later use, we remark that the third-order quantum term can be written equivalently as a self-interacting force term, involving the Bohm potential $\Delta\sqrt{n}/\sqrt{n}$,

$$\operatorname{div}(n\nabla^2\log n) = 2n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big). \tag{4}$$

When the collisions conserve mass and momentum only, the quantum equilibrium becomes $M[w] = \operatorname{Exp}(A - |p-v|^2/2)$. In this situation, a Chapman–Enskog expansion has been carried out by Brull and Méhats [9]. They obtain equations (2)-(3) with $T = 1$ and $S = 2nD(u)$.

3 Analysis

System (2)-(3) with $T = 1$ possesses a surprising property which has been exploited in [23] to prove the existence of solutions. More precisely, we consider the system

$$n_t + \operatorname{div}(nu) = 0, \quad x\in\mathbb{T}^d,\ t>0, \tag{5}$$

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

$$n(\cdot,0) = n_0, \quad (nu)(\cdot,0) = n_0u_0 \quad \text{in } \mathbb{T}^d, \tag{7}$$

where $\mathbb{T}^d$ is the d-dimensional torus ($d\le 3$). The function $p(n) = n^\gamma$ with $\gamma\ge 1$ is the pressure. Compared to (3), the quantum term is reformulated using (4). In the treatment of (5)-(7), we need to overcome several mathematical difficulties.

The first problem lies in the strongly nonlinear third-order differential operator and the dispersive structure of the momentum equation. In particular, as the maximum principle is not applicable, it is not clear how to obtain the positivity or nonnegativity of the particle density. In the literature, some ideas have been developed to overcome this problem. For instance, some artificial diffusion has been added to the mass equation such that the maximum principle can be applied [15]. Another idea is to introduce an additional pressure with negative powers of the density, which allows one to derive an L^∞ bound for $1/n$ [7].

The second 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 have been concerned with density-dependent viscosities, see, e.g., [5, 29] and references therein.

The third problem is the lack of suitable a priori estimates. Indeed, let us define the energy of (5)-(6) by the sum of the kinetic, internal, and quantum energies,

$$E_{\varepsilon^2}(n,u)=\int_{\mathbb{T}^d}\left(\frac{n}{2}|u|^2+H(n)+\frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2\right)dx, \tag{8}$$

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

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

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 *effective velocity*

$$w=u+\alpha\nabla\log n, \tag{9}$$

The term $\alpha\nabla\log n$ has been called in [19] the "kinematical quasivelocity". A computation shows [23] that the system (5)-(6) can be equivalently written as

$$n_t+\operatorname{div}(nw)=\alpha\Delta n, \tag{10}$$

$$(nw)_t+\operatorname{div}(nw\otimes w)+\nabla p(n)-\frac{\varepsilon_0}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)-n\nabla V=\alpha\Delta(nw), \tag{11}$$

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

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

The inequality [24]

$$\int_{\mathbb{T}^d}|\nabla^2\sqrt{n}|^2dx\le C\int_{\mathbb{T}^d}n|\nabla^2\log n|^2dx \tag{13}$$

with some constant $C>0$ provides an $L^2_{\mathrm{loc}}(0,\infty;H^2(\mathbb{T}^d))$ bound for $\sqrt{n}$. This bound is the key argument of the global existence analysis. The second advantage is that we may apply the maximum principle to the parabolic equation (10) to deduce strict positivity of the density n if n_0 is strictly positive and the velocity w is smooth.

The viscous quantum Euler model (10)-(11) is of interest by itself. Indeed, it has been derived from a Wigner–Fokker–Planck equation by a moment method [18]. The viscous terms $\alpha\Delta n$ and $\alpha\Delta(nw)$ arise from the moments of the Fokker–Planck collision operator. This operator also provides the momentum relaxation term $-nw/\tau$ to the right-hand side of the momentum equation, where $\tau>0$ is the relaxation time. For existence results for the viscous quantum Euler system, we refer to [11, 17, 18, 26].

Neglecting the viscous terms ($\alpha=0$), the two systems (5)-(6) and (10)-(11) reduce to the so-called quantum hydrodynamic model, see, e.g., [16, 22]. First mathematical results have been concerned with the local existence of solutions or the global existence of near-equilibrium solutions. For the stationary problem, only the existence of "subsonic" solutions has been achieved so far [21]. Recently, the global existence of weak transient solutions for general initial data has been shown by Antonelli and Marcati [2].

Interestingly, the effective velocity (9) has been used also in related models. First, Bresch and Desjardins employed it to derive new entropy estimates for viscous Korteweg-type and shallow-water equations [6]. Brenner [4] suggested the modified Navier–Stokes model

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

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 [26] to prove the existence of solutions to the one-dimensional stationary viscous quantum Euler problem with physical boundary conditions.

The strategy of the existence proof for (5)-(7) is as follows. First, the viscous quantum Euler system (10)-(11) is approximated by a projection of the infinite-dimensional momentum equation onto a finite system of ordinary differential equations on a Faedo-Galerkin space with dimension N, following the ideas of Feireisl in [15] and generalizing the one-dimensional approach in [17]. We need a second approximation parameter δ by adding the term $\delta(\Delta w-w)$ to the right-hand side of (11), which allows one to derive an H^1 estimate for w. The global existence of approximate solutions (n_δ,w_δ) follows from the energy estimate (12), which also provides some Sobolev estimates independent of (N,δ). The limits $N\to\infty$ and $\delta\to 0$ then give the following existence result; for a proof we refer to [23].

Theorem 2. *Let $d\le 3$, ε, $\alpha>0$, $p(n)=n^\gamma$ with $\gamma>3$ if $d=3$ and $\gamma\ge 1$ if $d=2$, $\nabla V\in L^\infty(0,\infty;L^\infty(\mathbb{T}^d))$, and (n_0,u_0) is such that $n_0\ge 0$ and $E_\varepsilon(n_0,u_0+\alpha\nabla\log n_0)$ is finite. Then there exists a weak solution (n,u) to* (5)-(7) *with the regularity*

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

satisfying (5) *pointwise and, for all* $T_0>0$ *and for all smooth test functions satisfying* $\phi(\cdot,T_0)=0$,

$$-\int_{\mathbb{T}^d} n_0^2 u_0\cdot\phi(\cdot,0)dx = \int_0^{T_0}\int_{\mathbb{T}^d}\Big(n^2u\cdot\phi_t - n^2\mathrm{div}(u)u\cdot\phi + nu\otimes nu:\nabla\phi \\ + \frac{\gamma}{\gamma+1}n^{\gamma+1}\mathrm{div}\,\phi - 2\varepsilon^2\Delta\sqrt{n}\big(2\sqrt{n}\nabla n\cdot\phi + n^{3/2}\mathrm{div}\,\phi\big) \\ + n^2\nabla V\cdot\phi - \nu nD(u):\big(n\nabla\phi+\nabla n\otimes\phi\big)\Big)dxdt. \qquad (14)$$

In the above theorem, the product "$A:B$" means summation over both indices of the matrices A and B. In order to control the behavior of the solutions when the particle density n vanishes, we need to define test functions for the momentum equation, which are, in some sense, supported on the set $\{n>0\}$. In fact, we have chosen in the weak formulation (14) as in [8] test functions of the form $n\phi$, where ϕ is some smooth function, in order to deal with the convection term.

The restriction $\gamma>3$ is needed to improve the uniform L^3 bound for n (obtained from the H^1 bound for $\sqrt{n}$) to an L^γ bound. This property helps us in the limit $\delta\to 0$ to achieve a suitable weak convergence result (see [23] for details).

Theorem 2 is proved in [23] for the case $\varepsilon^2>12\alpha^2$. This condition is necessary to obtain H^2 bounds for $\sqrt{n}$ via the viscous quantum Euler model from the new energy estimate (12). 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 [14]. Indeed, using (an approximation of) the test function $\Delta\sqrt{n}/\sqrt{n}$ in (10) leads to

$$\frac{d}{dt}\int_{\mathbb{T}^d}|\nabla\sqrt{n}|^2dx+\frac{\alpha}{4}\int_{\mathbb{T}^3}n|\nabla^2\log n|^2dx\le\frac{1}{4\alpha}\int_{R^3}n|\nabla w|^2dx. \qquad (15)$$

In view of the energy inequality (12), the right-hand side is uniformly bounded. By (13), this shows the desired H^2 bound for $\sqrt{n}$. Jiang and Jiang [20] have combined the inequalities (12) and (15) 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 (12) and (15) to conclude

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

Since $12\alpha^2-\varepsilon_0=\varepsilon^2>0$, we obtain an L^2 estimate for $\sqrt{n}|\nabla w|$. Going back to (15), 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 (13), the desired H^2 bound for $\sqrt{n}$.

4 Numerical simulation

In this section we present the results from our numerical simulation of a simple resonant tunneling diode, computed from the one-dimensional stationary quantum Navier–Stokes model (5)-(6) with $\gamma = 1$, coupled to the Poisson equation $\lambda^2 V_{xx} = n - C(x)$, $x \in (0,1)$, where λ is the Debye length and $C(x)$ is the doping concentration. The geometry of the diode is as follows. The length of the diode is 75 nm. It consists of two highly doped 25 nm GaAs regions near the contacts and a lightly doped 25 nm middle region. The middle region contains a quantum well of 5 nm length sandwiched between two 5 nm $Al_{0.3}Ga_{0.7}As$ barriers. This double barrier heterostructure is placed between two 5 nm GaAs spacer layers. The barrier height B is incorporated in the model by replacing V by $V + B$ in the momentum equation. The effective electron mass in GaAs is $m_{\text{eff}} = 0.067 \cdot m_0$ ($m_0 = 10^{-31}$ kg) and we have chosen $\alpha = \varepsilon$. For the unscaled model and the other physical parameters, we refer to [27]. The boundary conditions are

$$n(0) = C(0), \quad n(1) = C(1), \quad n_x(0) = n_x(1) = 0,$$
$$u_x(0) = u_x(1) = 0, \quad T(0) = T(1) = T_0, \quad V(0) = 0, \quad V(1) = U,$$

where $T_0 = 77$ K is the lattice temperature and U is the applied voltage.

We have discretized the stationary quantum Navier–Stokes–Poisson system using central finite differences on a uniform mesh with $N = 500$ points. Compared to previously approximated quantum fluid models [25, 26], we do not need any numerical stabilization. The resulting nonlinear discrete system is solved by the (undamped) Newton method, together with a continuation in the applied voltage with the voltage step $\triangle V = 1$ mV.

Figure 1 shows the dependence of the current-voltage characteristics on the number of the discretization points N. As expected, there is a region of negative differential resistance (NDR) in which the current density decreases although the applied voltage increases. It seems that the characteristics converge to some "limit curve" as $N \to \infty$, thus confirming numerical stability. The influence of the effective mass m_{eff} and the barrier height B is depicted in Figure 2. As observed in other quantum hydrodynamic simulations [25, 26], there is no NDR region using the physical effective mass, but the NDR effect is more pronounced for larger (unphysical) values. Furthermore, larger barrier heights enhance NDR.

Finally, we present the dependence of the model on the viscous parameter α; see Figure 3. When α is much smaller than ε, several NDR regions occur, whereas for α larger than ε, we observe only one NDR region. The electron density develops "wiggles" at the right barrier which are due to the NDR effect and which have been observed in the quantum hydrodynamic model with $\alpha = 0$.

A more complete numerical study and a numerical comparison with other quantum hydrodynamic models can be found in the work [27] in which the full quantum Navier–Stokes–Poisson system is solved.

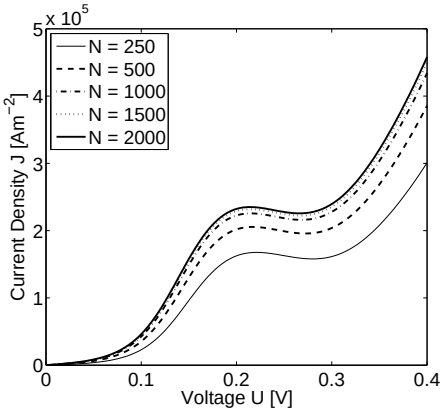

Fig. 1 Current-voltage characteristics for various values of the number N of discretization points.

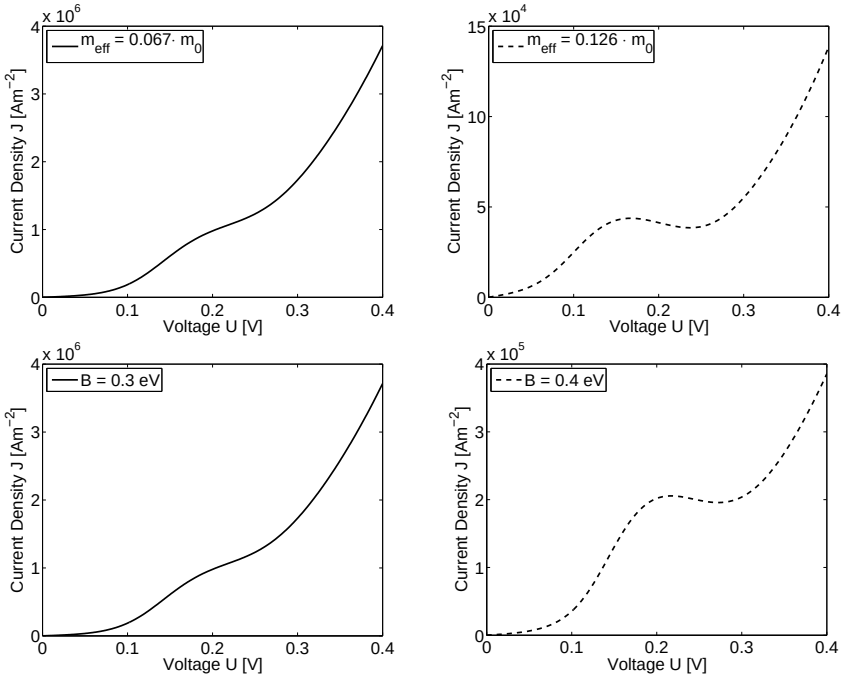

Fig. 2 Current-voltage characteristics for different effective masses m_{eff} and barrier heights B.

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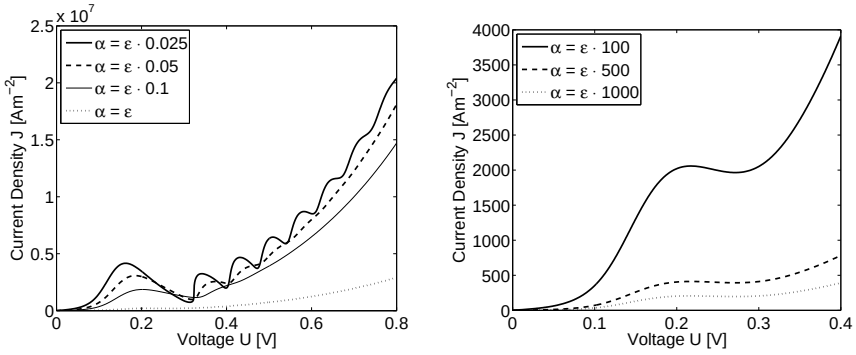

Fig. 3 Current-voltage characteristics for different values of α.

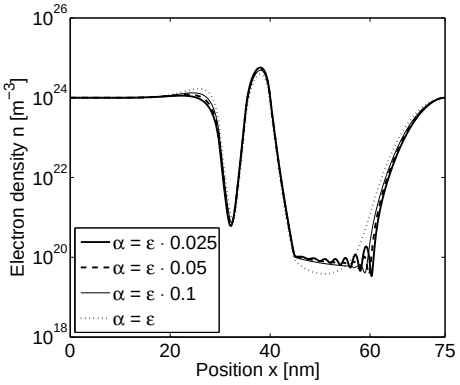

Fig. 4 Electron density for different values of α.

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