

ASC Report No. 02/2011

Full Compressible Navier-Stokes Equations for Quantum Fluids: Derivation and Numerical Solution

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www.asc.tuwien.ac.at ISBN 978-3-902627-04-9

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ISBN 978-3-902627-04-9

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FULL COMPRESSIBLE NAVIER-STOKES EQUATIONS FOR QUANTUM FLUIDS: DERIVATION AND NUMERICAL SOLUTION

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ABSTRACT. Navier-Stokes equations for compressible quantum fluids, including the energy equation, are derived from a collisional Wigner equation, using the quantum entropy maximization method of Degond and Ringhofer. The viscous corrections are obtained from a Chapman-Enskog expansion around the quantum equilibrium distribution and correspond to the classical viscous stress tensor with particular viscosity coefficients depending on the particle density and temperature. The energy and entropy dissipations are computed and discussed. Numerical simulations of a one-dimensional tunneling diode show the stabilizing effect of the viscous correction and the impact of the relaxation terms on the current-voltage characteristics.

1. Introduction. Degond and Ringhofer initiated in [11] a program to derive a model hierarchy for quantum fluids by extending the moment method of Levermore [23] to the quantum context. The moment equations are closed by taking that distribution function in the definition of the moments, which maximizes the quantum entropy (or, more precisely, free energy) under the constraints of given moments. In the classical setting, this approach was first used by Dreyer [13], later carried out by Levermore [23], and refined by Anile and coworkers for semiconductor device modeling [1].

By applying a hydrodynamic scaling in the quantum Liouville equation (or Wigner equation), Degond and Ringhofer formally derived nonlocal quantum hydrodynamic models [11] (also see the recent reviews [8, 9]). In contrast to the classical equations, the quantum stress tensor may be nondiagonal and the quantum heat flux may not vanish. Local quantum hydrodynamic equations were obtained by expanding the quantum equilibrium distribution in powers of the scaled Planck constant

2000 *Mathematics Subject Classification.* Primary: 35Q30, 76Y05; Secondary: 35Q40, 82D37.

Key words and phrases. Quantum Navier-Stokes equations, density-dependent viscosity, Chapman-Enskog expansion, finite differences, tunneling diode, semiconductors.

The first author acknowledges partial support from the Austrian Science Fund (FWF), grants P20214 and I395, and from the Austrian-French and Austrian-Spanish Projects of the Austrian Exchange Service (ÖAD). Both authors have been supported by the Austrian-Croatian Project of the ÖAD (HR 01/2010) and the Ministry of Science, Education, and Sports of the Republic of Croatia (MZOS).

[21, 22] (also see [7]). Similar model equations were derived by Gardner [15] who used another equilibrium distribution motivated from classical gas dynamics.

Quantum diffusion models can be derived from collisional Wigner equations [20]. In some physical applications, such as semiconductor theory, momentum is transferred to the crystal lattice such that only mass and energy are conserved. Then the mean momentum of the thermal equilibria vanishes and the hydrodynamic equations are not well adapted to the macroscopic fluid transport [9]. Instead, one may employ a diffusive scale in the Wigner equation with suitable scattering terms, which leads to quantum drift-diffusion and quantum energy-transport models, see [6, 10].

All these models were obtained by performing the zero-mean-free-path limit in the collisional Wigner equation. In the first-order approximation of the mean-free path, it is well known in classical gas dynamics that this leads to viscous corrections to the Euler equations. This idea was applied by Brull and Méhats in [4] to derive the *isothermal* quantum Navier-Stokes equations. In this paper, we complement the result of [4] by computing the *full* quantum Navier-Stokes equations, i.e. including the energy equation, and its local approximation. Moreover, we discuss the energy and entropy dissipation of the resulting model and present, for the first time, numerical results for these models.

To this end, we start from a collisional Wigner equation in the hydrodynamic scaling,

$$w_t + p \cdot \nabla_x w + \theta[V] = \frac{1}{\alpha}(M[w] - w) + \frac{\alpha}{\tau}(\Delta_p w + \operatorname{div}_p(pw)), \quad (1)$$

where $w(x, p, t)$ is the Wigner function in the phase-space variables $(x, p) \in \mathbb{R}^3 \times \mathbb{R}^3$ and time $t > 0$, α is the scaled mean-free path (which is assumed to be small compared to one), τ is a relaxation time, and $\theta[V]$ is a nonlocal potential operator, involving the scaled Planck constant ε (see Section 2.1 for a definition). The electric potential V may be a given function or self-consistently coupled to the particle density through the Poisson equation. The collision operator on the right-hand side of (1) consists of two terms: The dominant term is of relaxation type, i.e., the Wigner function has the tendency to tend to the quantum equilibrium or quantum Maxwellian $M[w]$ (see Section 2.1). The second term is a Caldeira-Leggett-type collision operator [5]. Its moments lead to momentum and energy relaxation expressions which are often used in quantum hydrodynamic equations [17].

Performing a Chapman-Enskog expansion $w = M[w] + \alpha g$ around the quantum Maxwellian gives nonlocal equations for the first moments of w , the particle density n , the momentum nu , and the energy density ne , including viscous corrections of order α . Local expressions in the particle density n , velocity u , and temperature T are obtained by expanding the higher-order moments in powers of ε^2 . Then, assuming further that the temperature variations and the vorticity $A(u) = \frac{1}{2}(\nabla u - \nabla u^\top)$ are of order ε^2 , i.e. $\nabla \log T = O(\varepsilon^2)$ and $A(u) = O(\varepsilon^2)$, the expansion up to order $O(\alpha^2 + \alpha\varepsilon^2 + \varepsilon^4)$ gives the following quantum Navier-Stokes system:

$$n_t + \operatorname{div}(nu) = 0, \quad x \in \mathbb{R}^3, \quad t > 0, \quad (2)$$

$$(nu)_t + \operatorname{div}(nu \otimes u) + \nabla(nT) - \frac{\varepsilon^2}{12} \operatorname{div}(n \nabla^2 \log n) - n \nabla V = \operatorname{div} S - \frac{nu}{\tau_0}, \quad (3)$$

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

$$= \operatorname{div}(Su) - \frac{2}{\tau_0} \left(ne - \frac{3}{2}n \right), \quad (4)$$

where $u \otimes u$ is a matrix with components $u_j u_k$, ∇^2 is the Hessian matrix, $\tau_0 = \tau/\alpha$, the energy density (up to terms of order $O(\varepsilon^4)$) is given by

$$ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\Delta \log n, \quad (5)$$

the viscous stress tensor S and the total heat flux q_0 are defined by

$$S = 2\alpha n T D(u) - \frac{2}{3}\alpha n T \operatorname{div} u \mathbb{I}, \quad q_0 = -\frac{5}{2}\alpha n T \nabla T - \frac{\varepsilon^2}{24}n(\Delta u + 2\nabla \operatorname{div} u), \quad (6)$$

$D(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$ is the symmetric part of the velocity gradient, and \mathbb{I} is the unit matrix in $\mathbb{R}^{3 \times 3}$.

The mass and momentum equations (2)-(3) with constant temperature have been derived by Brull and Méhats in [4]. The novelty of this paper is the derivation of the energy equation and the numerical solution of the full Navier-Stokes model.

In the following, we comment the form of the pressure, total heat flux, and the viscous corrections. The pressure $p(n, T) = nT$ can be interpreted as the Boyle law for a perfect gas [14]. The total heat flux q_0 consists of two contributions: one from the third-order moment $q = \int_{\mathbb{R}^3} \frac{1}{2}(p-u)|p-u|^2 M[w] dp / (2\pi\varepsilon)^3$ (see (15)), which is of quantum mechanical origin, and another contribution from the heat flux $\frac{5}{2}\alpha n T \nabla T$ (computed in Section 2.4), which arises from the Chapman-Enskog expansion. The heat conductivity equals $\kappa(n, T) = \frac{5}{2}\alpha n T$, expressing the Wiedemann-Franz law. This term is often used in numerical simulations as a stabilizing term in the quantum hydrodynamic equations, see e.g. [15, 22].

The viscous stress tensor for Newtonian fluids with vanishing bulk viscosity coefficient reads as $S = 2\mu(D(u) - \frac{1}{3}\operatorname{div} u \mathbb{I})$ [14]. In our model, the viscosity coefficient is equal to $\mu = \alpha n T$. Thus, in the semi-classical limit $\varepsilon \rightarrow 0$, we recover the classical Navier-Stokes equations with the above viscosity coefficient which can be also obtained from a Chapman-Enskog expansion of the classical BGK model.

The global-in-time existence of weak solutions to the barotropic quantum fluid model (2)-(3) with $T = 1$ was proved, in a one-dimensional setting, in [19] for $\varepsilon = \alpha$ and, in several space dimensions, in [18] for $\varepsilon > \alpha$, in [12] for $\varepsilon = \alpha$, and in [16] for $\varepsilon < \alpha$. Up to our knowledge, no analytical results are available for the system (2)-(4).

The paper is organized as follows. In Section 2, we perform the Chapman-Enskog expansion of the Wigner function and derive the local quantum Navier-Stokes equations (2)-(4). We show in Section 3 that the total energy, consisting of the thermal, kinetic, and quantum energy, is conserved for all time if $1/\tau = 0$. Furthermore, the fluid entropy is dissipated for incompressible fluids. Finally, numerical simulations of a one-dimensional tunneling diode and stationary current-voltage characteristics are presented in Section 4.

2. Derivation of the model. In this section, we derive the system (2)-(4) from the Wigner equation (1).

2.1. The Wigner-BGK equation. We recall the kinetic quantum model [3] introduced in the introduction:

$$w_t + p \cdot \nabla_x w + \theta[V]w = \frac{1}{\alpha}(M[w] - w) + \frac{\alpha}{\tau}(\Delta_p w + \operatorname{div}_p(pw)). \quad (7)$$

The pseudo-differential operator

$$(\theta[V]w)(x, p, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} (\delta V)(x, \eta, t) w(x, p', t) e^{i(p-p') \cdot \eta} dp' d\eta$$

with its symbol

$$(\delta V)(x, \eta, t) = \frac{i}{\varepsilon} \left(V \left(x + \frac{\varepsilon}{2} \eta, t \right) - V \left(x - \frac{\varepsilon}{2} \eta, t \right) \right)$$

models the influence of the electric potential $V = V(x, t)$, which is assumed to be a given function or selfconsistently coupled to the Poisson equation. Here, $\varepsilon > 0$ denotes the scaled Planck constant. In the semiclassical limit $\varepsilon \rightarrow 0$, the potential operator $\theta[V]w$ converges formally to its classical counterpart $\nabla_x V \cdot \nabla_p w$. We refer to [17] for some properties on the Wigner equation.

The first term on the right-hand side of (7) describes a relaxation process towards the quantum equilibrium state $M[w]$, the so-called quantum Maxwellian which has been introduced in [11]. It is the formal maximizer of the quantum free energy subject to the constraints of given mass, momentum, and energy. More precisely, let the quantum exponential and quantum logarithm be defined by

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

where W is the Wigner transform, W^{-1} its inverse, and \exp and \log are the operator exponential and logarithm, respectively, defined by their corresponding spectral decompositions [11]. The quantum free energy is given by

$$S(w) = -\frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} w(x, p, \cdot) \left((\text{Log } w)(x, p, \cdot) - 1 + \frac{|p|^2}{2} - V(x, \cdot) \right) dx dp.$$

Whereas the classical free energy is a function on the configuration space, the quantum free energy at given time is a real number, which underlines the nonlocal nature of quantum mechanics. For a given Wigner function w , let $M[w]$ be the formal maximizer of $S(f)$, where f has the same moments as w , i.e.

$$\int_{\mathbb{R}^3} w \left(\begin{array}{c} 1 \\ p \\ |p|^2/2 \end{array} \right) dp = \int_{\mathbb{R}^3} f \left(\begin{array}{c} 1 \\ p \\ |p|^2/2 \end{array} \right) dp.$$

If such a solution exists, it has the form

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

where A , v , and T are some Lagrange multipliers [11, 17]. The rigorous solvability of the constrained maximization problem is a delicate issue. It is shown in [25] that there exists a unique maximizer of S subject to a given local density $\int_{\mathbb{R}^3} f dp / (2\pi\varepsilon)^3$ in the one-dimensional setting. By definition, the quantum Maxwellian satisfies for all functions w

$$\int_{\mathbb{R}^3} (M[w] - w) \left(\begin{array}{c} 1 \\ p \\ |p|^2/2 \end{array} \right) dp = 0. \quad (8)$$

Physically, this means that the collision operator $Q(w) = (M[w] - w)/\alpha$ conserves mass, momentum, and energy.

2.2. Nonlocal moment equations. We introduce the notation

$$\langle g(p) \rangle = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} g(p) dp$$

for functions $g(p)$. Multiplying the Wigner equation (7) by 1, p , and $|p|^2/2$, respectively, integrating over $p \in \mathbb{R}^3$, and employing (8), we obtain the moment equations

$$\begin{aligned} \partial_t \langle w \rangle + \operatorname{div}_x \langle pw \rangle + \langle \theta[V]w \rangle &= 0, \\ \partial_t \langle pw \rangle + \operatorname{div}_x \langle p \otimes pw \rangle + \langle p\theta[V]w \rangle &= -\alpha\tau^{-1} \langle pw \rangle, \\ \partial_t \langle \tfrac{1}{2}|p|^2 w \rangle + \operatorname{div}_x \langle \tfrac{1}{2}p|p|^2 w \rangle + \langle \tfrac{1}{2}|p|^2 \theta[V]w \rangle &= -\alpha\tau^{-1} \langle |p|^2 w - 3w \rangle, \end{aligned}$$

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

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

The variable $u = (nu)/n$ is the macroscopic velocity and $e = (ne)/n$ the macroscopic energy. The moments on the right-hand side of the moment equations can be written as

$$-\frac{\alpha}{\tau} \langle pw \rangle = -\frac{nu}{\tau_0}, \quad -\frac{\alpha}{\tau} \langle |p|^2 w - 3w \rangle = -\frac{2}{\tau_0} \left(ne - \frac{3}{2}n \right),$$

where $\tau_0 = \tau/\alpha$, and the moments of the potential operator $\theta[V]$ can be simplified as shown in the following lemma.

Lemma 2.1. *The moments of the potential operator $\theta[V]$ become*

$$\langle \theta[V] \rangle = 0, \quad \langle p\theta[V]w \rangle = -n\nabla_x V, \quad (9)$$

$$\langle p \otimes p\theta[V]w \rangle = -2nu \otimes_s \nabla_x V, \quad \langle \tfrac{1}{2}|p|^2 \theta[V]w \rangle = -nu \cdot \nabla_x V, \quad (10)$$

$$\langle \tfrac{1}{2}p|p|^2 \theta[V]w \rangle = -(\langle p \otimes pw \rangle + ne\mathbb{I})\nabla_x V + \frac{\varepsilon^2}{8}n\nabla_x \Delta_x V, \quad (11)$$

where $a \otimes_s b = \frac{1}{2}(a \otimes b + b \otimes a)$ denotes the symmetrized tensor product and \mathbb{I} is the unit matrix in $\mathbb{R}^{3 \times 3}$.

The moments (9) are computed in Lemma 12.9 in [17], (11) is shown in Lemma 13.2 in [17], and (10) is proved in Lemma 1 in [25].

In order to calculate the moments $\langle p \otimes pw \rangle$ and $\langle \tfrac{1}{2}p|p|^2 w \rangle$, which appear in the moment equations, we use the Chapman-Enskog expansion

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

which defines the function g . The moments can be written as

$$\langle p \otimes pw \rangle = \langle p \otimes pM[w] \rangle + \alpha \langle p \otimes pg \rangle, \quad \langle \tfrac{1}{2}p|p|^2 w \rangle = \langle \tfrac{1}{2}p|p|^2 M[w] \rangle + \alpha \langle \tfrac{1}{2}p|p|^2 g \rangle, \quad (12)$$

Inserting the Chapman-Enskog expansion in the Wigner equation (7), we obtain an explicit expression for g :

$$\begin{aligned} g &= -\frac{1}{\alpha}(M[w] - w) = -w_t - p \cdot \nabla_x w - \theta[V]w + \alpha\tau^{-1}(\Delta_p w + \operatorname{div}_p(pw)) \\ &= -M[w]_t - p \cdot \nabla_x M[w] - \theta[V]M[w] + O(\alpha), \end{aligned} \quad (13)$$

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

It remains to compute the higher-order moments of $M[w]$ and g . To this end, we introduce the quantum stress tensor P and quantum heat flux q ,

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

Then, using the relations $\langle M[w] \rangle = \langle w \rangle = n$, $\langle pM[w] \rangle = nu$, and $\langle \frac{1}{2}|p|^2 M[w] \rangle = ne$, which follow from (8), we compute

$$\begin{aligned} P &= \langle p \otimes pM[w] \rangle - u \otimes \langle pM[w] \rangle - \langle pM[w] \rangle \otimes u + u \otimes u \langle M[w] \rangle \\ &= \langle p \otimes pM[w] \rangle - nu \otimes u, \end{aligned} \quad (14)$$

$$\begin{aligned} q &= \langle \frac{1}{2}p|p|^2 M[w] \rangle - \langle \frac{1}{2}|p|^2 M[w] \rangle u + \frac{1}{2}|u|^2 \langle pM[w] \rangle - \frac{1}{2}u|u|^2 \langle M[w] \rangle \\ &\quad - \langle p \otimes pM[w] \rangle u + u \otimes u \langle pM[w] \rangle \\ &= \langle \frac{1}{2}p|p|^2 M[w] \rangle - (P + ne\mathbb{I})u. \end{aligned} \quad (15)$$

Hence, by (12), we can write

$$\begin{aligned} \langle p \otimes pw \rangle &= P + nu \otimes u + \alpha \langle p \otimes pg \rangle, \\ \langle \frac{1}{2}p|p|^2 w \rangle &= (P + ne\mathbb{I})u + q + \alpha \langle \frac{1}{2}p|p|^2 g \rangle. \end{aligned}$$

This shows the following lemma.

Lemma 2.2. *Up to terms of order $O(\alpha^2)$, the moment equations of the Wigner equation read as follows:*

$$n_t + \operatorname{div}_x(nu) = 0, \quad (16)$$

$$(nu)_t + \operatorname{div}_x(P + nu \otimes u) - n \nabla_x V = \alpha \operatorname{div}_x S_1 - \frac{nu}{\tau_0}, \quad (17)$$

$$(ne)_t + \operatorname{div}_x((P + ne\mathbb{I})u) + \operatorname{div}_x q - nu \cdot \nabla_x V = \alpha \operatorname{div}_x S_2 - \frac{2}{\tau_0} \left(ne - \frac{3}{2}n \right), \quad (18)$$

where $\tau_0 = \tau/\alpha$ and S_1 and S_2 are given by

$$\begin{aligned} S_1 &= \partial_t \langle p \otimes pM[w] \rangle + \operatorname{div}_x \langle p \otimes p \otimes pM[w] \rangle + \langle p \otimes p\theta[V]M[w] \rangle, \\ S_2 &= \partial_t \langle \frac{1}{2}p|p|^2 M[w] \rangle + \operatorname{div}_x \langle \frac{1}{2}p \otimes p|p|^2 M[w] \rangle + \langle \frac{1}{2}p|p|^2 \theta[V]M[w] \rangle. \end{aligned}$$

These equations can be interpreted as a nonlocal quantum Navier-Stokes system. By expanding the quantum Maxwellian $M[w]$ in powers of ε^2 , we derive a local version of this system. Such an expansion has been already carried out in [22] for P , q , and ne . Under the assumptions that the temperature varies slowly and that the vorticity tensor $A(u)$ is small, in the sense of $\nabla_x \log T = O(\varepsilon^2)$ and $A(u) = \frac{1}{2}(\nabla u - \nabla u^\top) = O(\varepsilon^2)$, it is shown in [22] that

$$P = nT\mathbb{I} - \frac{\varepsilon^2}{12}n\nabla_x^2 \log n + O(\varepsilon^4), \quad (19)$$

$$q = -\frac{\varepsilon^2}{24}n(\Delta_x u + 2\nabla_x \operatorname{div}_x u) + O(\varepsilon^4),$$

$$ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\Delta_x \log n + O(\varepsilon^4). \quad (20)$$

(Notice that the formula for q in [22] contains a misprint.) Moreover, the Lagrange multiplier v is related to the macroscopic velocity u by [22]

$$nu = nv + O(\varepsilon^2). \quad (21)$$

In the following subsections, we derive local expressions for the viscous terms S_1 and S_2 up to order $O(\alpha\varepsilon^2 + \alpha^2)$.

2.3. Calculation of S_1 . We set $S_1 = S_{11} + S_{12} + S_{13}$, where

$$S_{11} = \partial_t \langle p \otimes p M[w] \rangle, \quad S_{12} = \operatorname{div}_x \langle p \otimes p \otimes p M[w] \rangle, \quad S_{13} = \langle p \otimes p \theta[V] M[w] \rangle.$$

It is sufficient to compute these expressions up to terms of order $O(\alpha)$ or $O(\varepsilon^2)$ since the expressions $\alpha \operatorname{div}_x S_1$ and $\alpha \operatorname{div}_x S_2$ are already of order $O(\alpha)$. By Lemma 2.1, we have

$$S_{13} = -2nu \otimes_s \nabla_x V. \quad (22)$$

For the calculation of S_{12} , we set $s = (p - v)/\sqrt{T}$ and employ the following expansions (see [22]).

Lemma 2.3. *It holds:*

$$\begin{aligned} \langle s M[w] \rangle &= O(\varepsilon^2), & \langle s \otimes s \otimes s M[w] \rangle &= O(\varepsilon^2), \\ \langle s \otimes s M[w] \rangle &= n\mathbb{I} + O(\varepsilon^2), & \langle s \otimes s |s|^2 M[w] \rangle &= 5n\mathbb{I} + O(\varepsilon^2). \end{aligned}$$

Taking into account (21) and Lemma 2.3, we infer that

$$\begin{aligned} \langle p_j p_k p_\ell M[w] \rangle &= \langle (v_j + \sqrt{T} s_j)(v_k + \sqrt{T} s_k)(v_\ell + \sqrt{T} s_\ell) M[w] \rangle \\ &= \langle v_j v_k v_\ell M[w] \rangle \\ &\quad + \sqrt{T} (v_k v_\ell \langle s_j M[w] \rangle + v_j v_\ell \langle s_k M[w] \rangle + v_j v_k \langle s_\ell M[w] \rangle) \\ &\quad + T (v_j \langle s_k s_\ell M[w] \rangle + v_k \langle s_j s_\ell M[w] \rangle + v_\ell \langle s_j s_k M[w] \rangle) \\ &\quad + T^{3/2} \langle s_j s_k s_\ell M[w] \rangle \\ &= nu_j u_k u_\ell + nT (u_j \delta_{k\ell} + u_k \delta_{j\ell} + u_\ell \delta_{jk}) + O(\varepsilon^2). \end{aligned} \quad (23)$$

Hence,

$$S_{12} = \operatorname{div}_x (nu \otimes u \otimes u) + \operatorname{div}_x (nT u) \mathbb{I} + 2 \nabla_x (nT) \otimes_s u + 2nTD(u) + O(\varepsilon^2), \quad (24)$$

where we recall that $D(u) = \frac{1}{2}(\nabla u + \nabla u^\top)/2$.

The calculation of S_{11} is more involved. By (14) and (19), we have

$$\langle p \otimes p M[w] \rangle = P + nu \otimes u = nT \mathbb{I} + nu \otimes u + O(\varepsilon^2),$$

and thus, the time derivative becomes

$$S_{11} = (nT \mathbb{I} + nu \otimes u)_t + O(\varepsilon^2) = \frac{2}{3}(ne)_t \mathbb{I} - \frac{1}{3}(n|u|^2)_t \mathbb{I} + (nu \otimes u)_t + O(\varepsilon^2).$$

Elementary computations show that

$$\begin{aligned} (n|u|^2)_t &= 2(nu)_t \cdot u + \operatorname{div}_x (nu) |u|^2, \\ (nu \otimes u)_t &= 2(nu)_t \otimes_s u + \operatorname{div}_x (nu) u \otimes u. \end{aligned} \quad (25)$$

Then, employing (18) and the expansions for P , ne , and q , i.e.

$$(ne)_t = -\operatorname{div}_x \left(\frac{5}{2} nT u + \frac{1}{2} nu |u|^2 \right) + nu \cdot \nabla_x V + O(\varepsilon^2 + \alpha),$$

we find that

$$\begin{aligned}
S_{11} &= \frac{2}{3}(ne)_t \mathbb{I} - \frac{2}{3}(nu)_t \cdot u \mathbb{I} + 2(nu)_t \otimes_s u + \operatorname{div}_x(nu) \left(u \otimes u - \frac{1}{3}|u|^2 \mathbb{I} \right) + O(\varepsilon^2) \\
&= -\frac{2}{3} \operatorname{div}_x \left(nu \left(\frac{5}{2}T + \frac{1}{2}|u|^2 \right) \right) \mathbb{I} + \frac{2}{3} nu \cdot \nabla_x V \mathbb{I} + \frac{2}{3} \operatorname{div}_x(nu \otimes u) \cdot u \mathbb{I} \\
&\quad + \frac{2}{3} \nabla_x(nT) \cdot u \mathbb{I} - \frac{2}{3} nu \cdot \nabla_x V \mathbb{I} - 2 \operatorname{div}_x(nu \otimes u) \otimes_s u - 2 \nabla_x(nT) \otimes_s u \\
&\quad + 2n \nabla_x V \otimes_s u + \operatorname{div}_x(nu) \left(u \otimes u - \frac{1}{3}|u|^2 \mathbb{I} \right) + O(\varepsilon^2 + \alpha).
\end{aligned}$$

The terms involving T simplify to

$$-\operatorname{div}_x(nTu) \mathbb{I} - \frac{2}{3} nT \operatorname{div}_x u \mathbb{I} - 2 \nabla_x(nT) \otimes_s u.$$

The terms involving third powers of u sum up to $-\operatorname{div}_x(nu \otimes u \otimes u)$. Hence,

$$\begin{aligned}
S_{11} &= -\operatorname{div}_x(nTu) \mathbb{I} - \frac{2}{3} nT \operatorname{div}_x u \mathbb{I} - 2 \nabla_x(nT) \otimes_s u - \operatorname{div}_x(nu \otimes u \otimes u) \\
&\quad + 2n \nabla_x V \otimes_s u + O(\varepsilon^2 + \alpha).
\end{aligned}$$

In view of (22) and (24), we conclude that

$$S_1 = 2nTD(u) - \frac{2}{3} nT \operatorname{div}_x u \mathbb{I} + O(\varepsilon^2 + \alpha).$$

2.4. Calculation of S_2 . Similarly as in the previous subsection, we set $S_2 = S_{21} + S_{22} + S_{23}$, where

$$S_{21} = \partial_t \langle \frac{1}{2} p |p|^2 M[w] \rangle, \quad S_{22} = \operatorname{div}_x \langle \frac{1}{2} p \otimes p |p|^2 M[w] \rangle, \quad S_{23} = \langle \frac{1}{2} p |p|^2 \theta[V] M[w] \rangle.$$

Formula (11) and the expansions (14), (19), and (20) show that

$$\begin{aligned}
S_{23} &= -(P + nu \otimes u + ne \mathbb{I}) \nabla_x V + O(\varepsilon^2) \\
&= -\left(\frac{5}{2} nT \mathbb{I} + \frac{1}{2} n|u|^2 \mathbb{I} + nu \otimes u \right) \nabla_x V + O(\varepsilon^2).
\end{aligned}$$

Next, we calculate the fourth moment $\langle \frac{1}{2} p \otimes p |p|^2 M[w] \rangle$. Setting $s = (p - v)/\sqrt{T}$ and employing Lemma 2.3 and (21), we obtain

$$\begin{aligned}
\langle \frac{1}{2} p \otimes p |p|^2 M[w] \rangle &= \langle \frac{1}{2} (v + \sqrt{T}s) \otimes (v + \sqrt{T}s) |v + \sqrt{T}s|^2 M[w] \rangle \\
&= \langle \frac{1}{2} v \otimes v |v|^2 M[w] \rangle + \sqrt{T} (v \otimes_s \langle sM[w] \rangle |v|^2 \\
&\quad + (v \otimes v) v \cdot \langle sM[s] \rangle) + T \left(\frac{1}{2} \langle s \otimes sM[w] \rangle |v|^2 \right. \\
&\quad + v \otimes v \langle \frac{1}{2} |s|^2 M[w] \rangle + 2 \langle (v \otimes_s s) v \cdot sM[w] \rangle \\
&\quad + T^{3/2} (v \otimes_s \langle s |s|^2 M[w] \rangle + \langle s \otimes s \otimes sM[w] \rangle \cdot v) \\
&\quad \left. + T^2 \langle \frac{1}{2} s \otimes s |s|^2 M[w] \rangle \right) \\
&= \frac{1}{2} nu \otimes u |u|^2 + \frac{1}{2} T |u|^2 \langle s \otimes sM[w] \rangle + \frac{1}{2} Tu \otimes u \langle |s|^2 M[w] \rangle \\
&\quad + 2Tu \otimes_s \langle s(u \cdot s) M[w] \rangle + \frac{1}{2} T^2 \langle s \otimes s |s|^2 M[w] \rangle + O(\varepsilon^2) \\
&= \frac{1}{2} nu \otimes u |u|^2 + \frac{1}{2} nT |u|^2 \mathbb{I} + \frac{7}{2} nT (u \otimes u) + \frac{5}{2} nT^2 \mathbb{I} + O(\varepsilon^2).
\end{aligned}$$

Therefore,

$$S_{22} = \frac{1}{2} \operatorname{div}_x (nu \otimes u |u|^2) + \frac{1}{2} \nabla_x (nT |u|^2) + \frac{7}{2} \operatorname{div}_x (nTu \otimes u) + \frac{5}{2} \nabla_x (nT^2) + O(\varepsilon^2).$$

It remains to calculate the time derivative of $\langle \frac{1}{2} p |p|^2 M[w] \rangle$. Setting $k = \ell$ in (23) and summing over j , we find that

$$\langle \frac{1}{2} p |p|^2 M[w] \rangle = \frac{5}{2} nTu + \frac{1}{2} nu |u|^2 + O(\varepsilon^2).$$

Hence,

$$\begin{aligned} S_{21} &= \partial_t \left(\frac{5}{2} nTu + \frac{1}{2} nu |u|^2 \right) + O(\varepsilon^2) = \partial_t \left(\frac{5}{3} ne u - \frac{1}{3} nu |u|^2 \right) + O(\varepsilon^2) \\ &= \frac{5}{3} (ne)_t u + \frac{5}{3} \left(\frac{3}{2} T + \frac{1}{2} |u|^2 \right) nu_t - \frac{1}{3} (n|u|^2)_t u - \frac{1}{3} |u|^2 nu_t + O(\varepsilon^2) \\ &= \frac{5}{3} (ne)_t u + \left(\frac{5}{2} T + \frac{1}{2} |u|^2 \right) nu_t - \frac{1}{3} (n|u|^2)_t u + O(\varepsilon^2). \end{aligned}$$

By (25) and $nu_t = (nu)_t + \operatorname{div}_x (nu)u$ (which is a consequence of (16)), it follows that

$$\begin{aligned} S_{21} &= \frac{5}{3} (ne)_t u + \left(\frac{5}{2} T + \frac{1}{2} |u|^2 \right) (nu)_t + \left(\frac{5}{2} T + \frac{1}{2} |u|^2 \right) \operatorname{div}_x (nu)u \\ &\quad - \frac{1}{3} \operatorname{div}_x (nu) |u|^2 u - \frac{2}{3} uu \cdot (nu)_t + O(\varepsilon^2) \\ &= \frac{5}{3} (ne)_t u + \left(\frac{5}{2} T + \frac{1}{2} |u|^2 \right) (nu)_t + \left(\frac{5}{2} T + \frac{1}{6} |u|^2 \right) \operatorname{div}_x (nu)u \\ &\quad - \frac{2}{3} uu \cdot (nu)_t + O(\varepsilon^2). \end{aligned}$$

Inserting the momentum equation (17) and the energy equation (18),

$$\begin{aligned} (ne)_t &= -\operatorname{div}_x \left(\frac{5}{2} nTu + \frac{1}{2} nu |u|^2 \right) + nu \cdot \nabla_x V + O(\varepsilon^2 + \alpha), \\ (nu)_t &= -\operatorname{div}_x (nT \mathbb{I} + nu \otimes u) + n \nabla_x V + O(\varepsilon^2 + \alpha), \end{aligned}$$

in the expression for S_{21} gives

$$\begin{aligned} S_{21} &= -\frac{25}{6} \operatorname{div}_x (nTu)u - \frac{5}{6} \operatorname{div}_x (nu |u|^2)u + \frac{5}{3} nu \cdot \nabla_x V u \\ &\quad - \left(\frac{5}{2} T + \frac{1}{2} |u|^2 \right) \operatorname{div}_x (nT \mathbb{I} + nu \otimes u) + \left(\frac{5}{2} T + \frac{1}{2} |u|^2 \right) n \nabla_x V \\ &\quad + \left(\frac{5}{2} T + \frac{1}{6} |u|^2 \right) \operatorname{div}_x (nu)u + \frac{2}{3} \operatorname{div}_x (nT \mathbb{I} + nu \otimes u) \cdot uu \\ &\quad - \frac{2}{3} nuu \cdot \nabla_x V + O(\varepsilon^2 + \alpha). \end{aligned}$$

The terms involving the potential V sum up to

$$nuu \cdot \nabla_x V + \frac{5}{2} nT \nabla_x V + \frac{1}{2} n |u|^2 \nabla_x V,$$

which equals $-S_{23}$ up to terms of order $O(\varepsilon^2)$. We simplify the terms involving T :

$$-\frac{7}{2} \operatorname{div}_x (nTu \otimes u) - \frac{2}{3} nTu \operatorname{div}_x u + nT (\nabla u + \nabla u^\top) u - \frac{5}{2} T \nabla_x (nT) - \frac{1}{2} \nabla_x (nT |u|^2).$$

Finally, we summarize all remaining terms involving fourth powers of u :

$$-\frac{1}{2}|u|^2 u \operatorname{div}_x(nu) - nu(u^\top \nabla uu) - \frac{1}{2}|u|^2(u \cdot \nabla)u = -\frac{1}{2}\operatorname{div}_x(nu \otimes u|u|^2).$$

We conclude that

$$\begin{aligned} S_{21} &= \left(\frac{5}{2}nT\mathbb{I} + \frac{1}{2}n|u|^2\mathbb{I} + nu \otimes u \right) \nabla_x V + 2nTD(u)u - \frac{2}{3}nT u \operatorname{div}_x u \\ &\quad - \frac{1}{2}\nabla_x(nT|u|^2) - \frac{7}{2}\operatorname{div}_x(nTu \otimes u) - \frac{5}{2}T\nabla_x(nT) - \frac{1}{2}\operatorname{div}_x(nu \otimes u|u|^2) \\ &\quad + O(\varepsilon^2 + \alpha). \end{aligned}$$

Summing S_{21} , S_{22} , and S_{23} , some terms cancel, and we end up with

$$S_2 = \frac{5}{2}nT\nabla_x T + 2nTD(u)u - \frac{2}{3}nT u \operatorname{div}_x u + O(\varepsilon^2 + \alpha).$$

Notice that, up to the Fourier heat term $(5/2)nT\nabla_x T$, S_2 equals S_1 times u .

We have proved (formally) the following result.

Theorem 2.4. *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 (1) are given by (2)-(4), where the energy density ne , viscous stress tensor S , and the total heat flux q_0 are given by (5) and (6).*

3. Energy and entropy estimates. In this section, we prove energy and entropy estimates for the quantum Navier-Stokes system (2)-(4). Let the electric potential V solve the Poisson equation

$$\lambda^2 \Delta V = n - C(x), \tag{26}$$

where $\lambda > 0$ is the scaled Debye length and $C(x)$ models fixed background ions (doping profile).

Proposition 1. *Let (n, nu, ne) be a smooth solution to (2)-(4) and let V be the solution to (26). We assume that the variables decay sufficiently fast to zero as $|x| \rightarrow \infty$ uniformly in t . Then the total mass $N(t) = \int_{\mathbb{R}^3} n(x, t) dx$ is conserved, i.e. $dN(t)/dt = 0$, and the total energy*

$$E(t) = \int_{\mathbb{R}^3} \left(ne + \frac{\lambda^2}{2} |\nabla V|^2 \right) dx$$

is dissipated according to

$$\frac{dE}{dt} + \frac{2}{\tau_0} \int_{\mathbb{R}^3} \left(\frac{3}{2}n(T-1) + \frac{1}{2}n|u|^2 + \frac{\varepsilon^2}{6} |\nabla \sqrt{n}|^2 \right) dx = 0.$$

In particular, without relaxation ($1/\tau_0 = 0$), the energy is conserved. Furthermore, the energy can be written as

$$E(t) = \int_{\mathbb{R}^3} \left(\frac{3}{2}nT + \frac{1}{2}n|u|^2 + \frac{\varepsilon^2}{6} |\nabla \sqrt{n}|^2 + \frac{\lambda^2}{2} |\nabla V|^2 \right) dx \geq 0.$$

The total energy is the sum of the thermal, kinetic, quantum, and electric energy.

Proof. The conservation of the mass N is clear. The dissipation of E follows from

$$\begin{aligned}
\frac{dE}{dt} &= \int_{\mathbb{R}^3} ((ne)_t + \lambda^2 \nabla V \cdot \nabla V_t) dx \\
&= \int_{\mathbb{R}^3} (nu \cdot \nabla V - \lambda^2 V (\Delta V)_t) dx - \frac{2}{\tau_0} \int_{\mathbb{R}^3} \left(ne - \frac{3}{2}n \right) dx \\
&= \int_{\mathbb{R}^3} (-\operatorname{div}(nu)V - Vn_t) dx - \frac{2}{\tau_0} \int_{\mathbb{R}^3} \left(\frac{3}{2}n(T-1) + \frac{1}{2}n|u|^2 + \frac{\varepsilon^2}{24} \frac{|\nabla n|^2}{n} \right) dx \\
&= -\frac{2}{\tau_0} \int_{\mathbb{R}^3} \left(\frac{3}{2}n(T-1) + \frac{1}{2}n|u|^2 + \frac{\varepsilon^2}{6} |\nabla \sqrt{n}|^2 \right) dx
\end{aligned}$$

using (26) and (2). \square

Next, we calculate the evolution of the thermal energy $\frac{3}{2}nT$. By (5), we find that

$$\frac{3}{2}(nT)_t = (ne)_t - \frac{1}{2}(n|u|^2)_t + \frac{\varepsilon^2}{24}(n\Delta \log n)_t. \quad (27)$$

We employ (4) and (25) to reformulate the first two terms on the right-hand side:

$$\begin{aligned}
(ne)_t &= \frac{5}{2} \operatorname{div}(-nTu + \alpha nT\nabla T) - \frac{1}{2} \operatorname{div}(nu|u|^2) + \operatorname{div}(Su) + nu \cdot \nabla V \\
&\quad + \frac{\varepsilon^2}{24} \operatorname{div}(nu\Delta \log n + 2n(\nabla^2 \log n)u + n\Delta u + 2n\nabla \operatorname{div} u) \\
&\quad - \frac{2}{\tau_0} \left(ne - \frac{3}{2}n \right), \\
-\frac{1}{2}(n|u|^2)_t &= -(nu)_t \cdot u - \frac{1}{2} \operatorname{div}(nu)|u|^2 \\
&= \operatorname{div}(nu \otimes u) \cdot u - \frac{1}{2} \operatorname{div}(nu)|u|^2 + \nabla(nT) \cdot u - \frac{\varepsilon^2}{12} \operatorname{div}(n\nabla^2 \log n) \cdot u \\
&\quad - nu \cdot \nabla V - (\operatorname{div} S)u + \frac{n}{\tau_0}|u|^2.
\end{aligned}$$

Since the third-order terms in u sum up to zero,

$$-\frac{1}{2} \operatorname{div}(nu|u|^2) + \operatorname{div}(nu \otimes u) \cdot u - \frac{1}{2} \operatorname{div}(nu)|u|^2 = 0,$$

the sum $(ne)_t - \frac{1}{2}(n|u|^2)_t$ simplifies to

$$\begin{aligned}
(ne)_t - \frac{1}{2}(n|u|^2)_t &= \operatorname{div} \left(-\frac{3}{2}nTu + \frac{5}{2}\alpha nT\nabla T \right) - nT \operatorname{div} u + S : \nabla u \\
&\quad - \frac{\varepsilon^2}{12} \operatorname{div}(n\nabla^2 \log n) \cdot u + \frac{\varepsilon^2}{24} \operatorname{div}(nu\Delta \log n + 2n(\nabla^2 \log n)u \\
&\quad + n\Delta u + 2n\nabla \operatorname{div} u) - \frac{2}{\tau_0} \left(\frac{3}{2}n(T-1) - \frac{\varepsilon^2}{24}n\Delta \log n \right), \quad (28)
\end{aligned}$$

where the double point “:” means summation over both matrix indices. We notice that

$$\begin{aligned} S : \nabla u &= \alpha n T \left((\nabla u + \nabla u^\top) : \nabla u - \frac{2}{3} (\operatorname{div} u)^2 \right) \\ &= \alpha n T \left(\frac{1}{2} (\nabla u + \nabla u^\top) : (\nabla u + \nabla u^\top) - \frac{2}{3} (\operatorname{div} u)^2 \right) \\ &= \alpha n T \left(2|D(u)|^2 - \frac{2}{3} (\operatorname{div} u)^2 \right). \end{aligned}$$

The remaining time derivative becomes, by (2),

$$(n\Delta \log n)_t = -\operatorname{div}(nu)\Delta \log n - n\Delta(\nabla \log n \cdot u + \operatorname{div} u).$$

Since

$$\begin{aligned} n\Delta(\nabla \log n \cdot u + \operatorname{div} u) &= n\nabla\Delta \log n \cdot u + 2n\nabla^2 \log n : \nabla u + \Delta u \cdot \nabla n + n\Delta \operatorname{div} u \\ &= \operatorname{div}(nu\Delta \log n + 2n(\nabla^2 \log n)u + n\Delta u) - \operatorname{div}(nu)\Delta \log n \\ &\quad - 2\operatorname{div}(n\nabla^2 \log n) \cdot u, \end{aligned}$$

it follows that

$$\frac{\varepsilon^2}{24}(n\Delta \log n)_t = -\frac{\varepsilon^2}{24}\operatorname{div}(nu\Delta \log n + 2n(\nabla^2 \log n) \cdot u + n\Delta u) + \frac{\varepsilon^2}{12}\operatorname{div}(n\nabla^2 \log n) \cdot u.$$

Inserting this identity and (28) into (27), we conclude that

$$\begin{aligned} \frac{3}{2}(nT)_t + \operatorname{div} \left(\frac{3}{2}nTu - \frac{5}{2}\alpha nT\nabla T - \frac{\varepsilon^2}{12}n\nabla \operatorname{div} u \right) \\ = -nT\operatorname{div} u + \alpha nT \left(2|D(u)|^2 - \frac{2}{3}(\operatorname{div} u)^2 \right) \\ - \frac{2}{\tau_0} \left(\frac{3}{2}n(T-1) - \frac{\varepsilon^2}{24}n\Delta \log n \right). \end{aligned} \quad (29)$$

This formulation allows us to formulate the evolutions of the thermal energy and entropy.

Proposition 2. *Let (n, nu, ne) be a smooth solution to (2)-(4). We assume that the variables decay sufficiently fast to zero as $|x| \rightarrow \infty$ uniformly in t . Then*

$$\begin{aligned} \frac{3}{2} \frac{d}{dt} \int_{\mathbb{R}^3} nT dx &= \int_{\mathbb{R}^3} \nabla(nT) \cdot u dx + \alpha \int_{\mathbb{R}^3} nT \left(2|D(u)|^2 - \frac{2}{3}(\operatorname{div} u)^2 \right) \\ &\quad - \frac{2}{\tau_0} \int_{\mathbb{R}^3} \left(\frac{3}{2}n(T-1) + \frac{\varepsilon^2}{6}|\nabla \sqrt{n}|^2 \right) dx, \end{aligned} \quad (30)$$

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^3} \left(n \log \frac{n}{T^{3/2}} + \frac{3}{2}nT \right) dx \\ = - \int_{\mathbb{R}^3} \left(\frac{5}{2}\alpha \frac{n}{T} |\nabla T|^2 + \alpha n \left(2|D(u)|^2 - \frac{2}{3}(\operatorname{div} u)^2 \right) + \frac{3}{\tau_0} \frac{n}{T} (T-1)^2 \right) dx \\ - \frac{\varepsilon^2}{12} \int_{\mathbb{R}^3} \left(\frac{n}{T^2} \nabla T \cdot \nabla \operatorname{div} u - \frac{1}{\tau_0} \frac{n}{T} (T-1) \Delta \log n \right) dx. \end{aligned} \quad (31)$$

The first integral on the right-hand side of (30) expresses the energy change due to the work of compression. In incompressible fluids, this term vanishes. The second integral is nonnegative since

$$2|D(u)|^2 - \frac{2}{3}(\operatorname{div} u)^2 = \frac{1}{2} \sum_{j \neq k} \left| \frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j} \right|^2 + \frac{4}{3}(\operatorname{div} u)^2 \geq 0.$$

The third integral represents the dissipation due to relaxation. The first term on the right-hand side of (31) expresses the dissipation due to temperature variations, viscosity, and relaxation, the second term vanishes for incompressible fluids without relaxation. In this situation, the entropy is nondecreasing.

Proof. The first identity follows immediately from (29) after integration over $x \in \mathbb{R}^3$ and integrating by parts in the terms $nT \operatorname{div} u$ and $n\Delta \log n$. For the proof of the second identity, we employ (2) and (29) to obtain

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^3} \left(n \log \frac{n}{T^{3/2}} + \frac{3}{2} nT \right) dx &= \frac{d}{dt} \int_{\mathbb{R}^3} \left(\frac{5}{2} n \log n - \frac{3}{2} n \log(nT) + \frac{3}{2} nT \right) dx \\ &= \int_{\mathbb{R}^3} \left(n_t \left(\log n - \frac{3}{2} \log T \right) - \frac{5}{2} n_t - \frac{3}{2T} (nT)_t + \frac{3}{2} (nT)_t \right) dx \\ &= \int_{\mathbb{R}^3} \left[-\operatorname{div}(nu) \left(\log n - \frac{3}{2} \log T \right) \right. \\ &\quad \left. + \frac{1}{T} \operatorname{div} \left(\frac{3}{2} nTu - \frac{5}{2} \alpha nT \nabla T - \frac{\varepsilon^2}{12} n \nabla \operatorname{div} u \right) + n \operatorname{div} u \right. \\ &\quad \left. - \alpha n \left(2|D(u)|^2 - \frac{2}{3} (\operatorname{div} u)^2 \right) \right. \\ &\quad \left. - \frac{2}{\tau_0} \left(1 - \frac{1}{T} \right) \left(\frac{3}{2} n(T-1) - \frac{\varepsilon^2}{24} n \Delta \log n \right) \right] dx. \end{aligned}$$

After integration by parts, some terms cancel and we infer that

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^3} \left(n \log \frac{n}{T^{3/2}} + \frac{3}{2} nT \right) dx &= - \int_{\mathbb{R}^3} \left(\frac{5}{2} \alpha \frac{n}{T} |\nabla T|^2 + \alpha n \left(2|D(u)|^2 - \frac{2}{3} (\operatorname{div} u)^2 \right) + \frac{3}{\tau} \frac{n}{T} (T-1)^2 \right) dx \\ &\quad - \frac{\varepsilon^2}{12} \int_{\mathbb{R}^3} \left(\frac{n}{T^2} \nabla T \cdot \nabla \operatorname{div} u - \frac{1}{\tau_0} \frac{n}{T} (T-1) \Delta \log n \right) dx. \end{aligned}$$

This concludes the proof. \square

4. Numerical simulations. In this section we present some numerical simulations of a simple one-dimensional resonant tunneling diode.

4.1. Geometry and scaling. The geometry of the tunneling diode is shown in Figure 1. The total length of the device is $L = 75$ nm. The diode consists of highly doped 25 nm GaAs regions near the contacts and a lightly doped middle (channel) region of 25 nm length. The channel contains a quantum well of 5 nm length sandwiched between two 5 nm $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers with Al mole fraction $x = 0.3$. The double barrier heterostructure is placed between two 5 nm GaAs spacer layers. The double barrier height is $B = 0.4$ eV if not otherwise specified. It is incorporated into the quantum Navier-Stokes equations by replacing the potential V by $V + B$ in the momentum and the energy equations.

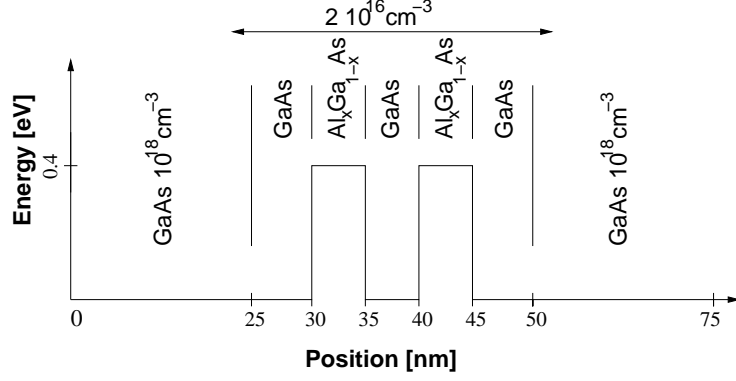


FIGURE 1. Geometry of the resonant tunneling diode and external potential modeling the double barriers.

In our simulations, we use the one-dimensional stationary full quantum Navier-Stokes equations, coupled to the Poisson equation for the electric potential. Including the physical parameters, the equations read as follows:

$$(nu)_x = 0, \quad (32)$$

$$\begin{aligned} m(nu^2)_x + k_B(nT)_x - \frac{\hbar^2}{12m}(n(\log n)_{xx})_x - qnV_x \\ = \frac{4}{3}k_B\alpha\tau_r(nTu_x)_x - \frac{mnu}{\tau_p}, \end{aligned} \quad (33)$$

$$\begin{aligned} \frac{5}{2}k_B(nTu)_x + \frac{1}{2}m(nu^3)_x - \frac{\hbar^2}{8m}(nu(\log n)_{xx} + nu_{xx})_x - qnuV_x \\ = \frac{5}{2}k_B\alpha\sigma(nTT_x)_x + \frac{4}{3}k_B\alpha\tau_r(nTuu_x)_x - \frac{1}{\tau_w}\left(ne - \frac{3}{2}k_BnT_0\right), \end{aligned} \quad (34)$$

$$\varepsilon_s V_{xx} = q(n - C), \quad (35)$$

where the energy density equals

$$ne = \frac{3}{2}k_BnT + \frac{m}{2}nu^2 - \frac{\hbar^2}{24m}(\ln n)_{xx}.$$

The physical constants in the above equations are the effective electron mass m , the Boltzmann constant k_B , the reduced Planck constant \hbar , the elementary charge q , and the semiconductor permittivity ε_s (see Table 1). The value for τ_0 given in Table 1 represents the low-energy momentum relaxation time from the low-field electron mobility in GaAs at 77 K (see [15]). The momentum and energy relaxation times are denoted by, respectively, τ_p and τ_w , and their values will be specified later. The parameter τ_r has the dimension of time and it is introduced to keep α dimensionless. We assume that τ_r is the time which a thermal electron needs to cross the device (see below). The parameter σ is defined by $\sigma = \kappa\tau_0k_B T_0/m$ with the thermal conductivity κ , and the lattice temperature T_0 .

We employ the following standard scaling:

$$\begin{aligned} x &= L\tilde{x}, & n &= C^*\tilde{n}, & V &= V^*\tilde{V}, \\ T &= T_0\tilde{T}, & C &= C^*\tilde{C}, & u &= u^*\tilde{u}, \end{aligned}$$

Parameter	Physical meaning	Value
q	elementary charge	$1.602 \cdot 10^{-19}$ As
m	effective electron mass	$0.067 \cdot 10^{-31}$ kg
k_B	Boltzmann constant	$1.3807 \cdot 10^{-23}$ kg m ² /s ² K
\hbar	reduced Planck constant	$1.0546 \cdot 10^{-34}$ kg m ² /s
ε_s	semiconductor permittivity	$12.9 \cdot 8.8542 \cdot 10^{-12}$ A ² s ⁴ /kg m ³
τ_0	relaxation time	$0.9 \cdot 10^{-12}$ s
T_0	lattice temperature	77 K

TABLE 1. Physical parameters for GaAs.

where C^* is the maximal doping value, $V^* = k_B T_0 / q$, and $(u^*)^2 = k_B T_0 / m$. The scaled Planck constant and the scaled Deby length are defined by

$$\varepsilon^2 = \frac{\hbar^2}{mL^2 k_B T_0}, \quad \lambda^2 = \frac{\varepsilon_s k_B T_0}{q^2 C^* L^2},$$

and we define $\tau_r = L / u^*$. This leads to the following equations in nondimensional form (omitting the tilde symbol)

$$(nu)_x = 0, \tag{36}$$

$$(nu^2)_x + (nT)_x - \frac{\varepsilon^2}{12}(n(\log n)_{xx})_x - nV_x = \frac{4}{3}\alpha(nTu_x)_x - \frac{nu}{\tau_1}, \tag{37}$$

$$\begin{aligned} & \frac{5}{2}(nTu)_x + \frac{1}{2}(nu^3)_x - \frac{\varepsilon^2}{8}(nu(\log n)_{xx} + nu_{xx})_x - nuV_x \\ & = \frac{5}{2}\alpha\kappa\tau(nTT_x)_x + \frac{4}{3}\alpha\tau(nTuu_x)_x - \frac{1}{\tau_2}\left(ne - \frac{3}{2}n\right), \end{aligned} \tag{38}$$

$$\lambda^2 V_{xx} = n - C, \quad x \in (0, 1), \tag{39}$$

where

$$\tau_1 = \frac{\tau_p}{\tau_r}, \quad \tau_2 = \frac{\tau_w}{\tau_r}, \quad \tau = \frac{\tau_0}{\tau_r}.$$

These equations are solved in the interval $(0, 1)$ with the following boundary conditions taken from [15]:

$$\begin{aligned} n(0) = C(0), \quad n(1) = C(1), \quad n_x(0) = n_x(1) = 0, \\ u_x(0) = u_x(1) = 0, \quad T(0) = T(1) = T_0, \quad V(0) = 0, \quad V(1) = U, \end{aligned}$$

where U is the applied voltage.

We discretize the quantum Navier-Stokes equations (36)-(39) using central finite differences on a uniform mesh with $N = 500$ points. This corresponds to a mesh size of $\Delta x = 1/500 = 0.002$. The resulting discrete nonlinear system is solved by a Newton method where no damping was needed. We follow the approach used in [22] and employ the continuation method for the applied voltage: first the system of equations is solved for applied voltage $U = 0$ V; then, the solution corresponding to the voltage U is taken as an initial guess for the solution of the system with applied voltage $U + U_{\text{step}}$. The voltage step is chosen as $U_{\text{step}} = 1$ mV.

4.2. Simulations of the isothermal model. First, we consider the isothermal quantum Navier-Stokes model [4, 18]

$$(nu)_x = 0, \quad (40)$$

$$(nu^2)_x + (nT)_x - \frac{\varepsilon^2}{12}(n(\log n)_{xx})_x - nV_x = 2\alpha(nu_x)_x - \frac{nu}{\tau_1}, \quad (41)$$

$$\lambda^2 V_{xx} = n - C, \quad x \in (0, 1). \quad (42)$$

We are interested in the influence of the relaxation term $-nu/\tau_1$ on the static current-voltage characteristics of the tunneling diode. In our tests, we have chosen the (augmented) effective mass $m = 0.126 \cdot m_0$, $m_0 = 10^{-31}$ kg, the barrier height is $B = 0.4$ eV, and the momentum relaxation time $\tau_p = \tau_0$, which yields $\tau_1 = \tau_0/\tau_r$.

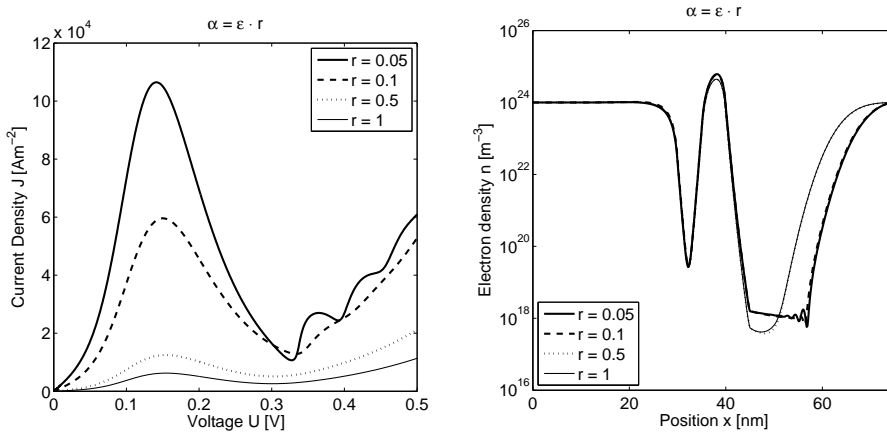


FIGURE 2. Current-voltage characteristics (left) and electron density (right) for the isothermal quantum Navier-Stokes model without relaxation term for various values of the viscosity α .

Figure 2 (left) shows the dependence of the viscosity parameter α on the current-voltage characteristics and the electron density when the relaxation term vanishes, i.e. $1/\tau_1 = 0$. As physically expected, the current density decreases for certain applied voltages, which is called negative resistance effect. An important parameter in applications is the peak-to-valley ratio, i.e. the ratio between the first local maximum and the next local minimum of the current density. We observe that the ratio increases for smaller values of the viscosity parameter α . Moreover, a small value for α produces multiple negative resistance effects, related to the appearance of “wiggles” in the electron density behind the right barrier (see Figure 2, right).

Next, we include the relaxation term $-nu/\tau_1$ in the momentum equation. Figure 3 shows the influence of this term on the current-voltage characteristics and the electron density. We observe that relaxation term eliminates the multiple negative resistance regions. The current density decreases with decreasing relaxation times τ_1 , and the electron density varies only near the right contact.

4.3. Simulations of the nonisothermal model without relaxation. We consider the full quantum Navier-Stokes model (36)-(39) without relaxation terms (i.e. $1/\tau_1 = 1/\tau_2 = 0$). We choose the viscosity parameter $\alpha = \varepsilon$ and the barrier height $B = 0.4$ eV. The influence of the effective electron mass on the current-voltage curve

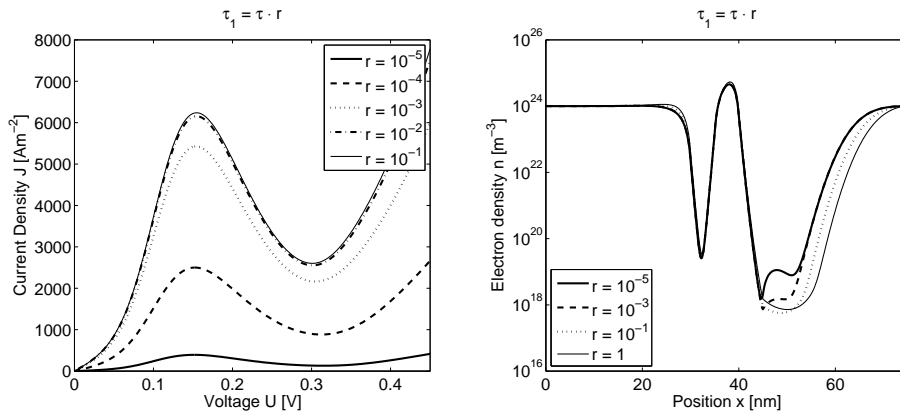


FIGURE 3. Current-voltage characteristics (left) and electron density (right) for the isothermal quantum Navier-Stokes model including relaxation for various values of the relaxation parameter τ_1 .

is illustrated in Figure 4 (top). It is well known that the peak-to-valley ratio increases with increasing values of the effective mass (see [24, Figure 6] for related numerical results). Figure 4 also shows the electron density and temperature for varying effective masses at the first peak (solid line) and the first valley (dashed line) of the current-voltage characteristics. Notice that the electron density is very small in the right barrier compared to the values at the contacts. Interestingly, the electron temperature is almost constant except in the right barrier where sharp temperature gradients appear. This shows that the assumption of low temperature variations, which has been used to simplify the model equations, is debatable in this case (see below for nonvanishing relaxation terms).

4.4. Simulations of the nonisothermal model with relaxation. Next, we consider the quantum Navier-Stokes model including relaxation terms. The relaxation times are given by the Baccarani-Wordeman expressions [2]

$$\tau_p = \tilde{\tau}_0 \frac{T_0}{T}, \quad \tau_w = \frac{\tau_p}{2} \left(1 + \frac{3k_B T}{m v_s^2} \right),$$

where $v_s = 2 \cdot 10^7$ cm/s is the saturation velocity and $\tilde{\tau}_0 = 100\tau_0$ is the low-energy momentum relaxation time. These expressions have been also employed by Gardner [15] in his quantum hydrodynamic simulations. We have chosen the value for $\tilde{\tau}_0$ for numerical reasons: With this value, the numerical scheme is stable with respect to changes of the other parameters (effective mass, viscosity etc.). We choose the barrier height $B = 0.4$ eV.

Figure 5 (top) verifies that the peak-to-valley ratio increases with the effective mass. The figure also shows the electron density and temperature for different values of the effective mass at the first peak (solid line) and the first valley (dashed line). Similarly as for the case without relaxation terms, in the first current valley, the electron density is relatively large in the quantum well but very small in the right barrier. On the other hand, the temperature changes drastically. Indeed, the particle temperature is almost constant except in the double-barrier structure.

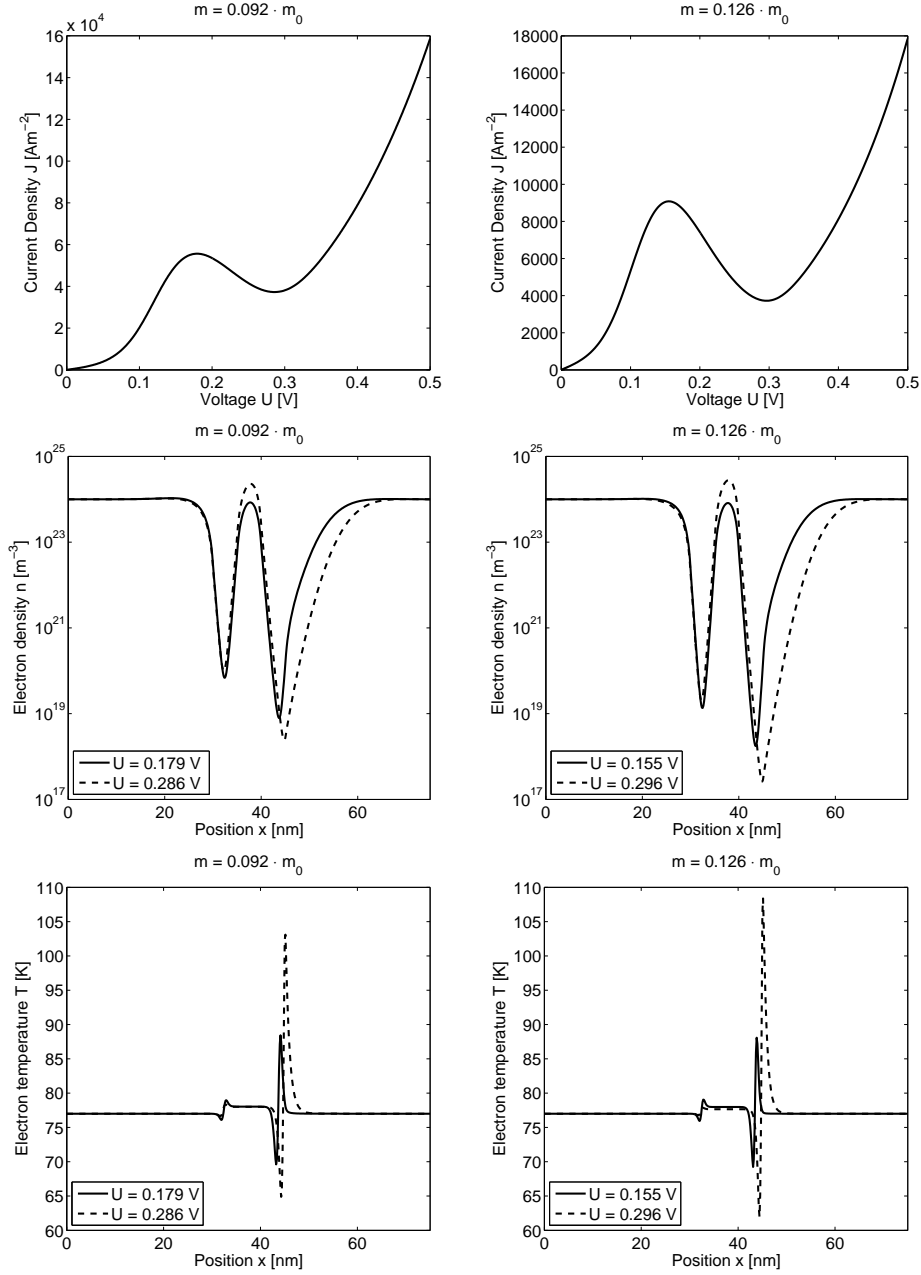


FIGURE 4. Current-voltage characteristics (top), electron density (middle), and electron temperature (bottom) for the nonisothermal quantum Navier-Stokes model without relaxation terms for different effective masses m .

Compared to the case without relaxation terms, the temperature variations are small and the relaxation eliminates the temperature oscillations.

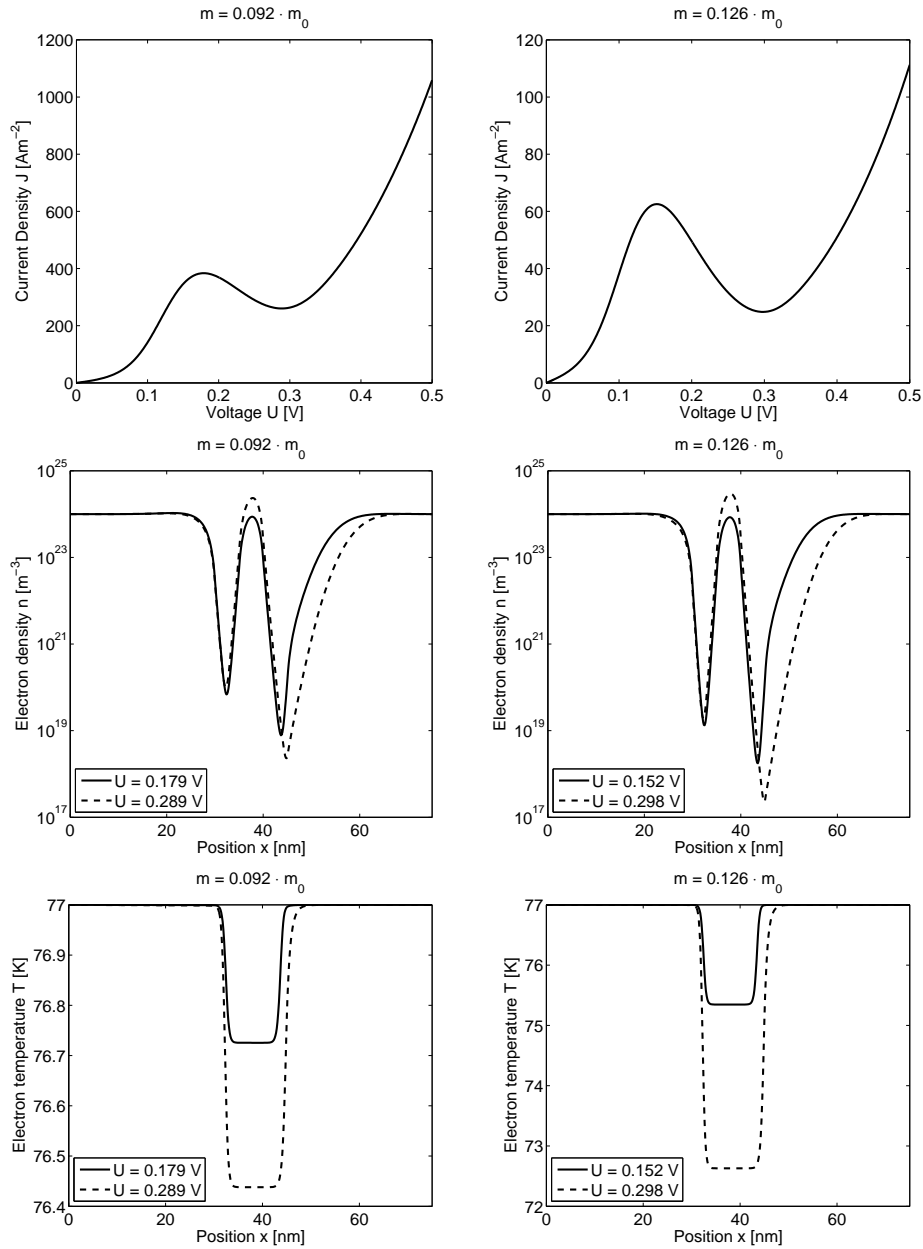


FIGURE 5. Current-voltage characteristics (top), electron density (middle), and electron temperature (bottom) for the nonisothermal quantum Navier-Stokes model with Baccarani-Wordeman relaxation terms for different effective masses m .

The dependence of the viscosity α on the current-voltage characteristics and the electron temperature is presented in Figure 6. As in the isothermal model, we find that the peak-to-valley ratio increases for smaller values of α . However, in contrast to the isothermal model, no multiple negative resistance regions occur and

the temperature has no sharp peaks, at least for α larger than ε (compare to Figure 2).

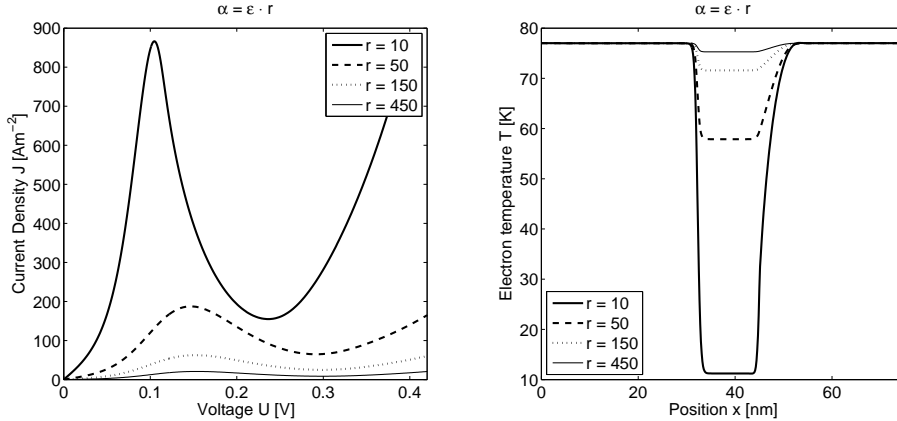


FIGURE 6. Current-voltage characteristics (left) and electron temperature at $U_0 = 0.45$ V (right) for the nonisothermal quantum Navier-Stokes model with Baccarani-Wordeman relaxation terms for various values of the viscosity α .

Up to now, we have used the same value of α in front of the thermal conductivity term as well as the viscosity terms in equations (36)-(38). We are interested in the influence of the thermal conductivity term

$$\frac{5}{2}\alpha_1\kappa\tau(nTT_x)_x$$

and the viscosity terms

$$\frac{4}{3}\alpha_2\tau(nTu_x)_x, \quad \frac{4}{3}\alpha_2\tau(nTuu_x)_x$$

on the current-voltage characteristics and the electron temperature. Figure 7 shows the results obtained by taking the fixed value of the thermal conductivity coefficient $\alpha_1 = 100\varepsilon$ and by varying the viscosity constant α_2 . Our numerical results are similar to those for the isothermal model; see Figure 2. For α much smaller than ε , there are multiple negative resistance regions in the current-voltage characteristics. Moreover, we observe oscillations in the electron temperature, which disappear for larger values of α_2 , see Figure 7 (bottom).

Finally, Figure 8 shows the influence of the thermal conductivity term on the current-voltage characteristics and the electron temperature. We have fixed the viscosity parameter $\alpha_2 = 100\varepsilon$, whereas the value of the thermal conductivity constant α_1 varies. It turns out that the thermal conductivity stabilizes the numerical scheme. Indeed, if the constant α_1 has been chosen too small, we observed strong oscillations in the electron density and the electron temperature became negative. Figure 8 (bottom) shows that the temperature becomes very small (the minimal value is about 0.05 K only) in the quantum well when the parameter α_1 is of the order of or smaller than ε .

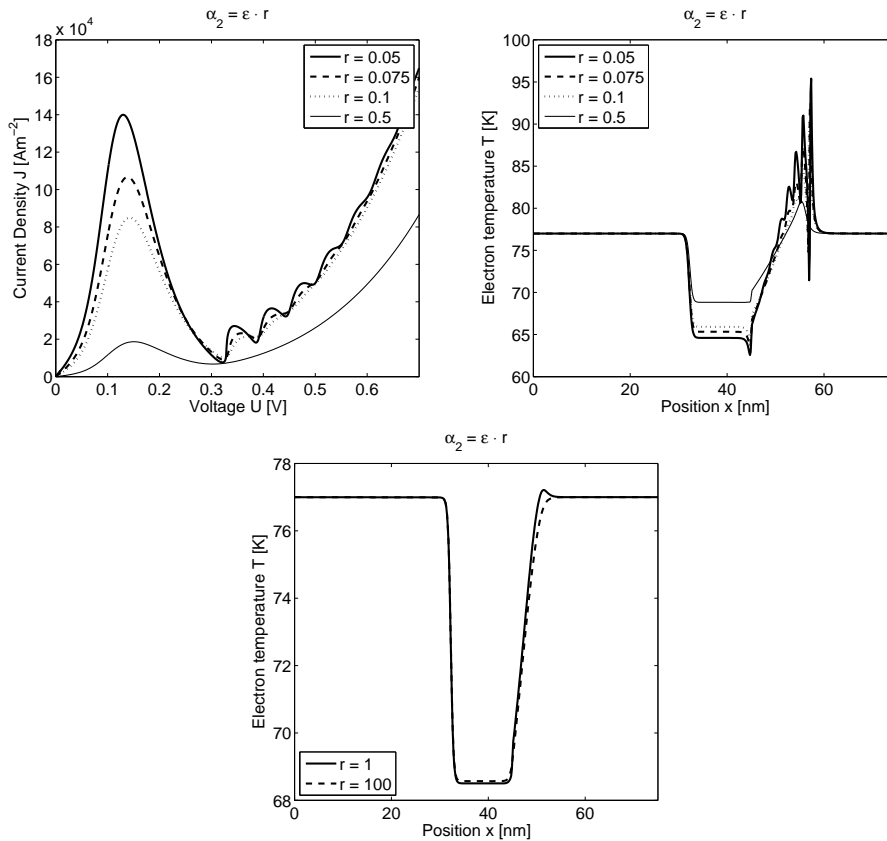


FIGURE 7. Current-voltage characteristics (top left) and electron temperature at $U_0 = 0.7$ V (top right and bottom) for the nonisothermal quantum Navier-Stokes model with Baccarani-Wordeman relaxation terms for various values of the viscosity α_2 .

REFERENCES

- [1] M. Anile, V. Romano, G. Russo, *Extended hydrodynamical model of carrier transport in semiconductors*, SIAM J. Appl. Math., 61 (2000), 74–101.
- [2] G. Baccarani and M. Wordeman, *An investigation of steady-state velocity overshoot effects in Si and GaAs devices*, Solid-State Electronics, 28 (1985), 407–416.
- [3] P. Bhatnagar, E. Gross and M. Krook, *A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems*, Phys. Rev., 94 (1954), 511–525.
- [4] S. Brull and F. Méhats, *Derivation of viscous correction terms for the isothermal quantum Euler model*, Z. Angew. Math. Mech., 90 (2010), 219–230.
- [5] A. Caldeira and A. Leggett, *Path integral approach to quantum Brownian motion*, Physica A, 121 (1983), 587–616.
- [6] P. Degond, S. Gallego, and F. Méhats, *On quantum hydrodynamic and quantum energy transport models*, Commun. Math. Sci. 5 (2007), 887–908.
- [7] P. Degond, S. Gallego, and F. Méhats, *Isothermal quantum hydrodynamics: derivation, asymptotic analysis, and simulation*, Multiscale Model. Simul., 6 (2007), 246–272.
- [8] P. Degond, S. Gallego, F. Méhats, and C. Ringhofer, *Quantum hydrodynamic and diffusion models derived from the entropy principle*, in: G. Allaire et al. (eds.), *Quantum transport*, pp. 111–168, Lecture Notes Math. 1946. Springer, Berlin, 2008.

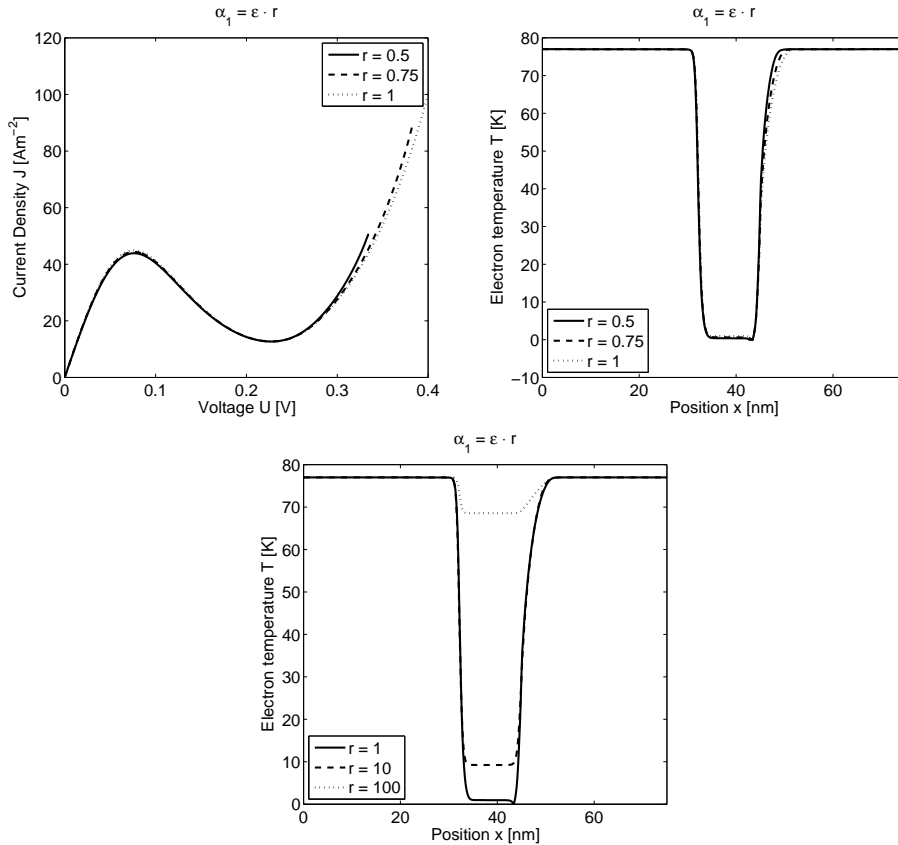


FIGURE 8. Current-voltage characteristics (top left) and electron temperature at $U_0 = 0.335$ V (top right and bottom) for the nonisothermal quantum Navier-Stokes model with Baccarani-Wordeman relaxation terms for various viscosities α_1 .

- [9] P. Degond, S. Gallego, F. Méhats, and C. Ringhofer, *Quantum diffusion models derived from the entropy principle*, in: L. Bonilla et al. (eds.), *Progress in Industrial Mathematics at ECMI 2006*, pp. 106–122, Mathematics in Industry 12. Springer, Berlin, 2008.
- [10] P. Degond, F. Méhats, and C. Ringhofer, *Quantum energy-transport and drift-diffusion models*, *J. Stat. Phys.*, 118 (2005), 625–665.
- [11] P. Degond and C. Ringhofer, *Quantum moment hydrodynamics and the entropy principle*, *J. Stat. Phys.*, 112 (2003), 587–628.
- [12] J. Dong, *A note on barotropic compressible quantum Navier-Stokes equations*, *Nonlin. Anal.*, 73 (2010), 854–856.
- [13] W. Dreyer, *Maximisation of the entropy in non-equilibrium*, *J. Phys. A*, 20 (1987), 6505–6517.
- [14] E. Feireisl, *Dynamics of Viscous Compressible Fluids*, Oxford University Press, Oxford, 2004.
- [15] C. Gardner, *The quantum hydrodynamic model for semiconductor devices*, *SIAM J. Appl. Math.*, 54 (1994), 409–427.
- [16] F. Jiang, *A remark on weak solutions to the barotropic compressible quantum Navier-Stokes equations*, to appear in *Nonlin. Anal.*, 2011.
- [17] A. Jüngel, *Transport Equations for Semiconductors*, Lecture Notes in Physics 773, Springer, Berlin, 2009.
- [18] A. Jüngel, *Global weak solutions to compressible Navier-Stokes equations for quantum fluids*, *SIAM J. Math. Anal.*, 42 (2010), 1025–1045.

- [19] A. Jüngel, *Effective velocity in compressible Navier-Stokes equations with third-order derivatives*, to appear in *Nonlin. Anal.*, 2011.
- [20] A. Jüngel, *Dissipative quantum fluid models*, preprint, Vienna University of Technology, Austria, 2010.
- [21] A. Jüngel and D. Matthes, *Derivation of the isothermal quantum hydrodynamic equations using entropy minimization*, *Z. Angew. Math. Mech.*, 85 (2005), 806–814.
- [22] A. Jüngel, D. Matthes, and J.-P. Milišić, *Derivation of new quantum hydrodynamic equations using entropy minimization*, *SIAM J. Appl. Math.*, 67 (2006), 46–68.
- [23] C. Levermore, *Moment closure hierarchies for kinetic theories*, *J. Stat. Phys.*, 83 (1996), 1021–1065.
- [24] T. Li, Z. Yu, Y. Wang, L. Huang, and C. Xiang, *Numerical simulation of negative differential resistance characteristics in $\text{Si}/\text{Si}_{1-x}\text{Ge}_x$ RTD at room temperature*, Proceedings of the 2005 IEEE Conference on Electron Devices and Solid-State Circuits, pp. 409–412, ISBN 0-7803-9339-2, 2005.
- [25] F. Méhats and O. Pinaud, *An inverse problem in quantum statistical physics*, *J. Stat. Phys.*, 140 (2010), 565–602.

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