A SIMPLIFIED QUANTUM ENERGY-TRANSPORT MODEL FOR SEMICONDUCTORS

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Abstract. The existence of global-in-time weak solutions to a quantum energy-transport model for semiconductors is proved. The equations are formally derived from the quantum hydrodynamic model in the large-time and small-velocity regime. They consist of a nonlinear parabolic fourth-order equation for the electron density, including temperature gradients; an elliptic nonlinear heat equation for the electron temperature; and the Poisson equation for the electric potential. The equations are solved in a bounded domain with periodic boundary conditions. The existence proof is based on an entropy-type estimate, exponential variable transformations, and a fixed-point argument. Furthermore, we discretize the equations by central finite differences and present some numerical simulations of a one-dimensional ballistic diode.

1. Introduction

The nanoscale structure of state-of-the-art semiconductor devices makes it necessary to incorporate suitable quantum corrections in the existing simulation tools. In order to reduce the computational cost, these tools are often based on macroscopic models for averaged physical quantities. In engineering applications, the quantum drift-diffusion equations [2] became very popular since they are capable to describe quantum confinement and tunneling effects in metal-oxide-semiconductor structures and to simulate ultrasmall semiconductor devices [25, 26]. Quantum drift-diffusion models have been derived from a Wigner-Boltzmann equation by a moment method [9]. The idea is to integrate the Wigner equation over the momentum space and to expand the Wigner distribution function around the quantum equilibrium by the Chapman-Enskog method [10]. This gives an evolution equation for the zeroth-order moment, the electron density, containing fourth-order derivatives.

Physically more precise models may be derived by taking into account more moments, for instance, the electron and energy densities, which leads to so-called quantum energy-transport models. In this paper, we will analyze a simplified version of a quantum energy-transport model. More precisely, we study the following scaled equations for the electron density n, the

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electron temperature T, and the selfconsistent electric potential V:

$$\partial_t n + \mathrm{div}\left(\frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) - \nabla(nT) + n\nabla V\right) = 0, \tag{1}$$

$$-\mathrm{div}(n\nabla T) = \frac{n}{\tau_e}(T_L(x) - T), \tag{2}$$

$$\lambda^2\Delta V = n - C(x). \tag{3}$$

The physical parameters are the scaled Planck constant ε, the energy relaxation time $\tau_e > 0$, and the Debye length λ. The doping profile $C(x)$ models fixed background charges in the semiconductor crystal, and the lattice temperature $T_L(x)$ is a given function. We refer to Section 2 for a derivation of the above model and the simplifications we have made. System (1)-(3) is solved in the multi-dimensional torus $\mathbb{T}^d \subset \mathbb{R}^d$ (thus imposing periodic boundary conditions), and we prescribe the initial datum

$$n(\cdot, 0) = n_0 \quad \text{in } \mathbb{T}^d. \tag{4}$$

Equation (1) is a generalization of the quantum drift-diffusion model since we take into account temperature gradients. The fourth-order differential term includes the so-called Bohm potential $\Delta\sqrt{n}/\sqrt{n}$ which is well known in quantum mechanics. The heat equation (2) is a simplification of the energy equation in the macroscopic quantum model; its right-hand side describes the relaxation to the lattice temperature T_L. If the lattice temperature is constant, $T = T_L$ solves the heat equation (2), and the system (1) and (3) reduces to the quantum drift-diffusion equations. Hence, temperature gradients are only due to variations of the lattice temperature. In (2), the heat conductivity is taken as $\kappa(n, T) = n$; we comment this (simpliying) choice at the end of Section 2.

Before we explain the main mathematical challenges to analyze (1)-(3) and state our main theorem, we review briefly related results. The stationary quantum drift-diffusion model (1) with $T =$ const. and (3) has been analyzed in [3, 21], and the existence of weak solutions with positive particle density has been shown. Existence of global-in-time weak solutions to the transient equations without the diffusion term $\nabla(nT)$ and for vanishing electric fields has been proved first in [20] in one space dimension and later in [14, 18] in multiple space dimensions. Global existence results for the full quantum drift-diffusion model in one space dimension can be found in [22] for physical boundary conditions, [6] for Dirichlet boundary conditions, and [7] for homogeneous Neumann boundary conditions.

There are much less analytical results for semiconductor models including temperature variations, due to a lack of suitable a priori estimates for the temperature. Earlier results have been concerned with the drift-diffusion equations with temperature-dependent mobilities but without temperature gradients [27] (also see [16]) or with nonisothermal systems containing simplified thermodynamic forces [1]. Later, temperature effects via the energy-transport model have been included, see [11, 15] for stationary solutions near the equilibrium, [5] for transient solutions close to thermal equilibrium, and [8] for systems with nondegenerate diffusion coefficients.

Up to our knowledge, there are no analytical results in the literature for quantum diffusion models *including* temperature variations. In particular, the model (1)-(3) is studied here for the first time.

The following mathematical difficulties have to be overcome. First, the fourth-order differential term in (1) prevents the use of the maximum principle and it is not clear how to define the Bohm potential term. This problem has been solved in [18, 20] by introducing the exponential variable $n = e^{y/2}$ which is positive if suitable bounds for y are available. The variable y is chosen since we can reformulate the fourth-order term as

$$\operatorname{div}\Big(n\nabla\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = \frac{1}{2}\nabla^2 : (n\nabla^2\log n) = \nabla^2 : (n\nabla^2 y), \tag{5}$$

where $\nabla^2\log n$ is the Hessian matrix of $\log n$ and the double point means summation over both matrix indices. The fourth-order term is symmetric in the variable y allowing for the use of the Lax-Milgram lemma in the linearized problem. Second, even without the fourth-order quantum term, the maximum principle does not apply to (1) due to the temperature gradients. There exist estimates for the entropy (or free energy) of the energy-transport model [8], but these estimates cannot be derived for the present model. Third, the fourth-order term (5) in y and the heat equation (2) are degenerate at $n = 0$. Fourth, for more physical boundary conditions, boundary integrals appear in the weak formulation of (1) which cannot be handled easily. The last problem is overcome by using periodic boundary conditions.

Our idea is to apply the maximum principle to the heat equation (2) together with entropy-type estimates. Indeed, assuming suitable bounds for T_L, the maximum principle for (2) shows that T is bounded from below and above by positive constants. Differentiating formally the "entropy" functional

$$H(t) = \int_{\mathbb{T}^d} n(\log n - 1)dx,$$

we obtain after a computation (see Section 3 for details)

$$\begin{aligned}\frac{dH}{dt} + \frac{\varepsilon^2}{12}\int_{\mathbb{T}^d} n|\nabla^2\log n|^2 + 4\int_{\mathbb{T}^d} T|\nabla\sqrt{n}|^2dx \\ = 2\int_{\mathbb{T}^d}\sqrt{n}\nabla\sqrt{n}\cdot\nabla T dx - \lambda^{-2}\int_{\mathbb{T}^d}(n - C(x))n dx,\end{aligned} \tag{6}$$

where we have employed the Poisson equation (3). The last integral is clearly bounded. The first integral on the right-hand side can be estimated from above by

$$\delta\int_{\mathbb{T}^d}|\nabla\sqrt{n}|^2dx + \frac{1}{\delta}\int_{\mathbb{T}^d} n|\nabla T|^2dx,$$

where $\delta > 0$. As T is bounded from below, the first integral can be absorbed by the last term on the left-hand side of (6) if $\delta > 0$ is chosen sufficiently small. For the second integral, the test function T in the weak formulation of (2) leads to

$$\int_{\mathbb{T}^d} n|\nabla T|^2dx = \frac{1}{\tau_e}\int_{\mathbb{T}^d} n(T_L(x) - T)T dx \le -\frac{1}{2\tau_e}\int_{\mathbb{T}^d} nT^2dx + \frac{1}{2\tau_e}\int_{\mathbb{T}^d} nT_L^2dx.$$

The last integral is bounded since the total mass $\int_{\mathbb{T}^d} n dx$ is constant in time, which is a consequence of the periodic boundary conditions. Then, putting together these estimates, our key estimate reads as follows:

$$\frac{dH}{dt} + \frac{\varepsilon^2}{12}\int_{\mathbb{T}^d} n|\nabla^2\log n|^2 + K_1\int_{\mathbb{T}^d}|\nabla\sqrt{n}|^2dx \le K_2 + \frac{1}{2\tau_e}\|T_L\|^2_{L^\infty(\mathbb{T}^d)}\int_{\mathbb{T}^d} n_0 dx, \tag{7}$$

where K_1, $K_2 > 0$ are some constants only depending on λ, C, and T_L.

We will show below that this estimate provides H^2 bounds for $\sqrt{n}$. However, no gradient bounds for T can be expected since we have only an L^2 bound for $\sqrt{n}\nabla T$ and an H^1 bound for $\sqrt{n}T$. Thus, the "right" variable for (2) is neither the temperature T nor the energy density nT but $\sqrt{n}T$. Notice that this situation is related to the analysis of the Korteweg-Navier-Stokes equations with density-dependent viscosities which vanish at vacuum [4]. In these equations, the third-order Korteweg term provides gradient estimates for n. However, due to the degeneracy of the viscosity coefficient, there is no estimate for the velocity u but for $\sqrt{n}\mathrm{div}\, u$ and $\sqrt{n}u$ only, see e.g. [4].

Our main result reads as follows.

Theorem 1. *Let $d \le 3$, ε, λ, $\tau_e > 0$, C, $T_L \in L^\infty(\mathbb{T}^d)$ with $0 < m_L \le T_L(x) \le M_L$ for $x \in \mathbb{T}^d$. Let the initial datum $n_0 \in L^1(\mathbb{T}^d)$ satisfy $n_0 \ge 0$ in $\mathbb{T}^d$, $\int_{\mathbb{T}^d} n_0 \log n_0 dx < \infty$, and $\int_{\mathbb{R}^d}(n_0 - C(x))dx = 0$. Then there exists a weak solution to (1)-(3) such that the regularity properties*

$$
\begin{aligned}
&n(\cdot,t) \ge 0, \quad 0 < m \le T(\cdot,t) \le M \ \text{a.e.},\\
&\sqrt{n} \in L^2_{\mathrm{loc}}(0,\infty; H^2(\mathbb{T}^d)) \cap L^\infty_{\mathrm{loc}}(0,\infty; L^2(\mathbb{T}^d)), \quad n \in W^{1,11/10}_{\mathrm{loc}}(0,\infty; H^{-2}(\mathbb{T}^d)),\\
&\sqrt{n}T \in L^2_{\mathrm{loc}}(0,\infty; H^1(\mathbb{T}^d)), \quad \sqrt{n}\nabla T \in L^2_{\mathrm{loc}}(0,\infty; L^2(\mathbb{T}^d)), \quad V \in L^2_{\mathrm{loc}}(0,\infty; H^2(\mathbb{T}^d)),
\end{aligned}
$$

where $m = m_L/2 > 0$ and $M = M_L + 1$, hold and the equations

$$
\partial_t n + \frac{\varepsilon^2}{12}\nabla^2 : \left(\sqrt{n}\nabla^2\sqrt{n} - \nabla\sqrt{n}\otimes\nabla\sqrt{n}\right) = \mathrm{div}(\nabla(nT) - n\nabla V), \tag{8}
$$

$$
-\mathrm{div}(n\nabla T) = \frac{n}{\tau_e}(T_L(x) - T), \tag{9}
$$

$$
\lambda^2\Delta V = n - C(x), \quad \int_{\mathbb{T}^d} V\,dx = 0, \tag{10}
$$

are satisfied in the sense of $L^1_{\mathrm{loc}}(0,\infty; H^{-2}(\mathbb{T}^d))$. The initial condition $n(\cdot,0) = n_0$ holds in the sense of $H^{-2}(\mathbb{T}^d)$. Moreover, the total mass is constant, $\int_{\mathbb{T}^d} n(x,t)dx = \int_{\mathbb{T}^d} n_0(x)dx$ for all $t > 0$.

Due to our weak regularity results, we can prove the existence of solutions in the formulation (8) only. We remark that the Poisson equation is uniquely solvable since $\int_{\mathbb{T}^d}(n(x,t) - C(x))dx = \int_{\mathbb{T}^d}(n_0(x)-C(x))dx = 0$. Furthermore, we notice that the bounds on T can be improved. In fact, the proof of Theorem 1 below shows that the bounds hold for $m = (1-\eta)m_L$, $M = M_L + \eta$ for any $\eta > 0$ and then, the limit $\eta \to 0$ yields $m_L \le T \le M_L$ in $\mathbb{T}^d$.

Theorem 1 is proved by semi-discretizing (1) in time, employing the Leray-Schauder fixed-point theorem, and working with the variables $\sqrt{n}$ and $y = 2\log n$. To solve the linearized problem in the variable y, we add to (1) the uniformly elliptic term $\delta(\Delta^2 y + y)$ since the operator (5) may degenerate at $n = 0$. Unfortunately, this additional term prevents the L^1 conservation of n which is needed in the key estimate (7). This problem is overcome by combining the L^1 estimate for n with estimates coming from the additional term $\delta(\Delta^2 y + y)$.

The paper is organized as follows. The next section is devoted to a formal derivation of the model (1)-(3). The proof of Theorem 1 is presented in Section 3. Section 4 is devoted to the numerical solution of (1)-(3) and the illustration of heating effects in a simple ballistic diode. We conclude in Section 5 and mention some open problems.

2. Derivation of the model equations

System (1)-(3) is deduced formally from the *quantum hydrodynamic equations*, which have been derived from the Wigner equation in [19]. The quantum hydrodynamic equations consist of balance equations for the electron density n, the electron mean velocity u, and the energy density ne:

$$\partial_t n + \operatorname{div}(nu) = 0, \tag{11}$$

$$\partial_t(nu) + \operatorname{div}(nu \otimes u) + \nabla(nT) - n\nabla V - \frac{\varepsilon^2}{6} n\nabla \frac{\Delta\sqrt{n}}{\sqrt{n}} = -\frac{nu}{\tau_p}, \tag{12}$$

$$\partial_t(ne) + \operatorname{div}\big((P + ne\mathbb{I})u\big) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) - nu \cdot \nabla V - \operatorname{div}(\kappa(n,T)\nabla T) = \frac{n}{\tau_e}(T_L - T), \tag{13}$$

selfconsistently coupled to the Poisson equation (3), where the matrix $u \otimes u$ has the components $u_i u_j$, τ_p is the (scaled) momentum relaxation time and $\kappa(n,T)$ the heat conductivity. The energy density ne and the stress tensor P are given by

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

where $\mathbb{I}$ is the identity matrix in $\mathbb{R}^{d\times d}$.

Compared to the model derived in [19], we have added the following expressions. First, we have included momentum and energy relaxation terms which are coming from Caldeira-Leggett-type collision operators in the kinetic Wigner-Boltzmann equation from which the quantum hydrodynamic equations have been derived [17]. Furthermore, we allow for the heat flux term $\operatorname{div}(\kappa(n,T)\nabla T)$ in the energy equation. The heat flux is usually taken into account in numerical simulations for stability reasons [12, 19]. It is necessary to obtain a positive definite diffusion matrix in the quantum energy-transport equations [17].

Quantum energy-transport equations are derived from system (11)-(13) after a diffusive rescaling and a relaxation-time limit. More precisely, we change the time scale $t \to t/\tau_p$ and scale the velocity as $u \to \tau_p u$, the thermal conductivity as $\kappa \to \tau_p\kappa$, and the energy relaxation time as $\tau_e \to \tau_e/\tau_p$, giving

$$\tau_p^2\partial_t(nu) + \tau_p^2\operatorname{div}(nu \otimes u) + \nabla(nT) - n\nabla V - \frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = -nu, \tag{14}$$

$$ne = \frac{d}{2}nT + \frac{\tau_p^2}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\Delta\log n,$$

and (11) and (13) remain unchanged. Then, performing the formal limit $\tau_p \to 0$, we arrive to the quantum energy-transport equations

$$\partial_t n + \operatorname{div}\left(\frac{\varepsilon^2}{6}n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) - \nabla(nT) + n\nabla V\right) = 0, \tag{15}$$

$$\partial_t(ne) + \operatorname{div}\big((P + ne\mathbb{I})u\big) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) - nu\cdot\nabla V - \operatorname{div}(\kappa nT\nabla T) = \frac{n}{\tau_e}(T_L - T), \tag{16}$$

where the energy density simplifies to

$$ne = \frac{d}{2}nT - \frac{\varepsilon^2}{24}n\Delta\log n.$$

The *simplified quantum energy-transport model* (1)-(2) is obtained from (11)-(13) in a slightly different relaxation-time limit. We rescale time and velocity as above but we do not rescale the thermal conductivity or the energy relaxation time. Then (11) and (14) remain unchanged and (13) is written as

$$\tau_p\Big(\partial_t(ne) + \operatorname{div}\big((P + ne\mathbb{I})u\big) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) - nu\cdot\nabla V\Big) - \operatorname{div}(\kappa(n,T)\nabla T) = \frac{n}{\tau_e}(T_L - T).$$

Performing the formal limit $\tau_p \to 0$ in the above equation and in (11) and (14), we deduce (1)-(2) with the choice $\kappa(n) = n$ for the heat conductivity.

Physically, we expect that the heat conductivity depends on the thermal energy $\frac{d}{2}nT$. Often, the function $\kappa(n,T) = nT$ is taken [12, 19]. Our choice $\kappa(n,T) = n$ has a purely technical reason. Indeed, having regularity for $\sqrt{n}T$ only, it seems to be difficult to treat the heat flux $nT\nabla T$ since the temperature appears quadratically, and we have only weak convergence results for the sequence of approximating temperatures.

3. Proof of Theorem 1

3.1. **Existence of a time-discrete solution.** We replace (1)-(3) by a semidiscrete system. To this end, let $\tau > 0$ be a time step and $\overline{w}$ be a given function. We wish to find a solution to the problem

$$\frac{1}{\tau}(w^2 - \overline{w}^2) + \frac{\varepsilon^2}{12}\nabla^2 : (w\nabla^2 w - \nabla w\otimes\nabla w) = \operatorname{div}\big(\nabla(w^2T) - w^2\nabla V\big), \tag{17}$$

$$-\operatorname{div}(w^2\nabla T) = \frac{w^2}{\tau_e}(T_L(x) - T), \tag{18}$$

$$\lambda^2\Delta V = \overline{w}^2 - C(x) \quad \text{in } \mathbb{T}^d. \tag{19}$$

Here, w represents the square root of the electron density at some time t and $\overline{w}$ the corresponding quantity at time $t - \tau$.

Lemma 2. *Let the assumptions of Theorem 1 hold and let $\overline{w} \in L^\infty(\mathbb{T}^d)$ satisfy $\int_{\mathbb{T}^d}(\overline{w}^2 - C(x))dx = 0$. Then there exists a weak solution $(w,T,V) \in H^2(\mathbb{T}^d)\times L^\infty(\mathbb{T}^d)\times H^2(\mathbb{T}^d)$ to (17)-(19) such that $wT \in H^1(\mathbb{T}^d)$, $w\nabla T \in L^2(\mathbb{T}^d)$, $\int_{\mathbb{T}^d}(w^2 - C(x))dx = 0$, and $w \geq 0$, $0 < m \leq T \leq M$ in $\mathbb{T}^d$, where $m = m_L/2$ and $M = M_L + 1$.*

Proof. The proof is performed in several steps.

Step 1: Definition of a regularized problem. The solution to (17)-(19) is obtained as the limit of solutions to a regularized problem. In particular, we add a strongly elliptic operator in $y = 2\log w$:

$$\frac{1}{\tau}(w^2 - \overline{w}^2) + \frac{\varepsilon^2}{12}\nabla^2 : (w^2\nabla^2 y) + \delta(\Delta^2 y + y) = \operatorname{div}\big(\nabla(w^2T) - w^2\nabla V\big), \tag{20}$$

$$-\operatorname{div}\big((w^2+\delta)\nabla T\big) = \frac{1}{\tau_e}(w^2+\delta)(T_L(x) - T), \tag{21}$$

$$\lambda^2\Delta V = \overline{w}^2 - C(x) \quad \text{in } \mathbb{T}^d, \tag{22}$$

where $\delta > 0$ is a regularization parameter. The fourth-order operator $\delta(\Delta^2 y + y)$ guarantees coercivity of the left-hand side of (20) with respect to y.

Step 2: Solution of the regularized problem. We solve (20)-(22) by employing the Leray-Schauder fixed-point theorem (see Theorem B.5 in [24]). Let $\sigma \in [0,1]$ and $w \in W^{1,4}(\mathbb{T}^d) \hookrightarrow$

$L^\infty(\mathbb{T}^d)$ (here we use the restriction on the space dimension $d \le 3$). Let $V \in H^2(\mathbb{T}^d)$ be the unique solution to the Poisson equation

$$\lambda^2 \Delta V = \overline{w}^2 - C(x) \quad \text{in } \mathbb{T}^d, \qquad \int_{\mathbb{T}^d} V dx = 0.$$

Notice that this problem is solvable since we have assumed that $\int_{\mathbb{T}^d}(\overline{w}^2 - C(x))dx = 0$. Next, let $T \in H^1(\mathbb{T}^d)$ be the unique solution to the linear equation

$$-\mathrm{div}\big((w^2+\delta)\nabla T\big) = \frac{1}{\tau_e}(\sigma w^2 + \delta)(T_L(x) - T) \quad \text{in } \mathbb{T}^d.$$

As the coefficient of the zeroth-order term $\tau_e^{-1}(\sigma w^2 + \delta)T$ is uniformly positive, this problem is uniquely solvable. Finally, introduce for y, $z \in H^2(\mathbb{T}^d)$ the forms

$$\begin{aligned} a(y,z) &= \frac{\varepsilon^2}{12}\int_{\mathbb{T}^d} w^2 \nabla^2 y : \nabla^2 z dx + \delta \int_{\mathbb{R}^d} (\Delta y \Delta z + yz) dx, \\ f(z) &= -\frac{\sigma}{\tau}\int_{\mathbb{T}^d} (w^2 - \overline{w}^2) z dx - \sigma \int_{\mathbb{T}^d} (\nabla(w^2 T) - w^2 \nabla V)\cdot \nabla z dx, \end{aligned}$$

The bilinear form a is continuous and coercive for $\delta > 0$, and the linear form f is continuous (since $\nabla(w^2T) \in L^2(\mathbb{T}^d)$). Consequently, the Lax-Milgram lemma provides the existence of a unique solution $y \in H^2(\mathbb{T}^d)$ to

$$a(y,z) = f(z) \quad \text{for all } z \in H^2(\mathbb{T}^d). \tag{23}$$

This defines the fixed-point operator $S : W^{1,4}(\mathbb{T}^d) \times [0,1] \to W^{1,4}(\mathbb{T}^d)$, $S(w,\sigma) = v := e^{y/2}$. Indeed, since $y \in H^2(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ in dimensions $d \le 3$, we have $v \in H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$.

We shall now verify the hypotheses of the Leray-Schauder theorem which provides a solution w to $S(w,1) = w$. The operator S is constant at $\sigma = 0$, $S(w,0) = 1$. By standard results for elliptic equations, S is continuous and compact since the embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$ is compact. It remains to show a uniform bound for all fixed points of $S(\cdot,\sigma)$. This is achieved by suitable entropy estimates.

Let $w \in H^2(\mathbb{T}^d)$ be a fixed point of $S(\cdot,\sigma)$ for some $\sigma \in [0,1]$. Then there exists $y \in H^2(\mathbb{T}^d)$ such that $w = e^{y/2}$. We derive first some bounds for T. With the test function $(T-M)^+ = \max\{0, T-M\} \in H^1(\mathbb{T}^d)$ in (21), where $M = \sup_{\mathbb{T}^d} T_L + 1$, we infer that

$$\begin{aligned} \int_{\mathbb{T}^d} (w^2+\delta)|\nabla(T-M)^+|^2 dx &= \frac{1}{\tau_e}\int_{\mathbb{T}^d} (\sigma w^2 + \delta)(T_L(x) - T)(T-M)^+ dx \\ &\le -\frac{1}{\tau_e}\int_{\mathbb{T}^d} (\sigma w^2 + \delta)(T-M)^+ dx \le 0. \end{aligned}$$

This implies that $(T-M)^+ = 0$ and hence $T \le M$ in $\mathbb{T}^d$. The test function $(T-m)^- = \min\{0, T-m\} \in H^1(\mathbb{T}^d)$ with $m = \frac{1}{2}\inf_{\mathbb{T}^d} T_L > 0$ leads to

$$\begin{aligned} \int_{\mathbb{T}^d} (w^2+\delta)|\nabla(T-m)^-|^2 dx &= \frac{1}{\tau_e}\int_{\mathbb{T}^d} (\sigma w^2 + \delta)(T_L(x) - T)(T-m)^- dx \\ &\le \frac{1}{2\tau_e}\inf_{\mathbb{T}^d} T_L \int_{\mathbb{T}^d} (\sigma w^2 + \delta)(T-m)^- dx \le 0, \end{aligned}$$

from which we conclude that $(T-m)^-=0$ and $T\ge m>0$ in $\mathbb{T}^d$. Furthermore, we employ the test function T in (21):

$$\begin{aligned}\int_{\mathbb{T}^d}(w^2+\delta)|\nabla T|^2dx &= \frac{1}{\tau_e}\int_{\mathbb{T}^d}(\sigma w^2+\delta)(T_L(x)-T)Tdx\\ &\le -\frac{1}{2\tau_e}\int_{\mathbb{T}^d}(\sigma w^2+\delta)T^2dx+\frac{1}{2\tau_e}\int_{\mathbb{T}^d}(\sigma w^2+\delta)T_L^2dx,\end{aligned}$$

which gives, since $M_L=\|T_L\|_{L^\infty(\mathbb{T}^d)}$,

$$\int_{\mathbb{T}^d}(w^2+\delta)|\nabla T|^2dx+\frac{\sigma}{2\tau_e}\int_{\mathbb{T}^d}(wT)^2dx\le\frac{1}{2\tau_e}M_L^2\int_{\mathbb{T}^d}(\sigma w^2+\delta)dx.$$

We derive an approximate L^2 bound for w by using the test function $z=1$ in (23):

$$\sigma\int_{\mathbb{T}^d}w^2dx=\sigma\int_{\mathbb{T}^d}\overline{w}^2dx-\delta\tau\int_{\mathbb{T}^d}ydx=\sigma\int_{\mathbb{T}^d}C(x)dx-\delta\tau\int_{\mathbb{T}^d}ydx, \tag{24}$$

Thus, the estimate on $w\nabla T$ becomes

$$\begin{aligned}\int_{\mathbb{T}^d}(w^2+\delta)|\nabla T|^2dx+\frac{\sigma}{2\tau_e}\int_{\mathbb{T}^d}(wT)^2dx &\le \frac{\sigma}{2\tau_e}M_L^2\int_{\mathbb{T}^d}C(x)dx-\frac{\delta\tau}{2\tau_e}M_L^2\int_{\mathbb{T}^d}ydx\\ &\quad+\frac{\delta}{2\tau_e}M_L^2\mathrm{meas}(\mathbb{T}^d).\end{aligned} \tag{25}$$

We proceed with the estimates for w. Taking the test function $y=2\log w$ in (23), we find that

$$\begin{aligned}&\frac{\varepsilon^2}{3}\int_{\mathbb{T}^d}(w^2+\delta)|\nabla^2\log w|^2dx+\delta\int_{\mathbb{T}^d}\big((\Delta y)^2+y^2\big)dx\\ &\quad=-\frac{\sigma}{\tau}\int_{\mathbb{T}^d}(w^2-\overline{w}^2)\log(w^2)dx-2\sigma\int_{\mathbb{T}^d}\big(\nabla(w^2T)-w^2\nabla V\big)\cdot\nabla\log w dx\\ &\quad\le-\frac{\sigma}{\tau}\int_{\mathbb{T}^d}\big(\phi(w^2)-\phi(\overline{w}^2)\big)dx-2\sigma\int_{\mathbb{T}^d}\Big(2T|\nabla w|^2+w\nabla T\cdot\nabla w-\frac{1}{2}\nabla(w^2)\cdot\nabla V\Big)dx,\end{aligned}$$

where we have employed the convexity of the function $\phi(s)=s(\log s-1)+1$, $\phi(s)-\phi(t)\le\phi'(s)(s-t)$ for all s, $t\ge 0$. Then, using the Poisson equation and the Young inequality, we obtain

$$\begin{aligned}&\frac{\sigma}{\tau}\int_{\mathbb{T}^d}\big(\phi(w^2)-\phi(\overline{w}^2)\big)dx+\frac{\varepsilon^2}{3}\int_{\mathbb{T}^d}(w^2+\delta)|\nabla^2\log w|^2dx+\delta\int_{\mathbb{T}^d}\big((\Delta y)^2+y^2\big)dx\\ &\qquad\le\sigma\int_{\mathbb{T}^d}\Big(-2m|\nabla w|^2+\frac{w^2}{2m}|\nabla T|^2-\frac{w^2}{\lambda^2}(\overline{w}^2-C(x))\Big)dx\\ &\qquad\le-2\sigma m\int_{\mathbb{T}^d}|\nabla w|^2dx+\frac{1}{2m}\int_{\mathbb{T}^d}w^2|\nabla T|^2dx+\frac{\sigma}{\lambda^2}\|C\|_{L^\infty(\mathbb{T}^d)}\int_{\mathbb{T}^d}w^2dx.\end{aligned}$$

The second term on the right-hand side is estimated by (25) and the last term can be bounded by (24), leading to

$$\begin{aligned}&\frac{\sigma}{\tau}\int_{\mathbb{T}^d}\big(\phi(w^2)-\phi(\overline{w}^2)\big)dx+\frac{\varepsilon^2}{3}\int_{\mathbb{T}^d}w^2|\nabla^2\log w|^2dx+\delta\int_{\mathbb{T}^d}\big((\Delta y)^2+y^2\big)dx\\ &\qquad\le-2\sigma m\int_{\mathbb{T}^d}|\nabla w|^2dx-\delta\tau K_1(m)\int_{\mathbb{T}^d}ydx+K_2(m),\end{aligned}$$

where the constants $K_i(m) > 0$ depend on $C(x)$, $T_L(x)$ etc. but not on σ, τ, or δ. Now, the integral over y^2 on the left-hand side dominates the integral over y on the right-hand side since

$$-\frac{\delta}{2}\int_{\mathbb{T}^d}(2\tau K_1(m)y + y^2)dx \le \delta\tau K_1(m)^2\mathrm{meas}(\mathbb{T}^d).$$

This yields our key (entropy) estimate

$$\begin{aligned}\frac{\sigma}{\tau}\int_{\mathbb{T}^d}\big(\phi(w^2)-\phi(\overline{w}^2)\big)dx + \frac{\varepsilon^2}{3}\int_{\mathbb{T}^d} w^2|\nabla^2\log w|^2dx \qquad\qquad \\ + \delta\int_{\mathbb{T}^d}(\Delta y)^2dx + \frac{\delta}{2}\int_{\mathbb{T}^d} y^2dx + 2\sigma m\int_{\mathbb{T}^d}|\nabla w|^2dx \le K,\end{aligned} \tag{26}$$

where $K > 0$ denotes here and in the following a generic constant not depending on y, T, τ, or δ. Hence, y and Δy are uniformly bounded in $L^2(\mathbb{T}^d)$ for any fixed $\delta > 0$. This implies that y and also $w = e^{y/2}$ are uniformly bounded in $H^2(\mathbb{T}^d)$. Then the Leray-Schauder theorem provides a solution w to $S(w,1) = w$, which we denote by w_δ. Obviously, w_δ satisfies (20). We denote by T_δ the solution to (21) and by V_δ the solution to (22).

Step 3: Lower bound for w_δ. By construction of w_δ, there exists $y_\delta \in H^2(\mathbb{T}^d)$ such that $w_\delta = \exp(y_\delta/2)$. Inequality (26) yields an H^2 bound for y_δ, depending on $\overline{w}$ and δ, $\|y_\delta\|_{H^2(\mathbb{T}^d)} \le K\delta^{-1/2}$. In combination with the embedding $H^2(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$, this gives $\|y_\delta\|_{L^\infty(\mathbb{T}^d)} \le K\delta^{-1/2}$. Consequently, w_δ is strictly positive,

$$w_\delta = \exp(y_\delta/2) \ge \exp(-K\delta^{-1/2}/2) > 0 \quad \text{in } \mathbb{T}^d.$$

Step 4: Uniform H^1 bound for $w_\delta T_\delta$. Estimate (26) shows that $\sqrt{\delta}\|y_\delta\|_{L^2(\mathbb{T}^d)}$ is uniformly bounded. Hence, by (25) with $\sigma = 1$,

$$\begin{aligned}\int_{\mathbb{T}^d}(w_\delta^2+\delta)|\nabla T_\delta|^2dx + \frac{1}{2\tau_e}\int_{\mathbb{T}^d}(w_\delta T_\delta)^2dx &\le K_1 + \delta K_2\|y\|_{L^1(\mathbb{T}^d)} \\ &\le K_1 + \delta K_3\|y\|_{L^2(\mathbb{T}^d)} \le K_4.\end{aligned} \tag{27}$$

Thus, in view of (26),

$$\int_{\mathbb{T}^d}|\nabla(w_\delta T_\delta)|^2dx \le 2\int_{\mathbb{T}^d} w_\delta^2|\nabla T_\delta|^2dx + 2M^2\int_{\mathbb{T}^d}|\nabla w_\delta|^2dx$$

is uniformly bounded. This provides a uniform bound for $w_\delta T_\delta$ in $H^1(\mathbb{T}^d)$.

Step 5: The limit $\delta \to 0$. By (26), the sequences $(\phi(w_\delta^2))$ and $(|\nabla w_\delta|^2)$ are bounded in $L^1(\mathbb{T}^d)$. Since $s \le \phi(s) + e - 1$ for all $s \ge 0$, the sequence (w_δ^2) is bounded in $L^1(\mathbb{T}^d)$ too. Next, we employ Lemma 2.2 of [18] which gives the inequality

$$\int_{\mathbb{T}^d} w_\delta^2|\nabla^2\log w_\delta|^2dx \ge K\int_{\mathbb{T}^d}(\Delta w_\delta)^2dx, \tag{28}$$

for some constant $K > 0$ (depending on the space dimension only). This inequality, together with the estimate (26), shows that (Δw_δ) is bounded in $L^2(\mathbb{T}^d)$. Since (w_δ) is bounded in $L^2(\mathbb{T}^d)$, we conclude that (w_δ) is bounded in $H^2(\mathbb{T}^d)$. Thus, for a subsequence which is not relabeled, as $\delta \to 0$,

$$\begin{aligned} w_\delta &\rightharpoonup w \quad \text{weakly in } H^2(\mathbb{T}^d), \\ w_\delta &\to w \quad \text{strongly in } W^{1,4}(\mathbb{T}^d)\end{aligned}$$

for some $w \in H^2(\mathbb{T}^d)$. In particular, since $w_\delta > 0$, we have $w \geq 0$ in $\mathbb{T}^d$. Furthermore,

$$w_\delta^2 \nabla^2 \log w_\delta = w_\delta \nabla^2 w_\delta - \nabla w_\delta \otimes \nabla w_\delta \rightharpoonup w \nabla^2 w - \nabla w \otimes \nabla w \quad \text{weakly in } L^2(\mathbb{T}^d).$$

By the δ-dependent bound for y_δ in (26),

$$\begin{aligned} \left|\sqrt{\delta}\langle(\Delta^2 y_\delta + y_\delta), z\rangle_{H^{-2},H^2}\right| &\leq \sqrt{\delta}\big(\|y_\delta\|_{H^2(\mathbb{T}^d)}\|z\|_{H^2(\mathbb{T}^d)} + \|y_\delta\|_{L^2(\mathbb{T}^d)}\|z\|_{L^2(\mathbb{T}^d)}\big) \\ &\leq K\|z\|_{H^2(\mathbb{T}^d)}, \end{aligned}$$

for any test function $z \in H^2(\mathbb{T}^d)$. Therefore,

$$\delta\big(\Delta^2 y_\delta + y_\delta\big) \rightharpoonup 0 \quad \text{weakly in } H^{-2}(\mathbb{T}^d).$$

The sequence (V_δ) is bounded in $H^2(\mathbb{T}^d)$ since (w_δ) is bounded in $L^4(\mathbb{T}^d)$. Moreover, (T_δ) is bounded in $L^\infty(\mathbb{T}^d)$. Unfortunately, we do not have better bounds for T_δ since we do not have a uniform lower bound for w_δ and the heat equation may degenerate in the limit $\delta \to 0$. However, we know from step 4 that $(w_\delta T_\delta)$ is bounded in $H^1(\mathbb{T}^d)$. As a consequence, up to subsequences,

$$\begin{aligned} V_\delta \to V &\quad \text{strongly in } W^{1,4}(\mathbb{T}^d), \\ T_\delta \rightharpoonup T &\quad \text{weakly* in } L^\infty(\mathbb{T}^d), \\ w_\delta T_\delta \rightharpoonup \theta &\quad \text{weakly in } H^1(\mathbb{T}^d), \end{aligned}$$

for some function $\theta \in H^1(\mathbb{T}^d)$. In fact, we can identify θ with wT since (w_δ) converges strongly to w in $L^2(\mathbb{T}^d)$ and (T_δ) converges weakly* to T in $L^\infty(\mathbb{T}^d)$, implying that

$$w_\delta T_\delta \rightharpoonup wT \quad \text{weakly in } L^2(\mathbb{T}^d).$$

It is clear that V solves the Poisson equation (19).

We claim that T is a solution to the heat equation (18). The above convergence results show that

$$w_\delta^2 \nabla T_\delta = w_\delta \nabla(w_\delta T_\delta) - w_\delta T_\delta \nabla w_\delta \rightharpoonup w\nabla(wT) - wT\nabla w = w^2 \nabla T \quad \text{weakly in } L^2(\mathbb{T}^d).$$

Furthermore, by (27), $(\sqrt{\delta}\nabla T_\delta)$ is bounded in $L^2(\mathbb{T}^d)$ and therefore, $\delta \nabla T_\delta \to 0$ strongly in $L^2(\mathbb{T}^d)$. This proves that

$$(w_\delta^2 + \delta)\nabla T_\delta \rightharpoonup w^2 \nabla T \quad \text{weakly in } L^2(\mathbb{T}^d).$$

Hence, T solves (18).

The above convergence results are sufficient to pass to the limit in the right-hand side of (20):

$$\begin{aligned} \int_{\mathbb{T}^d} \big(\nabla(w_\delta^2 T_\delta) - w_\delta^2 \nabla V_\delta\big)\cdot \nabla z dx &= \int_{\mathbb{T}^d} \big(w_\delta \nabla(w_\delta T_\delta) + w_\delta T_\delta \nabla w_\delta - w_\delta^2 \nabla V_\delta\big)\cdot \nabla z dx \\ &\to \int_{\mathbb{T}^d} \big(w\nabla(wT) + wT\nabla w - w^2 \nabla V\big)\cdot \nabla z dx \\ &= \int_{\mathbb{T}^d} \big(\nabla(w^2 T) - w^2 \nabla V\big)\cdot \nabla z dx, \end{aligned}$$

for $z \in H^1(\mathbb{T}^d)$. We have proved that (w, T, V) solves (17)-(19). Finally, the test function $z = 1$ in (17) yields

$$\int_{\mathbb{T}^d} w^2 dx = \int_{\mathbb{T}^d} \overline{w}^2 dx = \int_{\mathbb{T}^d} C(x) dx,$$

completing the proof. □

3.2. **A priori estimates.** Let an arbitrary final time $t_0 > 0$ be fixed. Define the step functions $(w^{(\tau)}, T^{(\tau)}, V^{(\tau)}) : [0, t_0) \to L^2(\mathbb{T}^d)^3$ recursively as follows. Let $w_0 = \sqrt{n_0}$, and for given $k \in \mathbb{N}$, let $(w_k, T_k, V_k) \in H^2(\mathbb{T}^d) \times L^\infty(\mathbb{T}^d) \times H^2(\mathbb{T}^d)$ be a solution to (17)-(19) with $\overline{w} = w_{k-1}$ (according to Lemma 2). Now we define $w^{(\tau)}(t) = w_k$ for $(k-1)\tau < t \le k\tau$ and similarly for $T^{(\tau)}$ and $V^{(\tau)}$. These step functions satisfy in $\mathbb{T}^d$

$$\frac{1}{\tau}\big((w^{(\tau)})^2 - (\sigma_\tau w^{(\tau)})^2\big) + \nabla^2 : \big(w^{(\tau)}\nabla^2 w^{(\tau)} - \nabla w^{(\tau)} \otimes \nabla w^{(\tau)}\big)$$
$$= \operatorname{div}\Big(\nabla\big((w^{(\tau)})^2 T^{(\tau)}\big) - (w^{(\tau)})^2 \nabla V^{(\tau)}\Big), \tag{29}$$

$$-\operatorname{div}\Big((w^{(\tau)})^2 \nabla T^{(\tau)}\Big) = \frac{(w^{(\tau)})^2}{\tau_e}(T_L(x) - T^{(\tau)}), \tag{30}$$

$$\lambda^2 \Delta V^{(\tau)} = (\sigma_\tau w^{(\tau)})^2 - C(x), \quad \int_{\mathbb{T}^d} V^{(\tau)} dx = 0, \tag{31}$$

where σ_τ denotes the shift operator $(\sigma_\tau w^{(\tau)})(t) = w^{(\tau)}(\cdot, t-\tau)$ for $\tau \le t < T$. In order to pass to the continuum limit $\tau \to 0$ in the above system, we need the following a priori estimates.

Lemma 3. *The functions* ($w^{(\tau)}$ *and* $T^{(\tau)}$) *satisfy*

$$\|w^{(\tau)}\|_{L^\infty(0,t_0;L^2(\mathbb{T}^d))} + \|w^{(\tau)}\|_{L^2(0,t_0;H^2(\mathbb{T}^d))} \le K,$$
$$\|T^{(\tau)}\|_{L^\infty(0,t_0;L^\infty(\mathbb{T}^d))} + \|w^{(\tau)}T^{(\tau)}\|_{L^2(0,t_0;H^1(\mathbb{T}^d))} \le K,$$

where $K > 0$ *is a generic constant not depending on* τ*.*

Proof. The bounds for $w^{(\tau)}$ are a consequence of (26), together with (28). The estimate for $T^{(\tau)}$ follows from the proof of Lemma 2, and the bound for $w^{(\tau)}T^{(\tau)}$ comes from step 4 of the proof. □

Lemma 4. *The following estimates hold:*

$$\big\|(w^{(\tau)})^2\big\|_{L^{11/10}(0,t_0;H^2(\mathbb{T}^d))} + \tau^{-1}\big\|(w^{(\tau)})^2 - (\sigma_\tau w^{(\tau)})^2\big\|_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} \le K, \tag{32}$$

$$\big\|w^{(\tau)}\big\|_{L^{8/d+2}(0,t_0;L^{8/d+2}(\mathbb{T}^d))} + \|V^{(\tau)}\|_{L^{4/d+1}(0,t_0;H^2(\mathbb{T}^d))} \le K, \tag{33}$$

where $K > 0$ *is a constant independent of* τ*.*

Proof. In Lemma 4.2 of [18], it is proved that the bounds of $(w^{(\tau)})$ in $L^\infty(0, t_0; L^2(\mathbb{T}^d))$ and $L^2(0, t_0; H^2(\mathbb{T}^d))$ imply that $(w^{(\tau)})^2$ is uniformly bounded in $L^{11/10}(0, t_0; H^2(\mathbb{T}^d))$ and that the fourth-order term in (29) is uniformly bounded in $L^{11/10}(0, t_0;\, H^{-2}(\mathbb{T}^d))$,

$$\big\|w^{(\tau)}\nabla^2 w^{(\tau)} - \nabla w^{(\tau)} \otimes \nabla w^{(\tau)}\big\|_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} \le K. \tag{34}$$

The same bounds show that $(w^{(\tau)})$ is bounded in $L^{8/d+2}(0, t_0; L^{8/d+2}(\mathbb{T}^d))$, since the Gagliardo-Nirenberg inequality with $\theta = d/(d+4)$ gives

$$\|w^{(\tau)}\|^{8/d+2}_{L^{8/d+2}(0,t_0;L^{8/d+2}(\mathbb{T}^d))} \le K \int_0^{t_0} \|w^{(\tau)}\|^{(8/d+2)\theta}_{H^2(\mathbb{T}^d)} \|w^{(\tau)}\|^{(8/d+2)(1-\theta)}_{L^2(\mathbb{T}^d)} dt$$
$$\le K \|w^{(\tau)}\|^{8/d}_{L^\infty(0,t_0;L^2(\mathbb{T}^d))} \int_0^{t_0} \|w^{(\tau)}\|^2_{H^2(\mathbb{T}^d)} dt \le K.$$

We infer from the Poisson equation that $(\Delta V^{(\tau)})$ is bounded in $L^{4/d+1}(0,t_0;L^{4/d+1}(\mathbb{T}^d))$, and using elliptic regularity, we deduce a bound for $V^{(\tau)}$ in $L^{4/d+1}(0,t_0;H^2(\mathbb{T}^d))$.

The estimates of Lemma 3 imply that

$$\begin{aligned}\big\|\Delta((w^{(\tau)})^2T^{(\tau)})\big\|_{L^2(0,t_0;H^{-2}(\mathbb{T}^d))} &\le \big\|(w^{(\tau)})^2T^{(\tau)}\big\|_{L^2(0,t_0;L^2(\mathbb{T}^d))} \\ &\le \|w^{(\tau)}\|^2_{L^4(0,t_0;L^4(\mathbb{T}^d))}\|T^{(\tau)}\|_{L^\infty(0,t_0;L^\infty(\mathbb{T}^d))} \le K. \end{aligned} \tag{35}$$

Since the embedding $H^1(\mathbb{T}^d) \hookrightarrow L^4(\mathbb{T}^d)$ is continuous in space dimensions $d \le 3$, the same holds for the embedding $L^{4/3}(\mathbb{T}^d) = (L^4(\mathbb{T}^d))^* \hookrightarrow H^{-1}(\mathbb{T}^d)$ for the dual spaces. This embedding, together with the Hölder inequality in x with $p = 3/2$ and $p' = 3$, gives

$$\begin{aligned}\big\|\mathrm{div}\big((w^{(\tau)})^2\nabla V^{(\tau)}\big)\big\|^{11/10}_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} &\le \big\|(w^{(\tau)})^2\nabla V^{(\tau)}\big\|^{11/10}_{L^{11/10}(0,t_0;H^{-1}(\mathbb{T}^d))} \\ \le K\int_0^{t_0}\big\|(w^{(\tau)})^2\nabla V^{(\tau)}\big\|^{11/10}_{L^{4/3}(\mathbb{T}^d)}dt &\le K\int_0^{t_0}\|w^{(\tau)}\|^{11/5}_{L^4(\mathbb{T}^d)}\|\nabla V^{(\tau)}\|^{11/10}_{L^4(\mathbb{T}^d)}dt.\end{aligned}$$

Next, we apply the Hölder inequality in t with $p = 70/37$ and $p' = 70/33$:

$$\begin{aligned}&\big\|\mathrm{div}\big((w^{(\tau)})^2\nabla V^{(\tau)}\big)\big\|^{11/10}_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} \\ &\quad\le K\|w^{(\tau)}\|^{11/5}_{L^{154/37}(0,t_0;L^4(\mathbb{T}^d))}\|\nabla V^{(\tau)}\|^{11/10}_{L^{7/3}(0,t_0;L^4(\mathbb{T}^d))} \le K,\end{aligned} \tag{36}$$

since $7/3 \le 4/d+1$ and $154/37 < 8/3+2$ in dimensions $d \le 3$. Estimates (34), (35), and (36) imply the estimate for the discrete time derivative of $w^{(\tau)}$, which finishes the proof. □

3.3. **The limit $\tau \to 0$.** The a priori estimates of the previous subsection are sufficient to pass to the limit $\tau \to 0$. First, the estimates (32) allow for the application of Aubin's lemma [23], showing that, up to a subsequence, $(w^{(\tau)})^2 \to n$ in $L^{11/10}(0,t_0;W^{1,4}(\mathbb{T}^d))$ as $\tau \to 0$ for some limit function n. Here we have used that the embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$ is compact in dimensions $d \le 3$. In particular, $(w^{(\tau)})$ converges pointwise a.e. As $(w^{(\tau)})^2$ is obviously nonnegative, so is n, and we can define the square root $\sqrt{n} \in L^{22/10}(0,t_0;L^\infty(\mathbb{T}^d))$ with $w^{(\tau)} \to \sqrt{n}$ pointwise a.e. The second estimate in (32) implies that, up to a subsequence,

$$\tau^{-1}\big((w^{(\tau)})^2 - (\sigma_\tau w^{(\tau)})^2\big) \rightharpoonup \partial_t n \quad \text{weakly in } L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d)).$$

Furthermore, the same arguments as in the proof of Lemma 4.3 in [18] show that $w^{(\tau)} \to \sqrt{n}$ strongly in $L^2(0,t_0;W^{1,4}(\mathbb{T}^d))$, which implies that

$$\begin{aligned} w^{(\tau)}\nabla^2 w^{(\tau)} &\rightharpoonup \sqrt{n}\nabla^2\sqrt{n} \quad \text{weakly in } L^1(0,t_0;L^2(\mathbb{T}^d)), \\ \nabla w^{(\tau)} \otimes \nabla w^{(\tau)} &\rightharpoonup \nabla\sqrt{n}\otimes\nabla\sqrt{n} \quad \text{weakly in } L^1(0,t_0;L^2(\mathbb{T}^d)).\end{aligned}$$

By Lemma 4, $(w^{(\tau)}T^{(\tau)})$ converges weakly (up to a subsequence) to some function θ in $L^2(0,t_0;H^1(\mathbb{T}^d))$. We can identify θ with $\sqrt{n}T$. Indeed, the pointwise a.e. convergence of $w^{(\tau)}$ to $\sqrt{n}$ and the boundedness of $(w^{(\tau)})$ in $L^{8/d+2}(0,t_0;L^{8/d+2}(\mathbb{T}^d))$ (see (33)) imply that $w^{(\tau)}$ converges strongly to $\sqrt{n}$ in $L^4(0,t_0;L^4(\mathbb{T}^d))$, since $8/d+2 < 4$ for $d \le 3$. Furthermore, $T^{(\tau)}$ converges weakly* to T in $L^\infty(0,t_0;L^\infty(\mathbb{T}^d))$. Hence, the product $w^{(\tau)}T^{(\tau)}$ converges weakly to $\sqrt{n}T$ in $L^4(0,t_0;L^4(\mathbb{T}^d))$, which shows that $\theta = \sqrt{n}T$. In particular, we infer that

$$w^{(\tau)}T^{(\tau)} \rightharpoonup \sqrt{n}T \quad \text{weakly in } L^2(0,t_0;H^1(\mathbb{T}^d)).$$

Moreover, $(w^{(\tau)}T^{(\tau)})$ is bounded in $L^\infty(0,t_0;L^2(\mathbb{T}^d))$, since $(w^{(\tau)})$ is bounded in $L^\infty(0,t_0;L^2(\mathbb{T}^d))$ and $T^{(\tau)}$ is bounded in $L^\infty(0,t_0;L^\infty(\mathbb{T}^d))$. Then, up to a subsequence,

$$w^{(\tau)}T^{(\tau)} \rightharpoonup^* \sqrt{n}T \quad \text{weakly* in } L^\infty(0,t_0;L^2(\mathbb{T}^d)).$$

The above convergence results, together with the strong convergence of $(w^{(\tau)})$ in $L^4(0,t_0;L^4(\mathbb{T}^d))$ and in $L^2(0,t_0;W^{1,4}(\mathbb{T}^d))$, imply that

$$\begin{aligned} \nabla\big((w^{(\tau)})^2T^{(\tau)}\big) &= w^{(\tau)}\nabla\big(w^{(\tau)}T^{(\tau)}\big) + w^{(\tau)}T^{(\tau)}\nabla(w^{(\tau)}) \\ &\rightharpoonup \sqrt{n}\nabla(\sqrt{n}T) + \sqrt{n}T\nabla\sqrt{n} = \nabla(nT) \\ &\quad \text{weakly in } L^{4/3}(0,t_0;L^{4/3}(\mathbb{T}^d)). \end{aligned} \tag{37}$$

The strong convergence of $(w^{(\tau)})$ in $L^4(0,t_0;L^4(\mathbb{T}^d))$ and the weak convergence of $(V^{(\tau)})$ (to some function V) in $L^2(0,t_0;W^{1,4}(\mathbb{T}^d))$ gives

$$(w^{(\tau)})^2\nabla V^{(\tau)} \rightharpoonup n\nabla V \quad \text{weakly in } L^{4/3}(0,t_0;L^2(\mathbb{T}^d)).$$

These limits allow us to perform the limit $\tau \to 0$ in (29), showing that $\sqrt{n}$ solves (8). We remark that the initial datum is satisfied by n in the sense of $H^{-2}(\mathbb{T}^d)$ since $n \in W^{1,11/10}(0,t_0;H^{-2}(\mathbb{T}^d)) \hookrightarrow C^0(0,t_0;H^{-2}(\mathbb{T}^d))$ and hence, $n(\cdot,0)$ is defined.

It remains to pass to the limit $\tau \to 0$ in the Poisson equation (31) and the heat equation (30). In view of (32), we have

$$\begin{aligned} &\big\|(\sigma_\tau w^{(\tau)})^2 - n\big\|_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} \\ &\quad \le \big\|(\sigma_\tau w^{(\tau)})^2 - (w^{(\tau)})^2\big\|_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} + \big\|(w^{(\tau)})^2 - n\big\|_{L^{11/10}(0,t_0;H^{-2}(\mathbb{T}^d))} \\ &\quad \le K_1\tau + K_2\big\|(w^{(\tau)})^2 - n\big\|_{L^{11/10}(0,t_0;L^2(\mathbb{T}^d))} \to 0 \quad \text{as } \tau \to 0, \end{aligned}$$

and we can perform the limit in the Poisson equation, showing that V is a solution to (10). Since $\nabla w^{(\tau)}$ converges strongly in $L^2(0,t_0;L^4(\mathbb{T}^d))$ and $w^{(\tau)}T^{(\tau)}$ converges weakly* in $L^\infty(0,t_0;L^2(\mathbb{T}^d))$, we obtain, together with (37),

$$\big(w^{(\tau)}\big)^2\nabla T^{(\tau)} = w^{(\tau)}\nabla\big(w^{(\tau)}T^{(\tau)}\big) - w^{(\tau)}T^{(\tau)}\nabla w^{(\tau)} \rightharpoonup \sqrt{n}\nabla(\sqrt{n}T) - \sqrt{n}T\nabla\sqrt{n} = n\nabla T$$

weakly in $L^{4/3}(0,t_0;L^{4/3}(\mathbb{T}^d))$. Thus, T solves (9). This completes the proof of Theorem 1.

4. Numerical results

In this section we present some numerical results for the simplified quantum energy-transport model in one space dimension:

$$n_t + \frac{\varepsilon^2}{12}\Big(n(\log n)_{xx}\Big)_{xx} - (nT)_{xx} + (nV_x)_x = 0, \tag{38}$$

$$-\kappa(nT_x)_x + \frac{1}{\tau_e}n(T-T_L) = 0, \tag{39}$$

$$\lambda^2 V_{xx} - n + C = 0, \tag{40}$$

where $x \in [0,1]$ and $t > 0$. The initial condition is $n(x,0) = C(x)$, $x \in (0,1)$. The parameters in the above equations are the scaled Planck constant ε, the Debye length λ, the heat-conduction constant κ, and the energy relaxation time τ_e. Notice that in contrast to the previous sections, we have introduced here the heat conductivity constant κ (see Section 2).

Parameter	Physical meaning	Value
q	elementary charge	$1.602 \cdot 10^{-19}$ As
m	effective electron mass	$0.067 \cdot 9.11 \cdot 10^{-31}$ 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 permitivity	$12.9 \cdot 8.8542 \cdot 10^{-12}$ A^{2}s^4/kg m^3
τ_0	momentum relaxation time	$0.9 \cdot 10^{-12}$ s

Table 1. Physical parameters for GaAs.

We consider periodic as well as the Dirichlet-Neumann boundary conditions, see below. In the numerical tests we simulate a GaAs n^+nn^+ diode, defined by the smooth doping profile

$$C(x) = 1 + 0.25(\tanh(100x - 60) - \tanh(100x - 40)), \quad x \in [0, 1].$$

We consider following two cases: (i) heating through the device contacts and (ii) heating in the interior of the device. Since we are interested in qualitative effects only, we choose the (artificial) scaled lattice temperature functions

$$\text{(i)} \quad T_L(x) = 4(a-1)(x^2 - x) + a, \quad \text{(ii)} \quad T_L(x) = -4(a-1)(x^2 - x) + 1,$$

where $a = 300/77$. The parameter a is chosen in such a way that, for the first function, the unscaled temperature equals 300 K at the boundary and 77 K at $x = \frac{1}{2}$ and vice versa for the second function. We have chosen here a characteristic temperature of $T_0 = 77$ K. The values of the remaining physical constants are given in Table 1.

In order to compute the values of the dimensionless parameters, we have to specify the scaling. Let L be a characteristic length, for instance the device length. We define the characteristic density, voltage, and time, respectively, by

$$C^* = \sup |C|, \quad V^* = \frac{k_B T_0}{q}, \quad t^* = \sqrt{\frac{mL^2}{k_B T_0}}. \tag{41}$$

The standard scaling (see for example [17]) gives

$$\varepsilon^2 = \frac{\hbar^2}{m k_B T_0 L^2}, \quad \lambda^2 = \frac{\epsilon_s V^*}{q C^* L^2}, \quad \kappa = \kappa_0 \tau_0 \frac{k_B T_0}{m}, \quad \tau_e = \frac{\tau_0}{t^*}.$$

For our numerical tests we have choosen $L = 75$ nm for the device length, $C^* = 10^{23}$ m^{-3} for the maximal doping concentration, and $\kappa_0 = 0.8$ for the thermal conductivity. Then

$$\varepsilon^2 \approx 3.05 \cdot 10^{-2}, \quad \lambda^2 \approx 8.42 \cdot 10^{-3}, \quad \kappa \approx 1.253 \cdot 10^{-2}, \quad \tau \approx 1.583.$$

The discretization of the model (38)–(40) using central finite differences reads as

$$\begin{aligned} \frac{n_i^{k+1} - n_i^k}{\triangle t} &= -\frac{\varepsilon^2}{12(\triangle x)^4} \Big[n_{i+1}^{k+1} \Big(u_{i+2}^{k+1} - 2u_{i+1}^{k+1} + u_i^{k+1} \Big) - 2n_i^{k+1} \Big(u_{i+1}^{k+1} - 2u_i^{k+1} + u_{i-1}^{k+1} \Big) \\ &\quad + n_{i-1}^{k+1} \Big(u_i^{k+1} - 2u_{i-1}^{k+1} + u_{i-2}^{k+1} \Big) \Big] + \frac{1}{(\triangle x)^2} \Big[n_{i+1}^{k+1} T_{i+1}^k - 2n_i^{k+1} T_i^k + n_{i-1}^{k+1} T_{i-1}^k \Big] \\ &\quad - \frac{1}{2(\triangle x)^2} \Big[(V_{i+1}^k - V_i^k) n_{i+1}^{k+1} + (V_{i+1}^k - 2V_i^k + V_{i-1}^k) n_i^{k+1} - (V_i^k - V_{i-1}^k) n_{i-1}^{k+1} \Big], \end{aligned} \tag{42}$$

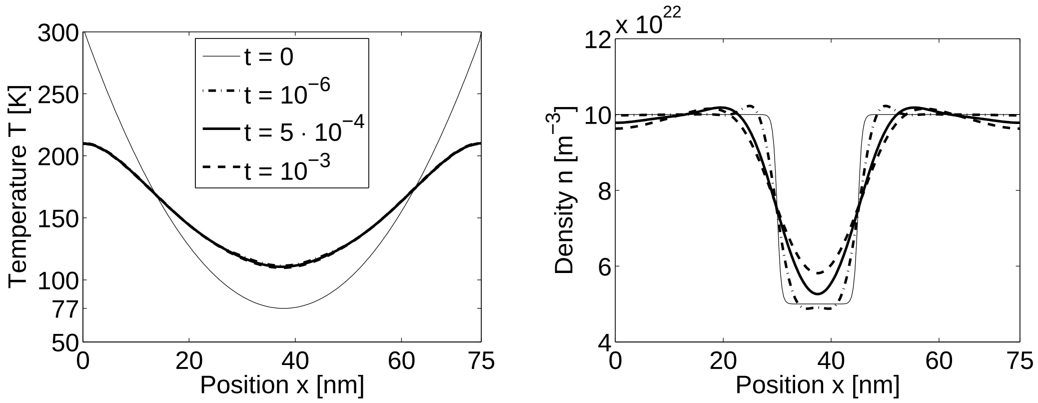

FIGURE 1. Periodic boundary conditions, case (i): Electron temperature (left) and electron density (right) at various times.

$$-\frac{(n_{i+1}^k+n_i^k)}{2}T_{i+1}^k+\Big(\alpha_T n_i^k+\frac{n_{i+1}^k+2n_i^k+n_{i-1}^k}{2}\Big)T_i^k-\frac{n_i^k+n_{i-1}^k}{2}T_{i-1}^k=\alpha_T n_i^k(T_L)_i, \tag{43}$$

$$\frac{\lambda^2}{(\Delta x)^2}(V_{i+1}^k-2V_i^k+V_{i-1}^k)=n_i^k-C_i, \tag{44}$$

where $u_i = \log(n_i)$, $i = 1,\dots,N-1$, $\alpha_T = (\triangle x)^2/(\kappa\tau_e)$. We used a uniform mesh with $N = 250$ points and $\triangle x = 1/N$. For the time step we have taken $\triangle t = 10^{-7}$. The system (42)–(44) is solved using an iterative semi-implicit numerical method. More precisely, given the electron density n^k at time step k, we solve the linear equations for the potential V^k and the temperature T^k. Then the values for T^k and V^k are employed in the nonlinear equation (42) for the particle density, which is solved by the Newton method. In this way we obtain the electron density n^{k+1} at time step $k+1$.

4.1. **Periodic boundary conditions.** Since the existence results in this paper are proved for periodic boundary conditions, we perform the first numerical tests for these boundary conditions. In order to assure the unique solvability of the Poisson equation, we impose the constraint $\int_0^1(n-C)dx = 0$.

First, we were interested how heating of the device through its contacts effects the device temperature. Figure 1 shows the electron temperature T (left) and particle density n (right) at various times. Notice that the values for the time are dimensionless; the characteristic time equals, according to (41), $t^* \approx 5.68\cdot 10^{-13}$ s. The temperature stabilizes extremely fast to its steady state. As expected, the heating through the contacts leads to a heating in the interior of the device and, because of the periodic boundary conditions, to an electron cooling in the n^+ regions at the contacts. The electron density becomes first smaller than the doping concentration (thin line) in the low-doped region, but it increases at larger times and finally reaches its steady state. Figure 2 illustrates the electron temperature and density in case (ii). In contrast to the previous case, the particle temperature T is smaller than T_L in the middle of the device, but larger at the contacts. This heating leads to an increase of the electron density at the contacts (right figure).

4.2. **Dirichlet-Neumann boundary conditions.** In this subsection, we consider more realistic boundary conditions for the one-dimensional n^+nn^+ diode studied in the previous

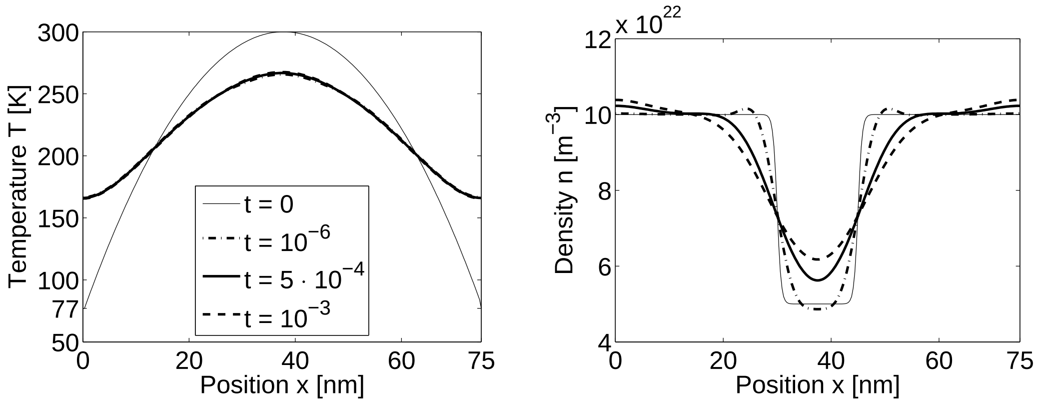

FIGURE 2. Periodic boundary conditions, case (ii): Electron temperature (left) and electron density (right) at various times.

subsection. We impose the following boundary conditions:

$$n(0) = C(0), \quad n(1) = C(1), \quad n_x(0) = n_x(1) = 0,$$
$$T(0) = T(1) = T_{\text{bc}}, \quad V(0) = 0, \quad V(1) = U,$$

where U is the applied potential and T_{bc} the given boundary temperature (300 K in case (i) and 77 K in case (ii)). The Dirichlet boundary conditions for the electron density express that the total space charge $C(x) - n$ vanishes at the boundary. Since $C(x)$ is nearly constant close to the boundary, we expect that $(C - n)_x \approx 0$ at $x = 0, 1$. This motivates the use of homogeneous Neumann boundary conditions for n. We are interested in the situation in which the device temperature at the contacts is constant, so we impose Dirichlet boundary conditions for the electron temperature T. Beside the Dirichlet conditions for V, no further constraint on V needs to be imposed.

The numerical results for the equilibrium situation $U = 0$ are presented in Figure 3 (case (i)) and in Figure 4 (case (ii)). The behavior of the temperature and density is similar to the previous subsection (except that now, the particle density cannot increase at the contacts since it is fixed). This is not surprising since the periodic case corresponds to some extend to the equilibrium situation.

In Figures 5 and 6, the particle temperatures and densities in case (i) and (ii), respectively, are shown for an applied voltage of $U = 1$ V. The temperature profile does not change significantly. On the other hand, the low-doped region in the diode is flushed by electrons, and the depletion region moves to the right due to the high electric field. The same behavior can be observed in the quantum drift-diffusion model in which the electron temperature is constant.

5. Conclusion and open problems

In this paper, we have shown the existence of global-in-time solutions to a simplified quantum energy-transport model. This is the first analytical result on a quantum diffusion model including temperature variations. The proof is based on exponential variable techniques employed in [18, 20], a fixed-point argument in the variables $\sqrt{n}$ and $\log n$, and the key entropy-type estimate (6). Moreover, some numerical results illustrate the heating behavior of a ballistic diode.

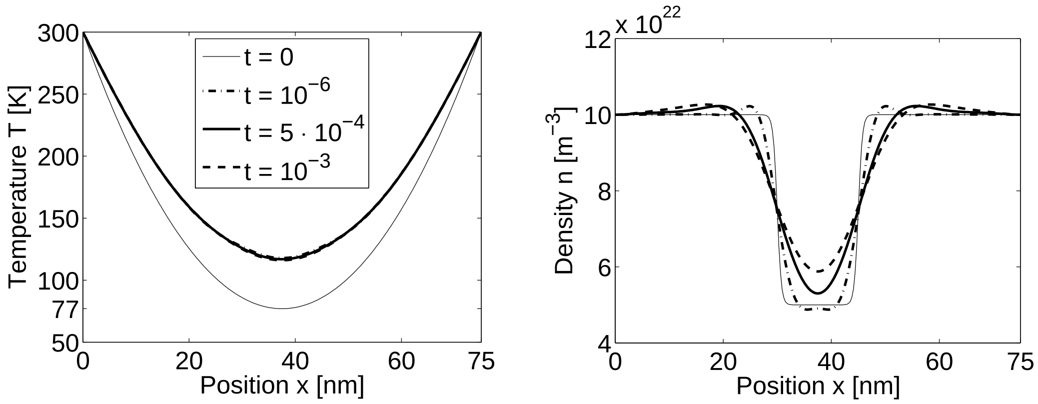

FIGURE 3. Dirichlet-Neumann boundary conditions, case (i), $U = 0$: Electron temperature (left) and electron density (right) at various times.

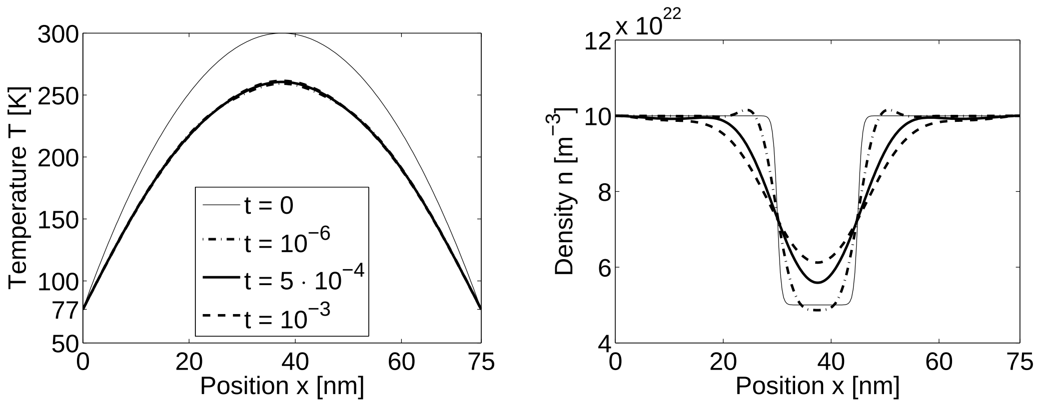

FIGURE 4. Dirichlet-Neumann boundary conditions, case (ii), $U = 0$: Electron temperature (left) and electron density (right) at various times.

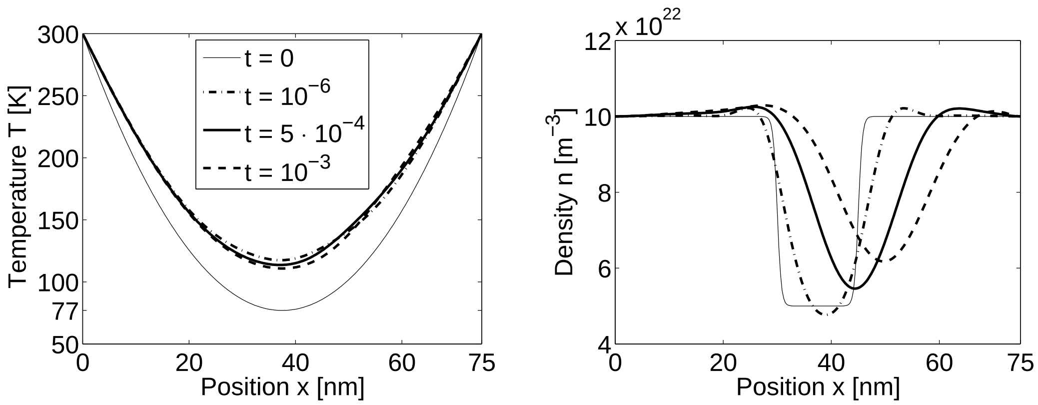

FIGURE 5. Case (i), Dirichlet-Neumann boundary conditions, $U = 1\,\mathrm{V}$: Electron temperature (left) and electron density (right) at various times.

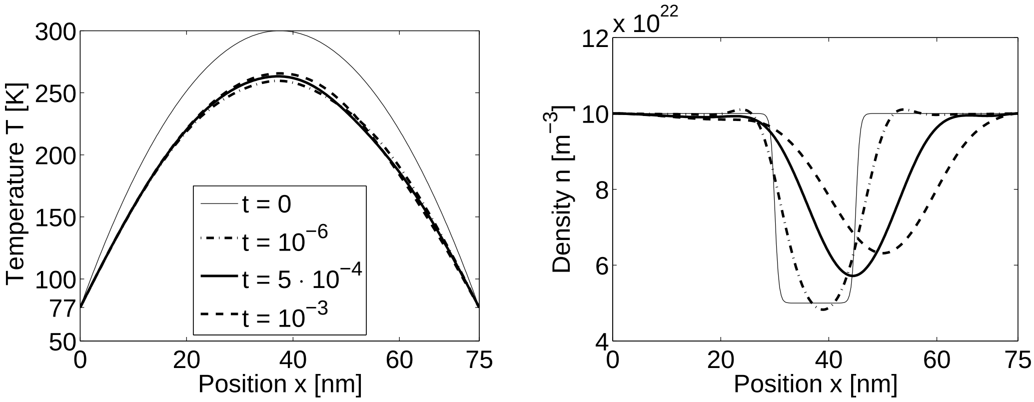

FIGURE 6. Case (ii), Dirichlet-Neumann boundary conditions, $U = 1\,\mathrm{V}$: Electron temperature (left) and electron density (right) at various times.

It is well known that, in real applications, thermal effects in semiconductors are becoming stronger in smaller devices due to large electric fields. Our result is slightly different. The numerical experiments show that the particle temperature depends only weakly on the model parameters. The reason is that the electron temperature is mainly governed by the lattice temperature through energy relaxation. A future investigation should take into account the full energy equation (16).

We have imposed several simplifications to the original quantum energy-transport model (15)-(16). First, the model (15)-(16) is special in the sense that it has been derived from the quantum hydrodynamic equations. There exists a class of quantum energy-transport models, derived directly from the Wigner-BGK equation [9, 17] and depending on the choice of the relaxation time model in the BGK collision operator. Second, the energy equation (16) has been significantly simplified, allowing us to use the maximum principle for the electron temperature. Third, we have chosen a rather simple model for the heat conductivity. Finally, we have imposed very simple periodic boundary conditions for the analytical results.

These comments lead us to the following open problems:

- Prove the global existence of solutions to the simplified model (1)-(3) with heat conductivity $\kappa(n, T) = nT$ instead of $\kappa(n, T) = n$.
- Prove the global existence of solutions to the simplified model (1)-(3) using more physical boundary conditions (for instance, $n = n_D$, $\nabla n \cdot \nu = 0$, $T = T_D$, $V = V_D$ on $\partial\Omega$, where $\Omega \subset \mathbb{R}^d$ is the semiconductor domain and ν the exterior unit normal vector to its boundary).
- Describe the long-time behavior of solutions to (1)-(3).
- Prove the semiclassical limit $\varepsilon \to 0$ in (1)-(3) (the problem is that we loose the H^2 bounds on $\sqrt{n}$).
- Prove the global existence of solutions to the full quantum energy-transport model (15)-(16).
- Analyze the quantum energy-transport models derived in [9] and reveal its mathematical structure.

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