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A Numerical Scheme for Quantum Hydrodynamics in a Semiconductor

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Dedicated to Professor Tai-Ping Liu on the occasion of his 60th birthday

Abstract

We study existence and numerical approximation of solutions to the quantum drift-diffusion equation arising in a semiconductor at the room temperature(i.e. at the high temperature). We obtain the existence of stational solutions by means of a numerically motivated solution map, introducing the generalized chemical potential(quasi-Fermi-level). This approach leads to an iterative solution method of the QDD equation coupled with the Poisson equation. An implicit semidiscretization of the time-dependent QDD equation is discussed. The new discretization in space of the QDD equation is proposed.

1 Introduction

The semiconductor transport in ultra-small structures at the room temperature(i.e. at the high temperature) is modeled by the quantum hydrodynamics. The quantum drift-diffusion model is viewed as one of the hierarchy of the quantum hydrodynamic models, which is derived from a moment expansion of Wigner-Boltzmann equation including collisional effects[1]. It is known that this model is a quantum corrected version of the classical drift-diffusion model, with $O(\hbar^2)$ corrections to the stress tensor[2]. We study the QDD system in a bounded domain $\Omega \subset R^d (d \geq 1)$ with piecewise smooth boundary, assuming Boltzmann statistics.

$$\epsilon\Delta\varphi = n - f, \tag{1}$$

$$\partial_t n + div(n\nabla(\varphi - ln(n) + \lambda^2\frac{\Delta\sqrt{n}}{\sqrt{n}})) = 0. \tag{2}$$

Here n is the electron density and the electrostatic potential φ. f is the density of ionized impurities. ϵ is the semiconductor permittivity. λ is the scaled Planck constant.

The fourth-order continuity equation (2) for the electron density is split into two second-order equations, using the generalized chemical potential(quasi-Fermi-level)$v =$

$\varphi - \ln(n) + \lambda^2 \frac{\Delta\sqrt{n}}{\sqrt{n}}$[2].

$$\epsilon\Delta\varphi = n - f, \tag{3}$$

$$\partial_t n + div(n\nabla v) = 0, \tag{4}$$

$$\lambda^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} - \ln(n) + \varphi = v. \tag{5}$$

In this paper we present the existence of stational solutions by means of a numerically motivated solution map, which leads to an iterative solution method of the QDD system. An implicit semidiscretization of the time-dependent QDD equation, which results in the elliptic system, is discussed. The new discretization in space of the elliptic system is proposed.

2 Existence of a solution and an iterative solution method

The analysis for the steady state of the QDD model was performed by a variational approach in the previous works[3],[4]. We obtain the existence of stational solutions by means of numerically motivated solution map. The result provides an iterative solution method of the QDD system. The analysis of stational solutions is based on the following assumptions.

(A.1) $\Omega \subset R^d$, d=1,2, or d=3 is a bounded domain with piecewise smooth boundary.

(A.2) $\partial\Omega\backslash(\partial\Omega_D \cup \partial\Omega_N)$ is a set of measure zero.

(A.3) There exists for all $f \in L^\infty(\Omega)$ and all $a, u_D \in W^{1,q}(\Omega)$ a function $u \in W^{1,q}(\Omega)$ with

$$div(a\nabla u) = f, \; u - u_D \in H_0^1(\Omega \cup \partial\Omega_N) \tag{6}$$

$$\|u\|_{W^{1,q}(\Omega)} \leq C(\|u_D\|_{W^{1,q}(\Omega)} + \|f\|_{L^\infty(\Omega)}). \tag{7}$$

Here $p, q \in (2, \infty]$ with $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$ such that $H^1(\Omega) \hookrightarrow L^p(\Omega)$ and $H^2(\Omega) \hookrightarrow W^{1,q}(\Omega)$.

(A.4) The Dirichlet boundary condition data $(\varphi_D, v_D, u_D) \in (H^1(\Omega) \cap L^\infty(\Omega))^3$, on $\partial\Omega_D$. The Neumann boundary conditions $\frac{\partial\varphi}{\partial\nu} = \frac{\partial v}{\partial\nu} = \frac{\partial u}{\partial\nu} = 0$, on $\partial\Omega_N$.

(A.5) $f \in L^\infty(\Omega)$.

We employ the exponetial transformation of variables $\rho = \sqrt{n} = e^u$ to construct the solution mapping. (5) is replaced by the equivalent form (9). In this case, if u is uniformly bounded, the positivity of the root-density $\rho = e^u$ is ensured.

$$\begin{aligned} \epsilon\Delta\varphi &= e^{2u} - f, & (8)\\ -\lambda^2\nabla(\rho\nabla u) + \rho u &= \frac{\rho}{2}(\varphi - v) \; in \; \Omega, & (9)\\ -div(n\nabla v) &= 0. & (10) \end{aligned}$$

The system is supplemented with the set of boundary conditions:

$$\varphi = \varphi_D, u = u_D, v = v_D, \text{ on } \partial\Omega_D, \tag{11}$$

$$\nabla\varphi \cdot \nu = \nabla u \cdot \nu = \nabla v \cdot \nu = 0 \text{ on } \partial\Omega_N. \tag{12}$$

To solve iteratively, we define the following solution mapping. Let w $\in L^2(\Omega)$ be given in Ω.

Algorithm 2.1 *(Solution map)*
(P1) Solve

$$\epsilon\Delta\varphi = e^{2w} - f, \tag{13}$$

subject to the boundary conditions(11),(12) for φ.
(P2) Solve

$$-div(e^{2w}\nabla v) = 0, \tag{14}$$

subject to the boundary conditions(11),(12) for v.
(P3) Solve

$$-2\lambda^2\nabla(e^w\nabla u) + 2e^w u = e^w(\varphi - v), \tag{15}$$

subject to the boundary conditions(11),(12) for u.

It readily follows from Lax-Milgram theorem that there exists a unique solution to each linear problem. Thus the mapping $T : X \to X$, $T(w) = u$, with $X = \{w \in L^2(\Omega) : -\underline{U} \leq w \leq \overline{U} \text{ in } \Omega\}$, is well defined. For $\overline{U}, \underline{U} > 0$, we define the cut-off function

$$Py := \begin{cases} \overline{U} & \text{if } y > \overline{U} \\ y & \text{if } -\underline{U} \leq y \leq \overline{U}. \\ -\underline{U} & \text{if } y < -\underline{U} \end{cases} \tag{16}$$

To obtain the L^∞ bounds for φ, u and v, we employ the following truncated system of (17)-(19) defined by the cut-off function.

$$\epsilon\Delta\varphi = e^{2Pu} - f, \tag{17}$$

$$-\lambda^2\nabla(e^{Pu}\nabla u) + e^{Pu}u = \frac{e^{Pu}}{2}(\varphi - v), \tag{18}$$

$$-\nabla(e^{2Pu}\nabla v) = 0, \tag{19}$$

subject to the boundary conditions (11)-(12). The proof of existence of solutions to the truncated system is based on the following a priori estimates. The result is obtained by applying Stampacchia's lemma[5] and maximum principle type arguments.

Lemma 2.1 *(A priori estimate) Let* $(\varphi, v, u) \in (H^1(\Omega) \cap L^\infty(\Omega))^3$ *be a weak solution to the truncated system. Then there exist positive constnants* $\underline{\varphi}, \overline{\varphi}, \underline{v}, \overline{v}, \underline{U}, \overline{U}$ *such that*

$$-\underline{\varphi} \leq \varphi \leq \overline{\varphi}, \ -\underline{v} \leq v \leq \overline{v}, \ -\underline{U} \leq u \leq \overline{U} \ in \ \Omega \tag{20}$$

where

$$\begin{aligned}
\overline{\varphi} &= \varphi_0 + c_1(\Omega, \epsilon)\|f\|, c_1(\Omega) > 0, && (21)\\
\underline{\varphi} &= \varphi_0 + c_2(\Omega, \epsilon)(e^{2\overline{U}} + \|f\|_\infty), c_2(\Omega) > 0, && (22)\\
\overline{v} &= \underline{v} = v_0, && (23)\\
\overline{U} &= max(\frac{\overline{\varphi} + \underline{v}}{2}, U_0), && (24)\\
\underline{U} &= max(\frac{\underline{\varphi} + \overline{v}}{2}, U_0), && (25)\\
\varphi_0 &= \sup_{\partial\Omega_D} |\varphi|, v_0 = \sup_{\partial\Omega_D} |v|, U_0 = \sup_{\partial\Omega_D} |u|. && (26)
\end{aligned}$$

Proof. Let $\psi \geq \varphi_0$. Selecting the test function $(\varphi - \psi)^+$, where $t^+ = max(t, 0)$,

$$\begin{aligned}
\int_\Omega \epsilon|\nabla(\varphi - \psi)^+|^2 dx &= -\int_\Omega (e^{2Pu} - f)(\varphi - \psi)^+ dx && (27)\\
&\leq \|f\|_\infty \|(\varphi - \psi)^+\|_1 (meas(\varphi > \psi))^{1/2}. && (28)
\end{aligned}$$

By a Poincare type inequality, we obtain

$$C_1(\Omega)\|(\varphi - \psi)^+\|_1 \leq \epsilon^{-1}\|f\|_\infty (meas(\varphi > \psi))^{1/2}, \ C_1 > 0. \tag{29}$$

Let $2 < r \leq 6$. By Sobolev's imbedding theorem, it follows for all $\eta > \psi$

$$\begin{aligned}
C_2(\Omega)^r \|(\varphi - \psi)^+\|_1^r &\geq \|(\varphi - \psi)^+\|_{0,r}^r && (30)\\
&\geq \int_{\{\varphi > \eta\}} (\varphi - \psi)^r dx && (31)\\
&\geq \int_{\{\varphi > \eta\}} (\eta - \psi)^r dx && (32)\\
&= (\eta - \psi)^r meas(\varphi > \eta). && (33)
\end{aligned}$$

For $\eta > \psi \geq \varphi_0$,

$$meas(\varphi > \eta) \leq K(\eta - \psi)^{-r}(meas(\varphi > \psi))^{r/2} \tag{34}$$

where $K = C(\Omega)^r \epsilon^{-r}\|f\|_\infty^r$. Applying Stampacchia's lemma for $g(\eta) = meas(\varphi > \eta)$:

$$g(\varphi_0 + \psi^*) = 0 \ with \ \psi^* = c_1(\Omega, \epsilon)\|f\|_\infty, \ where \ c_1(\Omega, \epsilon) = C(\Omega)\epsilon^{-1}. \tag{35}$$

We obtain $\varphi \leq \varphi_0 + \psi^* = \varphi_0 + c_1(\Omega, \epsilon)\|f\|_\infty \equiv \overline{\varphi}$. We need a upper bound for u to find a lower bound for φ. Let $\overline{U} = max(\frac{\overline{\varphi}+\underline{v}}{2}, U_0)$. For $u \geq \overline{U}$, the maximum principle gives a lower bound for v.

$$
\begin{aligned}
0 = \int_\Omega -div(e^{2Pu}\nabla v)(-v-\underline{v})^+ &= \int_\Omega e^{2Pu}|\nabla(-v-\underline{v})^+|^2 dx && (36)\\
&= \int_\Omega e^{2Pu}|\nabla(-v-\underline{v})^+|^2 dx && (37)\\
&\geq \int_\Omega e^{2\overline{U}}|\nabla(-v-\underline{v})^+|^2 dx && (38)
\end{aligned}
$$

We obtain $v \geq -\underline{v}$. Selecting the test function $(u-\overline{U})^+ \in H_0^1(\Omega \cup \partial\Omega_N)$,

$$\int_\Omega \lambda^2 e^{Pu}|\nabla(u-\overline{U})^+|^2 dx + \int_\Omega e^{Pu}(2u-(\varphi-v))(u-\overline{U})^+ dx = 0. \qquad (39)$$

Then we have the following estimates

$$\int_\Omega e^{Pu}(2u-(\varphi-v))(u-\overline{U})^+ dx \geq \int_\Omega e^{\overline{U}}(2\overline{U}-(\overline{\varphi}+\underline{v}))(u-\overline{U})^+ dx \geq 0. \qquad (40)$$

It follows that $u \leq \overline{U}$. Using $(-\varphi-\psi)^+$ *with* $\psi \geq \varphi_0$,

$$
\begin{aligned}
\int_\Omega \epsilon|\nabla(-\varphi-\psi)^+|^2 dx &= \int_\Omega (e^{2Pu}-f)(-\varphi-\psi)^+ dx && (41)\\
&\leq \int_\Omega (e^{2\overline{U}}+\|f\|_\infty)(-\varphi-\psi)^+ dx && (42)
\end{aligned}
$$

We recall the Stampacchia's lemma.

$$meas(-\varphi > \varphi_0 + \psi^*) = 0, \psi^* = e^{2\overline{U}} + c_2(\Omega, \epsilon)\|f\|_\infty. \qquad (43)$$

This implies $\varphi \geq -(\varphi_0 + \psi^*) \equiv -\underline{\varphi}, \psi^* = e^{2\overline{U}} + c_2(\Omega,\epsilon)\|f\|_\infty$. Let $\underline{U} = max(\frac{\underline{\varphi}+\overline{v}}{2}, U_0)$. Similarly we obtain $v \leq \overline{v}$ from the maximum principle arguments. Applying the test function $(-u-\underline{U})^+ \in H_0^1(\Omega \cup \partial\Omega_N)$, we obtain $u \geq -\underline{U}$. □

Theorem 2.1 *(Existence of a weak solution) There exists a solution of the boundary value problem (17)-(19) with the boundary conditions (11) and (12) in the regularity class of $H^1(\Omega) \cap L^\infty(\Omega)$.*

Proof. The mapping T is well-defined. It can be seen that the mapping T is continuous and compact. In fact, $\|u\|_1$ is bounded. Selecting the test function $u - u_D \in H_0^1(\Omega \cup \partial\Omega_N)$,

$$
\begin{aligned}
&\textstyle\int_\Omega \lambda^2 e^{Pw}|\nabla(u-u_D)|^2 dx + \int_\Omega \lambda^2 e^{Pw}\nabla u_D \nabla(u-u_D)dx + \int_\Omega e^{Pw}u(u-u_D)dx\\
&\qquad = \int_\Omega \frac{e^{Pw}}{2}(\varphi-v)(u-u_D)dx. && (44)\\
C_1\|u-u_D\|_1^2 &\leq \int_\Omega e^{Pw}|\nabla(u-u_D)|^2 dx && (45)\\
&\leq C_2 e^{\overline{U}}(\overline{U} + \frac{\overline{\varphi}+\overline{v}}{2} + \|u_D\|_1)\|u-u_D\|_1. && (46)
\end{aligned}
$$

Similarly, by (13) and (14) we conclude uniform H^1 bounds for φ and v. The Schauder fixed point theorem gives the existence of a fixed point,i.e., a solution (φ, u, v) to (8)-(10). $\square$

Lemma 2.2 *(Pinnau) The quantum operator* $A(n) = -\frac{\Delta\sqrt{n}}{\sqrt{n}}$ *is monotonic with respect to the* $L^p(\Omega)$*-norm.*

Proof. The operator A(n) is Gateâux differetiable. For $h \in [0,1]$, let $\xi := n_1 - h(n_1 - n_2)$. By the mean value theorem,

$$\langle A(n_1) - A(n_2), n_1 - n_2 \rangle = \langle A'(\xi), n_1 - n_2 \rangle. \tag{47}$$

The straight forward calculation gives

$$\langle A'(\xi), n_1 - n_2 \rangle = \int_\Omega \xi |\nabla (\frac{n_1 - n_2}{\xi})|^2 dx. \tag{48}$$

From [4, lemma 24], there exists a constant $C > 0$ such that

$$\langle A'(\xi), n_1 - n_2 \rangle \geq C \|n_1 - n_2\|_{L^p}^2. \tag{49}$$

where $p, q \in (2, \infty]$ satisfies $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$. $\square$

Theorem 2.2 *The mapping T is a contraction with respect to the* $L^p(\Omega)$*-norm.*

Proof. Let $w_1, w_2 \in X = \{w \in L^2(\Omega) : -\underline{U} \leq w \leq \overline{U} \ in \ \Omega\}$ and let $v_i, i = 1, 2$ be the solution of

$$-\nabla(e^{2w}\nabla v) = 0. \tag{50}$$

Taking the difference and employing Hölder's inequality, we get

$$\|v_1 - v_2\|_{H^1} \leq C \|\nabla v_2\|_{L^q} \|e^{2w_1} - e^{2w_2}\|_{L^p} \tag{51}$$

where $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$. We have from the elliptic estimate

$$\|v_1 - v_2\|_{H^1} \leq C \|v_D\|_{W^{1,q}} \|w_1 - w_2\|_{L^p}. \tag{52}$$

Let $(u_i, \varphi_i), i = 1, 2$ be the solution of

$$\epsilon \Delta \varphi = e^{2u} - f, \tag{53}$$

$$-\lambda^2 \frac{\nabla(\rho \nabla u)}{\rho} + u = \frac{1}{2}(\varphi - v), \ \rho = e^u. \tag{54}$$

Selecting the test fuction $n_1 - n_2 \in H_0^1(\Omega \cup \partial\Omega_N)$,

$$0 = -\lambda^2 \int_\Omega (\frac{\nabla^2 \rho_1}{\rho_1} - \frac{\nabla^2 \rho_2}{\rho_2})(n_1 - n_2)dx + \frac{1}{2}\int_\Omega (\ln(n_1) - \ln(n_2))(n_1 - n_2)dx$$

$$-\frac{1}{2}\int_\Omega (\varphi_1 - \varphi_2)(n_1 - n_2)dx + \frac{1}{2}\int_\Omega (v_1 - v_2)(n_1 - n_2)dx \tag{55}$$

$$= I_1 + I_2 + I_3 + I_4. \tag{56}$$

We estimate term wise.

$$I_1 = \langle A'(\xi), n_1 - n_2 \rangle \geq C\|n_1 - n_2\|_{L^p}^2, \tag{57}$$

$$I_2 \geq 0, \tag{58}$$

$$I_3 = \int_\Omega |\nabla(\varphi_1 - \varphi_2)|^2 dx \geq 0, \tag{59}$$

$$I_4 \leq \|v_1 - v_2\|_{L^2}\|n_1 - n_2\|_{L^p}. \tag{60}$$

Combining these estimates, we have

$$\|u_1 - u_2\|_{L^p} \leq C\|n_1 - n_2\|_{L^p} \leq \|v_1 - v_2\|_{H^1}. \tag{61}$$

From (52), we finally obtain

$$\|u_1 - u_2\|_{L^p} \leq C\|v_D\|_{W^{1,q}}\|w_1 - w_2\|_{L^p}. \tag{62}$$

The assertion follows by choosing $\|v_D\|_{W^{1,q}} \leq V_0 < 1$ small enough. □

3 Discretization in time

Let $\tau_k = t_k - t_{k-1} > 0$ be the time step. Set the initial condition $\rho_0 = \sqrt{n_0}$. For $k \in N$, we discretize (3),(4) and (9), employing an implicit time discretization by a backward Euler scheme as follows.

$$\frac{n^k - n^{k-1}}{\tau_k} + div(n^k \nabla v^k) = 0, \tag{63}$$

$$-2\lambda^2 \nabla(\rho^k \nabla u^k) + 2\rho^k u^k = \rho^k(\varphi^k - v^k), \tag{64}$$

$$\epsilon \Delta \varphi^k = n^k - f, \tag{65}$$

subject to the simplified boundary conditions:

$$\varphi^k = 0, u^k = u_D, \nabla v^k \cdot v = 0 \ on \ \partial\Omega. \tag{66}$$

The transient problem is replaced by a sequence of elliptic problems. As pointed out in the previous works[6], the following entropy dissipation property is presented.This provides the stability bounds of the approximate solutions.

Lemma 3.1 *(Discrete entropy estimate). Let $(\varphi^k, u^k, v^k) \in H_0^1(\Omega) \times H^1(\Omega) \times H^1(\Omega)$ be a solution of (63)-(65) subject to the boundary conditions (66). Then the following entropy (free energy) estimates holds:*

$$S^k \leq S^{k-1} \tag{67}$$

where $S^k = \lambda^2 \int_\Omega |\nabla \rho^k|^2 dx + \int_\Omega (n^k(\ln(n^k) - 1) + 1)dx + \frac{\epsilon}{2} \int_\Omega |\nabla \varphi^k|^2 dx.$

Proof. The straightforward calculation using the chemical potential v^k as a test function gives the entropy estimates. □

4 Discretization in space

Finally, we propose a new nonlinear scheme to the QDD equation[7] for discretization in space. The QDD equation is discretized by conservative difference schemes. The simulation region Ω is partitioned into computational cells Ω_i, i.e., $\Omega = \cup_i \Omega_i$. Assuming that the flux $J = e^G \nabla \eta$ in (63), where $\eta = exp(-v)$ and $G = \varphi + \lambda^2 \frac{\Delta \rho}{\rho}$, and the flux $F = \rho \nabla u$ in (64), we obtain by Green's formula over each computational cell Ω_i that

$$\int_{\Omega_i} n_t dx - \int_{\partial \Omega_i} e^G \frac{\partial \eta}{\partial \nu} ds = 0, \tag{68}$$

$$\int_{\partial \Omega_i} \lambda^2 \rho \frac{\partial u}{\partial \nu} ds - \int_{\Omega_i} \rho u dx = -\frac{1}{2} \int_{\Omega_i} \rho(\varphi - v) dx. \tag{69}$$

The numerical fluxes $J_{i+1/2}$ and $F_{i+1/2}$ yield

$$J_{i+1/2} \text{ or } F_{i+1/2} = \frac{\theta_{i+1} - \theta_i}{\int_{\Omega_i} e^{-\theta} dx}, \; \theta = G \text{ or } u. \tag{70}$$

Substituting in (68) and (69) the average fluxes $J_{1\pm 1/2}$ and $F_{1\pm 1/2}$ leads to a class of conservative schemes, following Tikhonov and Samarskii in [8]. In this case, the key ingredient is to find an explicit integration of the exponetial function with respect to the potentials. Assuming the piecewise-linear representation of θ, we have

$$\int_{\Omega_i} e^{-\theta} dx = \frac{h e^{-\theta_i}}{B(\theta_{i+1} - \theta_i)} \tag{71}$$

where B is the Bernoulli function. This yields the fully discrete system as follows.

$$\frac{n_i^k - n_i^{k-1}}{\tau_k} = \frac{B(G_{i+1}^k - G_i^k) n_{i+1}^k - (B(G_i^k - G_{i+1}^k) + B(G_i^k - G_{i-1}^k)) n_i^k + B(G_{i-1}^k - G_i^k) n_{i-1}^k}{h^2}, \tag{72}$$

$$-\frac{\rho_{i+1}^k B(u_{i+1}^k - u_i^k)(u_{i+1}^k - u_i^k) - \rho_i^k B(u_i^k - u_{i-1}^k)(u_i^k - u_{i-1}^k)}{h^2} + \Lambda_i^k u_i^k = \frac{\Lambda_i^k}{2}(\varphi_i^k - v_i^k), \tag{73}$$

where $\Lambda = \int_{\Omega_i} \rho dx$. This nonlinear scheme is a consistent generalization of the Scharffeter-Gummel scheme to the classical drift-diffusion equation[7].

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