ZERO RELAXATION TIME APPROXIMATION OF THE QUANTUM DRIFT-DIFFUSION EQUATION FROM NONLINEAR SCHRÖDINGER EQUATIONS

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Abstract. We show the existence of the weak solution of the quantum drift-diffusion system in the semiconductor devise simulation. We introduce a system of the damped nonlinear Schrödinger equation with the Poisson equation and show the global existence of the weak solution in the energy class. By the energy inequality with L^2 conservation law, we may derive the zero relaxation time approximation and the limiting function solves the quantum drift-diffusion system in a weak sense.

1. The quantum drift-diffusion system

In this short note, we consider the solvability of the Cauchy problem of the following quantum drift-diffusion equation:

$$\begin{cases} \partial_t\rho - \operatorname{div}\cdot\left(\nabla\rho - \mu\rho\nabla\psi - 2b\rho\nabla\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right) = 0, & t>0, x\in\mathbb{R}^n, \\ -\Delta\psi = \dfrac{1}{\kappa^2}(\rho+g), \quad x\in\mathbb{R}^n, \\ \rho(0,x) = \rho_0(x). \end{cases} \tag{1.1}$$

where $\rho = \rho(t,x)$ is nonnegative function denoting the charge density and $\psi = \psi(t,x)$ is the electric scaler fields. The given function $g(x)$ denotes the background charge and μ, κ, b are given positive constants.

As one of the simplest model for the carrier transport problem for the semiconductor devise simulation, the following elliptic parabolic system with the drift effect, called as *drift-diffusion system* is presented:

$$\begin{cases} \partial_t n - \mu_1\Delta n + \nabla(n\nabla\psi) = 0, & t>0, x\in\mathbb{R}^n, \\ \partial_t p - \mu_2\Delta p - \nabla(p\nabla\psi) = 0, & t>0, x\in\mathbb{R}^n, \\ -\Delta\psi = n - p + g, \quad x\in\mathbb{R}^n, \\ n(0,x) = n_0(x) > 0, \qquad p(0,x) = p_0(x) > 0, \quad x\in\mathbb{R}^n, \end{cases} \tag{1.2}$$

where $n(t,x)$ and $p(t,x)$ denote the density of negative and positive charges and ψ denotes the electric potential, respectively. μ_1 and μ_2 are positive constants standing for the mobility.

This equation originally appeared as the simplest model for the semiconductor device simulation. It is understood that the microscopic dynamics of the charge transfer is governing by the damped compressible Euler equation with the equation of continuity of the density of the charge.

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Let $\rho = \rho(t, x)$ be the density of charge and $J_\rho(t, x)$ be a current of charge. If we introduce the velocity vector of the charge $u(t, x)$, the fluid mechanical view of the semiconductor devise is described by the following system:

$$\begin{cases} \partial_t\rho + \text{div }(\rho u) = 0, \\ \partial_t(\rho u) + \nabla(\rho u \otimes u) + \nabla P(\rho) + \rho\nabla\psi = -\frac{1}{\tau}\rho u, \\ -\Delta\psi = \frac{4\pi}{\kappa^2}(\rho + g), \end{cases} \tag{1.3}$$

where g denotes a given back ground charge and τ denotes the relaxation time. We assume the barotropic condition on the pressure term $P = P(\rho)$. The adiabatic assumption says that the pressure is a function of some powered of the density function ρ. Here we assume the Einstein law $P(\rho) = \frac{k_BT}{q}\rho$, where T is the temperature, q is a unit charge and k is the Boltzmann constant. By a simple scaling : $t \to t'/\tau$, $u \to \tau u'$ and singular limiting process called as *zero-relaxation time limit* $\tau \to 0$ yields the simplest approximation for the semiconductor simulation model called the drift-diffusion equations with Darcy's law. Namely we deduce the following model for the monopolar semiconductor charge simulation:

$$\begin{cases} \partial_t\rho + \nabla\cdot J_\rho = 0, \qquad J_\rho = -\mu(\frac{k_BT}{q}\nabla\rho + \rho\nabla\psi) \\ -\Delta\psi = \frac{4\pi}{\kappa^2}(\rho + g), \end{cases}$$

If the design of the semiconductor is based on both the positive and negative charges, the bipolar model should be introduced and the system is generalized as following system:

$$\begin{cases} \partial_t n - \nabla\cdot J_n = 0, \quad J_n = \mu_n(\frac{k_BT}{q}\nabla n - n\nabla\psi) \\ \partial_t p + \nabla\cdot J_p = 0, \quad J_p = -\mu_p(\frac{k_BT}{q}\nabla p + p\nabla\psi) \\ -\Delta\psi = \frac{4\pi}{\kappa^2}(p - n + g), \end{cases}$$

The equation (1.2) is simplified form of this bipolar model. The first analytic result concerning the existence of a simplified stationary version of the system obtained by Mock [9] (cf. Biler [2]).

If the structure of the semiconductor devise enters much smaller scale, the quantum effect should necessarily appear. Here we consider the model which takes the quantum effect in the electric current into an account called as the *Quantum drift-diffusion model*: Introducing the corrected quantum current:

$$J_n = -\rho\nabla\left(\log\rho - \mu\psi - 2b\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right) \tag{1.4}$$

where $b > 0$ is a small parameter associated with the Plank constant $\hbar$ as

$$b = \frac{\hbar^2}{2mq}$$

where q is the unit charge and m is the approximated mass of the particles.

Consider the following initial value problem with the quantum drift-diffusion equation:

$$
(1.5)\qquad \begin{cases} \partial_t \rho - \operatorname{div}\ \cdot \left(\nabla\rho - \mu\rho\nabla\psi - 2b\rho\nabla\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}} \right) = f, \qquad t>0, x\in\mathbb{R}^n, \\ -\Delta\psi = \dfrac{1}{\kappa^2}(\rho+g), \quad x\in\mathbb{R}^n, \\ \quad \rho(0,x) = \rho_0(x). \end{cases}
$$

Note that for the bipolar model, we have a natural extension to the quantum model which will be described as follows:

$$
(1.6)\qquad \begin{cases} \partial_t n - \operatorname{div}\ \cdot \left(\nabla n - \mu_1 n\nabla\psi - 2bn\nabla\dfrac{\Delta\sqrt{n}}{\sqrt{n}} \right) = f, \qquad t>0, x\in\mathbb{R}^n, \\ \partial_t p + \operatorname{div}\ \cdot \left(-\nabla p - \mu_2 p\nabla\psi + 2bp\nabla\dfrac{\Delta\sqrt{p}}{\sqrt{p}} \right) = f, \qquad t>0, x\in\mathbb{R}^n, \\ -\Delta\psi = \dfrac{1}{\kappa^2}(p-n+g), \quad x\in\mathbb{R}^n, \\ \quad n(0,x) = n_0(x), \qquad p(0,x) = p_0(x). \end{cases}
$$

The external force f is normally given as a function of x and n and p but for simplicity, we treat it as a given function.

For simplicity we assume the external force f and back ground charge g are vanishing and we consider a simpler system such as;

$$
(1.7)\qquad \begin{cases} \partial_t \rho - \operatorname{div}\ \cdot \left(\nabla\rho - \mu\rho\nabla\psi - 2b\rho\nabla\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}} \right) = 0, \qquad t>0, x\in\mathbb{R}^n, \\ -\Delta\psi = \rho, \quad x\in\mathbb{R}^n, \\ \quad n(0,x) = n_0(x). \end{cases}
$$

The existence and well-posedness issue on the problem (1.5) seems to be very complicated since the principal term of the first equation is fourth order quasilinear parabolic equation and degeneracy is depending on both $\nabla\rho$ and ρ. See [1], [5], [6], [7].

On the other hand, the origin for the quantum drift-diffusion equation is the Schrödinger equation, it is natural to introduce related nonlinear Schrödinger equation in order to show the existence of the solution to (1.5). Analogous way to the zero relaxation time approximation from the dumped Euler equation to the classical drift-diffusion equation, we consider the following damped nonlinear Schrödinger- Poisson equation:

$$
(1.8)\qquad \begin{cases} i\partial_t\psi + \Delta\psi - f\big(|\psi|^2\big)\psi - (\lambda\Phi - i\tau^{-1}\log\dfrac{\psi}{|\psi|})\psi = 0, \quad t\ge 0, x\in\mathbb{R}^n, \\ \quad -\Delta\Phi = |\psi|^2, \quad t\ge 0, x\in\mathbb{R}^n, \\ \quad \psi(0,x) = \psi_0(x), \quad t\ge 0, x\in\mathbb{R}^n, \end{cases}
$$

where nonlinearity $f(\cdot)$ is typically given either by

$$
f(s) = \log s \text{ or } \quad f(s) = s^{\frac{p-1}{2}}
$$

and the parameter $\lambda = \pm 1$ determines that the system is either repulsive or attractive case. After establishing the time global wellposedness on the above nonlinear Schrödinger equation, we use the Madelung transform to derive so called the dispersive compressible Euler system and by the zero relaxation time limit $\tau \to 0$ with the change of variables as $t \to \tau t'$ and $\theta(t,x) \to \tau\theta'(t,x)$, where $\theta = -i \log \frac{\psi}{|\psi|}$ we derive the existence of the solution of the quantum drift-diffusion system.

2. The existence of solution of the nonlinear Schrödinger equations

The time local well posedness of the nonlinear Schrödinger equation (1.8) is nowaday well understood. Due to Kato-Yajima result ([8], [10]), we have the following (cf. [3]):

Definition. We call a pair of the exponents (θ, q) as H^s -admissible of the Strichartz estimate if

$$\frac{n}{q} + \frac{2}{\theta} = 1 + s.$$

Proposition 2.1. *Let (θ, q) be an L^2 admissible pair of the Strichartz estimate. For $1 < p < 1 + \frac{4}{n-2}$ and $\psi_0 \in H^1(\mathbb{R}^n)$, there exists a global solution of (1.8) in $\psi \in C([0,T); H^1) \cap W^{1,\theta}(0,T; W^{1,p})$. Moreover if the initial data is in $\psi \in H^{2k}(\mathbb{R}^n)$ then $\psi \in C^k([0,\infty); H^{2k}(\mathbb{R}^n))$.*

The solution is constructed by the integral equation:

$$\begin{cases} \psi(t) = e^{it\Delta}\psi_0 - \int_0^t e^{i(t-s)\Delta} \left\{ f(|\psi(s)|^2) + \lambda\Phi(s) + i\tau^{-1}\log\frac{\psi(s)}{|\psi(s)|} \right\} \psi(s)ds, \\ \Phi(t) = \int_{\mathbb{R}^n} G(x-y)|\psi(t,y)|^2 dy, \end{cases} \tag{2.9}$$

We then derive the global existence of the solution obtained in the above Proposition 2.1. Indeed, we have the following a priori estimate:

Proposition 2.2. *Let $F(s) = \int_0^s f(s)ds$. Then we have the following conservation laws:*

$$\|\psi(t)\|_2^2 = \|\psi_0\|_2^2,$$
$$E(\psi(t)) \le E(\phi_0),$$

where

$$E(\psi) \equiv \|\nabla\psi\|_2^2 + \int_{\mathbb{R}^n} F\big(|\psi|^2\big)dx + \frac{\lambda}{2}\int_{\mathbb{R}^n} \Phi|\psi|^2 dx.$$

Proof of Proposition 2.2. The energy identity

$$E(\psi(t)) + \int_0^t \frac{2}{\tau}\left[\mathrm{Im}\int_{\mathbb{R}^n} \bar{\psi}\nabla\theta\cdot\nabla\psi dx\right]dt = E(\phi_0)$$

can be derived via the gauge transform of the solution: $\phi(t,x) = \psi(t.x)e^{i\sigma(t,x)}$. According to the energy estimate obtained in the above, we may derive the a priori bound for the weak solution of (1.8) in $C([0,\infty); H^1)$. In deed, it is easy to check that the damping term

$$\int_0^t \frac{2}{\tau}\left[\mathrm{Im}\int_{\mathbb{R}^n} \bar{\psi}\nabla\theta\cdot\nabla\psi dx\right]dt$$

is non-negative if we write it by the polar coordinate expression $\psi(t,x) = \sqrt{\rho(t,x)}e^{i\theta(t,x)}$. It should be noted that since

$$\begin{aligned}\mathrm{Im}\int_{\mathbb{R}^n} \bar{\psi}\nabla\theta\cdot\nabla\psi dx =&\mathrm{Im}\int_{\mathbb{R}^n} \sqrt{\rho}e^{-i\theta}\nabla\theta\cdot\big(\nabla\sqrt{\rho}+i\sqrt{\rho}\nabla\theta\big)e^{i\theta}dx\\ =&\int_{\mathbb{R}^n}\rho|\nabla\theta|^2 dx\ge 0,\end{aligned}$$

we have the energy estimate

$$E(\psi(t))\le E(\psi_0).$$

□

3. the Madelung transform

Let $\psi(t,x)$ solves the following nonlinear Schrödinger equation:

$$\begin{cases} i\partial_t\psi+\Delta\psi = i\tau^{-1}\log\dfrac{\psi}{|\psi|}\psi + f(|\psi|^2)\psi+\lambda\Phi\psi,\\ -\Delta\Phi = |\psi|^2,\\ \psi(0,x)=\psi_0. \end{cases}$$

By setting a new unknown functions $\rho(t,x)$ and $\theta(t,x)$ as

$$\psi(t,x)=\sqrt{\rho}e^{i\theta(t,x)}.$$

It maybe worth to notice that

$$\theta(t,x) = -i\log\left(\frac{\psi}{\sqrt{\rho}}\right)$$

this means that ρ and ψ exactly determines θ. The transformed equation can be computed as follows:

$$\begin{aligned}0=&i\partial_t\psi+\Delta\psi+i\tau^{-1}\log\frac{\psi}{|\psi|}\psi-\Big(\lambda\Phi+f(|\psi|^2)\Big)\psi\\ =&e^{i\theta}\Bigg[-\sqrt{\rho}\partial_t\theta-\frac{1}{4\rho^{3/2}}|\nabla\rho|^2+\frac{1}{2\sqrt{\rho}}\Delta\rho-\sqrt{\rho}|\nabla\theta|^2-\sqrt{\rho}\tau^{-1}\theta-\lambda\sqrt{\rho}\Phi-\sqrt{\rho}f(\rho)\\ &+i\sqrt{\rho}^{-1}\left(\frac{1}{2}\partial_t\rho+\nabla\rho\cdot\nabla\theta+\rho\Delta\theta\right)\Bigg].\end{aligned}$$

Then the real and imaginary term part has to be 0 and the resulting equations are by dividing by $\sqrt{\rho}$,

$$\begin{cases}\partial_t\rho+2\mathrm{div}\ (\rho\nabla\theta)=0, \quad t>0, x\in\mathbb{R}^n,\\ \partial_t\theta+|\nabla\theta|^2+\tau^{-1}\theta+f(\rho)+\lambda\Phi-\dfrac{1}{2\rho}\Delta\rho+\dfrac{1}{4\rho^2}|\nabla\rho|^2=0, \quad t>0, x\in\mathbb{R}^n,\\ -\Delta\Phi=\rho, \quad t>0, x\in\mathbb{R}^n.\end{cases}$$

Note that

$$\begin{aligned}-\frac{1}{2\rho}\Delta\rho =&-\frac{1}{2}\mathrm{div}\ \frac{1}{\rho}\nabla\rho+\frac{1}{2}\frac{|\nabla\rho|^2}{\rho^2}\\ =&-\frac{1}{2}\Delta\log\rho-\frac{1}{2}\big|\nabla\log\rho\big|^2\end{aligned}\tag{3.10}$$

and thus

$$
(3.11)\qquad \begin{aligned} -\frac{1}{2\rho}\Delta\rho+\frac{1}{4\rho^2}|\nabla\rho|^2 =& -\frac{1}{2}\Delta\log\rho-\frac{1}{4}\big|\nabla\log\rho\big|^2\\ =& -\Delta\log\sqrt{\rho}-\big|\nabla\log\sqrt{\rho}\big|^2. \end{aligned}
$$

Or by taking a derivative

$$
\begin{cases} \partial_t\rho+2\text{div }(\rho\nabla\theta)=0,\\ \partial_t\nabla\theta+\nabla|\nabla\theta|^2+\tau^{-1}\nabla\theta=-\nabla\left(f(\rho)+\lambda\Phi-\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right),\\ -\Delta\Phi=\rho. \end{cases}
$$

This equation yields the so-called dispersive compressible Euler equation:

$$
\begin{cases} \partial_t\rho+2\text{div }(\rho v)=0,\\ \partial_t(\rho v)+2\nabla(\rho v\otimes v)+\dfrac{1}{\tau}\rho v=-\rho\nabla\left(f(\rho)+\lambda\Phi-\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right),\\ -\Delta\Phi=\rho. \end{cases}
$$

By changing the unknown function such as $t\to t'/\tau$, $v\to\tau v'$ we see that the system is given by

$$
\begin{cases} \partial_t\rho+2\text{div }(\rho v')=0,\\ \tau^2(\partial_t(\rho v')+2\nabla(\rho v'\otimes v'))+\rho v'=-\rho\nabla\left(f(\rho)+\lambda\Phi-\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right),\\ -\Delta\Phi=\rho. \end{cases}
$$

Combining the a priori estimate deduced from the energy estimate, we may take a weak limit of the $\tau\to 0$ and the limiting function is subject to solve the system

$$
\begin{cases} \partial_t\rho+2\text{div }(\rho v')=0,\\ \rho v'=-\rho\nabla\left(f(\rho)+\lambda\Phi-\dfrac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right),\\ -\Delta\Phi=\rho, \end{cases}
$$

we obtain the weak solution of the quantum drift-diffusion system (1.7).

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