INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 13, Number 6, Pages 898–925

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Computing and Information

STATIONARY SOLUTIONS TO HYBRID QUANTUM HYDRODYNAMICAL MODEL OF SEMICONDUCTORS IN BOUNDED DOMAIN

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Abstract. In this paper we study the behaviour of a micro-sized semiconductor device by means of a hybrid model of hydrodynamic equations. First of all, taking into account the quantum effects in the semiconductor device, we derive a new model called the hybrid quantum hydrodynamic model (H-QHD) coupled with the Poisson equation for electric potential. In particular, we write the Bohm potential in a revised form. This new potential is derived heuristically by assuming that the energy of the electrons depends on the charge density n and on ∇n just in a restricted part of the device domain, whereas the remaining parts are modeled classically. Namely, the device is designed with some parts that feel the quantum effects and some parts do not. The main target is to investigate the existence of the stationary solutions for the hybrid quantum hydrodynamic model. Since the quantum effect is regionally degenerate, this will also makes the working equation regionally degenerate regarding its ellipticity, and the corresponding solutions are weak only. This paper seems the first framework to treat the equation with regionally degenerate ellipticity. In order to prove the existence of such weak solutions, we first construct a sequence of smooth QHD solutions, then prove that such a sequence weakly converges and its limit is just our desired weak solution for the hybrid QHD problem. The Debye length limit is also studied. Indeed, we prove that the weak solutions of the hybrid QHD weakly converge to their targets as the spacial Debye length vanishes. Finally, we carry out some numerical simulations for a simple device, which also confirm our theoretical results.

Key words. Hybrid quantum hydrodynamic model, 4th-order degenerate elliptic equations, stationary solutions, existence, uniqueness, classical limit, hybrid limit.

1. Introduction

In the last decades, the characteristic size of semiconductor devices have gradually reduced up to few hundreds of nanometers. Under these conditions, quantum effects can no longer be neglected, because they play an important role in the functioning of the devices. However, quantum effects are usually localized in a small region of the device, while the rest of the domain can be treated classically, with remarkable reduction of the computational costs. Therefore, the hybrid models are developed in order to provide a strictly quantum description wherever necessary.

Simply speaking, the word *hybrid* emphasizes a mathematical approach for which one models a part of the device by using quantum equations (such as Schrödinger equation, quantum drift-diffusion (QDD) or quantum hydrodynamic (QHD)), and the other parts by using classical models, for example hydrodynamical (HD) or drift diffusion (DD). The main problem is which kind of transmission conditions must be prescribed at the interface between classical and quantum zones of the device. The pioneering study in the hybrid coupling between quantum and classical systems is the paper of N. Ben Abdallah [4], where a suitable set of transmission conditions, linking classical Boltzmann equation and stationary Schrödinger equations, is discussed. Since then, the relevant research has gradually become a hot spot. In [7], Baro *et al* study a one-dimensional stationary Schrödinger drift-diffusion

Received by the editors June 5, 2016.
2000 *Mathematics Subject Classification.* 35L50, 35L60, 35L65, 76R50.

including collisions. To link quantum zone and classical region, they prescribe the continuity of current density at the interface. In [5] Ben Abdallah, Méhats and Vauchelet introduce a hybrid drift-diffusion-Schrödinger-Poisson (DDSP) model, and later in [24] the optimal parallelization strategy of numerical solutions of the same model is performed. In [3] and [17], the DDSP model is applied to study the electrons transport in strongly confined structures, such as nanotubes. At the interface between classical and quantum domains, they impose the continuity of the total current. In [11], the hydrodynamic hybrid model is studied by prescribing the continuity of the charge density, where a small jump of the current density is accepted and justified from the physical point of view, by using scaling arguments.

As discussed above, many different strategies can be adopted to establish a physically reasonable set of interface conditions. The concept of hybrid model introduces an error at the interface, due to the arbitrary choice to neglect the quantum effects from a certain point on. Therefore, the choice of suitable transmission conditions allows us to preserve the continuity of certain physical quantities while others have to be sacrificed. Hence the great variety of conditions that can be found in the related literature.

In this paper, we first propose a hybrid model matching classical and quantum hydrodynamical equations, that is derived by introducing a modified form of the Bohm potential. As we know, both the classical and the quantum hydrodynamic models have been extensively studied, see, for example [2,8,10,12–16,18–20,22,23] and references therein. However, just very few results are presently available concerning the hybrid approach to the hydrodynamic model. Therefore, it will be quite interesting to theoretically study this hybrid quantum hydrodynamical model (H-QHD model). We introduce a quantum effect function $Q(x)$ where $Q > 0$ holds in the region of the device with quantum effect and $Q = 0$ for the region without quantum effect. As we will show later on, this makes the governing equations regionally degenerated for its ellipticity and the solutions are necessarily weak. Therefore, when studying the H-QHD case, compared with the regular cases of HD and QHD, some peculiar difficulties will appear. More precisely speaking, the governing steady-state equation of the H-QHD will be a 4th-order elliptic equation with regional degeneracy, and its leading coefficients involve $Q(x) \geq 0$ and $Q'(x)$. That is, in some part of the domain the equation is 4th-order elliptic, but in the other part it degenerates to be 2nd-order elliptic. In particular, when $Q(x)$ is the Heaviside function (the physical case), $Q'(x) = \infty$ will be at the jump discontinuous points of $Q(x)$. This makes the theoretical study on the existence of the H-QHD solutions and their regularity to be totally different from both the 4th-order uniform elliptic equation (the QHD model) and the 2th-order uniform elliptic equation (the HD model), and causes us some essential difficulties. To overcome such obstacles, we first introduce a sequence of smooth approximating functions $Q_q(x) \geq q > 0$ satisfying $Q_q \to Q$ as $q \to 0$, which modifies the governing equation to be uniformly elliptic, then we prove the existence of the solutions to the modified H-Q_qHD equation, where, when $q = 0$, we denote the H-Q_0HD as the H-QHD. Then, by rigorously proving the uniform boundedness of the solutions for the H-Q_qHD model with respect to q and by carrying out compactness analysis, we may expect that the approximating (smooth) solutions of the H-Q_qHD model will weakly converge to their target functions, which are just the weak solutions of the original H-QHD model. To the best of our knowledge, this paper is the first framework to treat the equation with regional degeneracy of ellipticity.