

Stationary and Transient Simulations for a One-Dimensional Resonant Tunneling Diode[†]

Xin Hu^{1,2}, Shaoqiang Tang^{1,*} and Maxime Leroux³

¹ *CAPT, College of Engineering, Peking University, Beijing 100871, China.*

² *Applied and Computational Mathematics, California Institute of Technology, Pasadena, CA 91125, USA.*

³ *Department of Physics, ENS de Lyon, 69364 Lyon cedex 07, France.*

Received 7 March 2008; Accepted (in revised version) 25 May 2008

Available online 10 July 2008

Abstract. We investigate the validity of stationary simulations for semiconductor quantum charge transport in a one-dimensional resonant tunneling diode via fluid type models. Careful numerical investigations to a quantum hydrodynamic model reveal that the transient simulations do not always converge to the steady states. In particular, growing oscillations are observed at relatively large applied voltage. A dynamical bifurcation is responsible for the stability interchange of the steady state. Transient and stationary computations are also performed for a unipolar quantum drift-diffusion model.

PACS: 02.60.Cb, 73.63.-b, 02.30.Jr

Key words: Quantum effects, charge transport, dissipation, transient/stationary computation.

1 Introduction

Miniaturization of semiconductor devices maintains a continuing trend in microelectronics industry, approaching the nanometer length scale [15]. In the modeling and simulations for nano-devices, it is crucial to incorporate the quantum effects in a proper manner. Because a complete description at the quantum mechanics level would require immense computing power, one usually makes a compromise between the numerical cost and the modeling accuracy. Due to their simplicity in formulation and similarity to the governing equations for classical devices, fluid type models have been widely explored, both theoretically and numerically [16, 20, 21]. However, these models involve strong nonlinearity

[†]Dedicated to Professor Xiantu He on the occasion of his 70th birthday.

*Corresponding author. *Email addresses:* lanxin@acm.caltech.edu (X. Hu), maotang@pku.edu.cn (S. Tang), maxime.leroux@ens-lyon.fr (M. Leroux)

and high order spatial derivatives representing quantum effects. Rigorous mathematical analysis are desirable and challenging. We refer to [1, 17, 19, 22] and references therein for more details. There then arises an urgent demand to justify fluid type models, which are typically derived in a formal way using closure assumptions, temporal and spatial scalings, etc. Careful numerical studies are an indispensable tool to serve this purpose, namely, to validate a model or to identify its effective range.

In this paper, we are concerned with the dynamical stability of steady states for fluid type models. To be more specific, we take a resonant tunneling diode (RTD) in one space dimension to investigate a quantum hydrodynamic (QHD) model, and a quantum drift-diffusion (QDD) model. RTD is a simple device that bears distinct quantum features. With a double potential barrier, the electric current decreases when the applied voltage increases in a certain range. This negative differential resistance (NDR) is caused by the quantum tunneling effect. Comparing transient and stationary QHD simulations, we observe that the steady states lose dynamical stability at moderate applied voltage. At a higher voltage, the transient solutions exhibit both spatial and temporal oscillations. Even the average current density differs from the stationary computations. A dynamical bifurcation occurs for the governing partial differential equations. The role of dissipation is a common issue for discussing instabilities. Actually, interplay between the quantum mechanism and the dissipative mechanism has been explored in a viscous quantum hydrodynamic (vQHD) model [17, 18]. On the other hand, steady states are stable in all our numerical experiments for the QDD model, where the diffusion dominates. However, the QDD model fails to reproduce the NDR phenomenon.

This study poses, likely for the first time, a question on whether stationary computations are always reliable in producing the current-voltage (I-V) curves for nano devices. As a matter of fact, almost all semiconductor quantum charge transport simulations have been performed with stationary problems, e.g. by using the Gummel iterations [8, 13, 23].

The rest of the paper is organized as follows. First, we sketch the derivation for the QHD model and the QDD model in Section 2. Then we describe the numerical algorithm for the QHD model in Section 3, and some numerical results are presented in Section 4. We briefly discuss the numerical scheme and simulations for the QDD model in Section 5. Finally, we make some further discussions in Section 6.

2 QHD model

Dynamics of carrier transport is governed by the Wigner-Poisson system at the quantum level [10, 21]:

$$\frac{\partial w}{\partial t} + \frac{p}{m} \cdot \nabla_x w + \frac{q}{m} \theta[V](w) = Q(w), \quad (2.1)$$

$$\varepsilon_s \Delta V = q \left(\int_{\mathbb{R}} w dp - C(x) \right), \quad (2.2)$$