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A POSITIVITY-PRESERVING FINITE ELEMENT METHOD FOR QUANTUM DRIFT-DIFFUSION MODEL*

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Abstract

In this paper, we propose a positivity-preserving finite element method for solving the three-dimensional quantum drift-diffusion model. The model consists of five nonlinear elliptic equations, and two of them describe quantum corrections for quasi-Fermi levels. We propose an interpolated-exponential finite element (IEFE) method for solving the two quantum-correction equations. The IEFE method always yields positive carrier densities and preserves the positivity of second-order differential operators in the Newton linearization of quantum-correction equations. Moreover, we solve the two continuity equations with the edge-averaged finite element (EAFE) method to reduce numerical oscillations of quasi-Fermi levels. The Poisson equation of electrical potential is solved with standard Lagrangian finite elements. We prove the existence of solution to the nonlinear discrete problem by using a fixed-point iteration and solving the minimum problem of a new discrete functional. A Newton method is proposed to solve the nonlinear discrete problem. Numerical experiments for a three-dimensional nano-scale FinFET device show that the Newton method is robust for source-to-gate bias voltages up to 9V and source-to-drain bias voltages up to 10V.

Mathematics subject classification: 35J60, 35Q81, 49M15, 49M37, 65N30.
Key words: Quantum drift-diffusion model, Positivity-preserving finite element method, Newton method, FinFET device, High bias voltage.

1. Introduction

As the size of modern semiconductor devices goes to nanometers, quantum mechanical phenomena become prominent and must be considered in numerical simulations. Classical drift-diffusion (DD) equations are not enough to describe these quantum effects arising, for example, from strong electron confinement at the interface between silicon and silicon-dioxide [8, 18]. In [1–3], Ancona and Iafrate derived a macroscopic model, called quantum drift-diffusion (QDD) model, which generalizes the classical DD model by incorporating quantum corrections to quasi-Fermi levels. Since then, the model has been used widely for simulating semiconductor devices.

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In 1997, Unterreiter studied the thermal equilibrium solution of a generic bipolar QDD model. He proved that the energy functional of the system has a unique minimizer which is the thermal equilibrium solution to the QDD model, and that the QDD model is reduced to classical DD model as the quantum-correction parameter $\varepsilon \to 0$ [17]. In 1998, Ben Abdallah and Unterreiter studied a bipolar QDD model which includes generation-recombination terms. They proved the existence of solutions for a general setting including the case in thermal equilibrium [5].

In the numerical aspect, Pinnau and Unterreiter first studied the finite element method for bipolar QDD model [13]. They proposed a quasi-gradient method for the thermal equilibrium model and proved the strong convergence of iterative solutions under H^1-norm. For the computation of current-voltage characteristics, they proposed an extended Gummel-iteration and proved the convergence of iterative solutions for small applied voltages. In 2004, Pinnau analyzed the exponentially fitted finite element scheme for one-dimensional unipolar QDD model. He proved the existence of discrete solutions and derived uniform error bounds which allow for the semiclassical limit [15]. We also refer to [14] for a review on the QDD model. In [8], de Falco, Gatti, Lacaita, and Sacco proposed a generalized Gummel iteration and a finite element method for solving the QDD model. They simulated a nanoscale MOSFET device which has a two-dimensional geometry. In [9], de Falco, Jerome, and Sacco delivered an analysis for the generalized Gummel algorithm and proved the existence of the solution to the QDD model by using fixed-point iteration and extremum principles.

The QDD model is a coupled system of five nonlinear elliptic equations: one for the electric potential, two for quasi-Fermi levels of electrons and holes, and the other two for quantum corrections to quasi-Fermi levels. Numerical solutions for the QDD model are very challenging, particularly, in the case of high bias voltages. Theoretical analysis and efficient numerical methods are far from satisfactory. For high bias voltages, the convergence of fixed-point iterations could be slow and inefficient in practical simulations. It is known that Newton-type iterations are more efficient than fixed-point iterations if the initial guess is close to the true solution. Our purpose in this paper is to propose a Newton method for solving the QDD model. Combining with the IEFE discretization for quantum-correction equations and the EAFE discretization for continuity equations, the Newton method is convergent and robust for high bias voltages in simulating a three-dimensional FinFET device.

Another issue for the QDD model or the DD model is how to preserve the positivity of numerical carrier densities. A popular way to deal with the issue is to express the electron density as an exponential function $n = \exp(u)$ and compute the numerical approximation u^h of u. This yields a positive density $n^h = \exp(u^h)$ naturally. Similar ideas have been used to other models. We refer to [7, 10, 11] for nonlinear fourth order parabolic equation, to [4, 15] for QDD equations, and to [6, 12, 16] for Poisson-Nernst-Planck (PNP) equations. However, this technique will transform all linear terms of n into nonlinear terms of u. Newton-type linearization of these nonlinear terms usually break the symmetry and positivity of the problem and lead to an indefinite problem. Here we propose an IEFE method to descretize square roots of carrier densities. The method preserves the positivity of second-order differential operators in the Newton linearization of quantum-correction equations.

In this paper, we propose a robust numerical method for solving the QDD model. The merits of the method are summarized as follows.

1. We express the square roots of carrier densities as $\rho = \exp(\psi_n)$ and $\sigma = \exp(\psi_p)$ for two potential functions ψ_n and ψ_p and derive an equivalent QDD model. We propose an IEFE method to discretize the second-order terms $-\Delta e^{\psi_n}$ and $-\Delta e^{\psi_p}$ so that the Newton-