Journal of Computational and Applied Mathematics 223 (2009) 790–800

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Convergent finite element discretizations of the density gradient equation for quantum semiconductors

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ARTICLE INFO

Article history:
Received 11 May 2007
Received in revised form 13 February 2008

Keywords:
Quantum semiconductors
Density gradient equation
Nonlinear finite element method
Consistency
Convergence
Numerics

ABSTRACT

We study nonlinear finite element discretizations for the density gradient equation in the quantum drift diffusion model. In particular, we give a finite element description of the so-called nonlinear scheme introduced by Ancona. We prove the existence of discrete solutions and provide a consistency and convergence analysis, which yields the optimal order of convergence for both discretizations. The performance of both schemes is compared numerically, in particular, with respect to the influence of approximate vacuum boundary conditions.

1. Introduction

During the last decade, quantum corrections of the well-known drift diffusion (DD) model for semiconductor devices [16–18] gained considerable attention in the mathematics and engineering community [20,9,29]. Most common is the so-called quantum drift diffusion (QDD) model proposed in [5,8,3], which is also known as the density gradient (DG) model. It proved its reliability especially in the simulation of MOSFET devices [29,10,9,7,6] and is also well understood from the mathematical point of view [28,1,22,19,14,15,20]. This great success is also underlined by its inclusion in commercial software packages, e.g. by Silvaco or Lucent. Hence, the QDD model is a good candidate to be the successor of the classical DD model, since it adds quantum effects to the DD model in a general, compact and computationally efficient manner [9,29].

The scaled unipolar, stationary QDD model on the bounded domain $\Omega = (0, 1)$ reads [20]

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + \log(n) + V = F, \tag{1.1a}$$

$$\partial_x(n\partial_x F) = 0, \tag{1.1b}$$

$$-\lambda^2 \partial_{xx} V = n - C_{\text{dop}} \tag{1.1c}$$

for the electron density n, the quantum quasi-Fermi potential F and the electrostatic potential V. The parameter ε is the scaled Planck constant, λ is the scaled Debye length and the function C_{dop} represents the concentration of fixed background ions. The system (1.1a)–(1.1c) is subject to Dirichlet boundary conditions modeling the Ohmic contacts of the device

$$n = n_D, \qquad V = V_D := V_{eq} + V_{\text{ext}} \qquad F = F_D := F_{eq} + V_{\text{ext}} \quad \text{on } \partial\Omega, \tag{1.1d}$$

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doi:10.1016/j.cam.2008.03.010

where n_D, V_{eq} and F_{eq} are the equilibrium values of the charge concentrations, the potential and the quasi-Fermi level, respectively, and V_{ext} is the external applied voltage. Note that the scaled constants are in general quite small, i.e. $\varepsilon^2, \lambda^2 = O(10^{-2\ldots-4})$, such that boundary or internal layers might occur [3].

Several discretization schemes have been proposed for the solution of the coupled, nonlinear partial differential equations (1.1). These can be classified into linear and nonlinear schemes, depending on the respective discretization of (1.1a). Following the discussion in [4], *linear* discretization schemes use linear ansatz functions for the electron density n (or for $s = \sqrt{n}$), while *nonlinear* schemes use nonlinear ansatz functions, e.g., exponentials. A typical linear scheme is the linear conservative scheme based on finite differences presented in [4]. However, due to the quantum effects that occur inside the device, the density might change by several orders of magnitude. Thus, such schemes require very fine grids in order to obtain reliable results, which implies a significant computational cost. To cope with such difficulties, nonlinear schemes have to be used, like the finite difference nonlinear scheme [4], which has proved its efficiency in solving coarse grid device examples involving quantum effects. An alternative numerical treatment of (1.1a) is proposed in [12]. Here, with the aim of fulfilling a maximum principle, first a suitable linearization is performed using a damped Newton method and then piecewise linear finite elements are employed to discretize the linearized problem. Another line of research is presented in [21,23], where the existence of a discrete solution for the coupled problem, as well as error bounds and uniform convergence for a Scharfetter–Gummel type discretization are investigated [13,25].

Although, the finite difference nonlinear scheme has been applied with success [4,9], no numerical analysis is so far available. In this paper, we embed this question into the context of finite element discretizations and study their respective consistency and convergence. Choosing appropriate quadrature rules we recover Ancona's nonlinear scheme [4]. In [27] the effect of approximate vacuum boundary conditions is studied and an improved scheme is suggested. Here, we present a different approach based on finite elements, which is also not affected by the boundary condition and yields even simpler discrete nonlinear systems.

This paper is organized as follows. In Section 2, we present the two different discretization schemes for the DG Eq. (1.1a). The existence of discrete solutions, as well as consistency and convergence results for the discretization schemes are discussed in Section 3. Finally, numerical tests for a metal insulator semiconductor (MIS) diode, underlining the theoretical results, are presented in Section 4. Concluding remarks are given in Section 5.

2. The finite element approach

In this section we introduce an exponential variable transform for the density, which has already proved very helpful in the analysis of the transient problem [14,15]. The construction of the nonlinear difference scheme in [4] relies on the same idea and is motivated by replacing the 'fast' density variable n with the 'slow' one $u = \log(n)$. In the following we write the transformed DG equation in weak form and perform the finite element discretization.

We consider here only the boundary value problem for the DG equation

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + \log(n) + V = 0, \tag{2.1a}$$

$$n(0) = \alpha \qquad n(1) = \beta. \tag{2.1b}$$

on the bounded domain $\Omega = (0, 1)$ and for a given potential $V \in H^1(\Omega)$. Further, we assume $\alpha, \beta > 0$.

After multiplication by $\sqrt{n}$ and using an exponential transformation $n = \mathrm{e}^{2u}$, in order to resolve better the large variations of the carrier density in the vicinity of inversion layers [3], we obtain the transformed problem in terms of the new unknown u

$$-\varepsilon^2 \partial_{xx}\mathrm{e}^u + \mathrm{e}^u(2u + V) = 0, \tag{2.2a}$$

$$u(0) = \frac{1}{2}\log(\alpha) \qquad u(1) = \frac{1}{2}\log(\beta). \tag{2.2b}$$

The weak formulation now reads: Find $u \in u_D + H_0^1(\Omega)$ such that

$$\varepsilon^2 \int_\Omega \mathrm{e}^u \partial_x u \partial_x \phi \,\mathrm{d}x + \int_\Omega (2u + V)\mathrm{e}^u \phi \,\mathrm{d}x = 0 \quad \text{for all } \phi \in H_0^1(\Omega), \tag{2.3}$$

where u_D is an $H^1(\Omega)$-extension of the boundary data.

Concerning the existence and uniqueness of solutions to the DG equation, different results are available in the literature [20], which depend on the specific formulation of the problem. In terms of the logarithmic variable u, we have the following.

Proposition 2.1. *Let $V \in H^1(\Omega)$ and choose constants $\overline{V}, \underline{V} \in \mathbb{R}$ such that*

$$\underline{V} \le V(x) \le \overline{V} \quad \textit{for all } x \in \Omega.$$