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NUMERICAL STUDIES OF I-V CHARACTERISTICS IN RESONANT TUNNELING DIODES: A SURVEY OF CONVERGENCE*

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Abstract

Resonant tunneling diodes (RTDs) exhibit a distinctive characteristic known as negative resistance. Accurately calculating the tunneling bias energy is indispensable for the design of quantum devices. This paper conducts a thorough investigation into the current-voltage (I-V) characteristics of RTDs utilizing various numerical methods. Through a series of numerical experiments, we verified that the transfer matrix method ensures robust convergence in I-V curves and proficiently determines the tunneling bias for energy potential functions with discontinuities. Our numerical analysis underscores the significant impact of variations in effective mass on I-V curves, emphasizing the need to consider this effect. Furthermore, we observe that increasing the doping concentration results in a reduction in tunneling bias and an enhancement in peak current. Leveraging the unique features of the I-V curve, we employ shallow neural networks to accurately fit the I-V curves, yielding satisfactory results with limited data.

Mathematics subject classification: 65L05, 65Z05, 81Q05, 34C60.
Key words: Schrödinger equation, Transfer matrix methods, Resonant tunneling diodes, Tunneling bias.

1. Introduction

Resonant tunneling diodes are considered to be among the quantum devices with significant potential for practical applications. The RTD is a two-terminal negative resistance nano-device based on the quantum tunneling phenomenon, which has the remarkable advantages of fast response speed, high operating frequency, low voltage, and low power consumption. An RTD consists of a double barrier and a single well connected to an emitter and a collector [11]. RTDs

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are studied in both theory and experiments, and their accurate simulation is very important for developing reliable design tools for quantum devices [20].

Usually, three approaches are used to model quantum transport in RTDs: the wave function [8], the Green function [9, 19], and the Wigner function [13–15]. The Green function method is equivalent to the wave function method for ballistic transport. The Wigner function is defined by the wave function and is very complicated due to the inclusion of the effects of varying effective mass. Thus, the wave function method based on the Schrödinger equation is applied in this paper to study the convergence of I-V curves of RTDs.

The finite difference method (FDM) is a widely used method for the numerical simulation of quantum structures. Employed in solving the Schrödinger equations and the Schrödinger-Poisson system, FDM has demonstrated significant and impactful applications. Cahay and Datta [8] employed FDM to effectively simulate the negative resistance phenomenon in RTDs. Arnold [3, 5] introduced a discrete transparent boundary condition based on discrete dispersion relations, extending its utility to the time-dependent Schrödinger equation [2, 4]. Additionally, the finite-difference time-domain method (FDTD) has been successfully utilized in solving the Schrödinger equation in three dimensions, incorporating modified formulas at the incident boundary to achieve numerical solutions through iterative processes [22]. Applications of FDM include its utilization in iteration schemes for the Schrödinger-Poisson system, where FDM has been employed to explore steady-state I-V characteristics [20]. Various iteration techniques have been adopted, including Broyden's method [21], Gummel's iteration with a non-uniform mesh [12], and Newton's iterative method combined with the successive over-relaxation (SOR) method [10].

The transfer matrix method (TMM) has proven to be a versatile tool for investigating bound and scattering states in quantum structures, offering superior accuracy in comparison to FDM [1]. One of the most noteworthy applications of the TMM is to describe the effective solution of the Schrödinger equation with arbitrary potential energy functions, with a specific emphasis on capturing the variation in the effective mass of electrons across different substances during computational processes [17]. Importantly, the numerical accuracy of TMM in solving the Schrödinger equation is substantiated and confirmed in the work presented in [16]. The efficacy of TMM extends comprehensively to a range of applications, including investigations of quantum spin systems [7], fermion models [23], and gamma-rays [6]. TMM was proposed to solve the Schrödinger equation solely, but has never been used in simulation of semiconductor devices.

In the course of our study, we employ TMM, FDM, and the finite volume method (FVM) to solve the Schrödinger equation and the coupled Schrödinger-Poisson system in RTDs. Our investigative results highlight the pronounced convergence of TMM, and notably excelling in accurately capturing tunneling bias energy when compared to the performance of FDM and FVM. Furthermore, our examination delves into the effects stemming from variations in effective mass and doping density on the I-V curves, further contributing to the comprehension and optimization of RTD characteristics. Additionally, we train a neural network with simulation data to predict I-V characteristics across various bias voltages and Fermi energy values, achieving excellent predictive accuracy with a relatively simple network architecture.

This paper is organized as follows. In Section 2, we introduce the structure of 1-D prototype RTDs and the Schrödinger-Poisson system. In Section 3, the numerical methods and the algorithm of the solver for the coupled system are presented. Numerical results are given and explained in Section 4. Finally, our conclusions are given in Section 5.