Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.OA-2024-0140

Vol. **18**, No. 4, pp. 881-902
November 2025

A Highly Efficient Adaptive Mesh Refinement Algorithm for the 1D Schrödinger-Poisson Problem

Meili Guo[1], Haiyan Jiang[1], Tiao Lu[2,3] and Wenqi Yao[4,*]

[1] *School of Mathematics and Statistics, Beijing Institute of Technology, Beijing 100081, P.R. China*
[2] *CAPT, LMAM, School of Mathematical Sciences, Peking University, Beijing 100871, P.R. China*
[3] *Chongqing Research Institute of Big Data, Peking University, Chongqing 401121, P.R. China*
[4] *School of Mathematics, South China University of Technology, Guangzhou 510641, P.R. China*

Received 15 December 2024; Accepted (in revised version) 6 May 2025

Abstract. The one-dimensional stationary Schrödinger equation, coupled with the transparent boundary conditions and self-consistently linked to the Poisson equation, is a well-established model for describing quantum effects. In this paper, we introduce a general framework for constructing arbitrarily high-order finite difference schemes on arbitrary grids, whether they are uniform or nonuniform, inspired by the analytic discrete transparent boundary conditions [M. Guo *et al.*, arXiv:2411.13175]. To enhance the accuracy of approximations while keeping computational costs low, we develop an optimal mesh refinement strategy that balances the need to resolve intervals with large gradient and high curvature of the potential function. We further propose an adaptive mesh refinement algorithm to solve the 1D Schrödinger-Poisson problem, incorporating a third-order compact finite difference discretization of the Schrödinger-Poisson system based on nonuniform grids, and a given mesh refinement strategy. Numerical experiments on a resonant tunneling diode are conducted to validate the algorithm's high efficiency and to study the I-V characteristic curve of the device.

AMS subject classifications: 34L40, 65L10, 65L50

Key words: 1D Schrödinger-Poisson problem, adaptive mesh refinement, transparent boundary condition, compact finite difference scheme, resonant tunneling diode.

---

*Corresponding author. *Email addresses:* guomeili@bit.edu.cn (M. Guo), tlu@pku.edu.cn (T. Lu), hyjiang@bit.edu.cn (H. Jiang), yaowq@scut.edu.cn (W. Yao)

1. Introduction

With the rapid advancement of semiconductor fabrication technology, quantum transparent models have emerged as valuable tools for understanding the electrical properties of nanoscale devices. As a representative quantum device, the resonant tunneling diode (RTD) has been extensively studied both experimentally and theoretically due to its distinctive features, such as negative differential resistance [9, 22]. To simulate the behavior of an RTD, several equivalent approaches have been proposed in the literature [3, 8, 12, 14, 21, 25].

In this paper, we utilize the one-dimensional stationary Schrödinger equation, self-consistently coupled with the Poisson equation incorporating electric neutrality boundary conditions, to model the RTD. To confine the Schrödinger equation in a bounded region, the transparent boundary conditions (TBCs) [19] have been usually considered. The TBCs assume the device is connected to two contacts acting like quantum mechanical reservoirs. The existence and uniqueness of the solution to the 1D Schrödinger equation equipped with the TBCs have also been studied in [2].

Numerically, the discretization of the TBCs is crucial for solving the Schrödinger equation, and considerable efforts have been dedicated to this topic in the literature [1, 11, 15]. Among these works, the discrete transparent boundary conditions (DTBCs) proposed by Arnold [1] are particularly noteworthy. In that study, it was revealed that "normal" discretizations of the TBCs, such as the standard central finite difference discretization, tend to produce unphysical spurious oscillations when the potential approaches zero. This issue arises because conventional approaches overlook the form of the true solution of the Schrödinger equation in unbounded regions when constructing the discrete representation of the TBCs. To address this problem, the DTBCs were introduced in conjunction with a second-order central finite difference discretization of the Schrödinger equation. Recently, we enhanced the accuracy of the DTBCs to fourth order [13], which was named as the D4TBCs, by implementing a fourth-order compact finite difference scheme for the Schrödinger equation.

Unfortunately, the DTBCs family, including the DTBCs and the D4TBCs, encounters significant challenges when higher-order schemes are required or when local mesh refinement is desired. This limitation arises because the DTBCs family can only be constructed on a uniform mesh grid, necessitating the solution of the same high-order algebraic equation for their construction. Besides, the accuracy order of the DTBCs family is limited by the order of scheme used to discretize the Schrödinger equation. As an alternative, we proposed a novel discretization scheme for the TBCs, referred to as the analytic discrete transparent boundary conditions (aDTBCs) [13]. In this paper, we propose a general version of the aDTBCs, which is named as the gaDTBCs, to facilitate the introduction of arbitrarily high-order finite difference schemes of the Schrödinger equation on arbitrary (uniform or nonuniform) grids. Despite exhibiting negligible weak oscillations, compared with the DTBCs family, the gaDTBCs offer three significant advantages: 1) no discretization errors; 2) elimination of the need to solve algebraic equations; and 3) independence from uniform mesh grids.