Numer. Math. Theor. Meth. Appl. Vol. **16**, No. 3, pp. 701-719
doi: 10.4208/nmtma.OA-2022-0164 August 2023

Green Function Method for Quantum Transport Based on the Generalized Fourier Transform

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Received 19 October 2022; Accepted (in revised version) 7 February 2023

Abstract. The rigorous relations between the propagators of transient Schrödinger equations and stationary Green functions are established. Based on the generalized Fourier transform, non-singular transparent boundary condition for transient problem is proposed in a representation of Green functions. The unified framework of Green function method is presented for converting an open boundary problem into a bounded boundary problem. Numerical scheme for time-dependent Schrödinger equation with non-singular transparent boundary condition is designed to simulate the propagations of a free Gaussian wave packet and the resonant tunnelling through double barriers. Numerical results validate the effectiveness of non-singular transparent boundary condition.

AMS subject classifications: 42A38, 65M80, 81-10, 81U26

Key words: Schrödinger equation, Green function, generalized Fourier transform, transparent boundary condition.

1. Introduction

Greatly advanced semiconductor technology leads to fabricating structures into the size of the mean free path. Typical devices like RTDs and MOSFETs in nano-meter scale have been studied both theoretically and experimentally. The classical mechanics is no longer suitable to describe the behavior of carrier transport correctly and quantum effects should be taken into account. The Schrödinger equation governs wave function on which imposed basic postulations in quantum mechanics and describes the behavior of quantum particles. Green function method is very popular in solving Schrödinger equation for all observables can be represented by the wave functions as well as Green functions [7, 9].

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Green function method provides a reasonable unified framework for quantum transport simulations [8, 9]. It was initially proposed by some theoretical physicists to describe the entropy generation process in channel by using theory of multi-body perturbation. Due to the complexity of multi-body theory and the heavy burden of calculation, it is difficult to solve practical problems [15,20]. Usually, multi-body problems are converted into approximate single-body problems. The framework of Green function is easily generalized to high-dimension cases and non-equilibrium states. It can also provide a reasonable conceptual method to handle the scattering effects [16]. Particularly, Green function method can provide a unified treatment for stationary open boundary problems [11]. A proper artificial boundary condition is particularly important for numerical simulation of quantum transport in the nano-size device with external reservoirs. Since the boundary condition must be coupled with the interior solution, the boundary condition should be well-posed, stable, and can annihilate all incident waves so as not to produce any reflections to affect the interior solution. These boundary conditions are usually coined as transparent (absorbing, radiation, non-reflecting or open) boundary conditions [10, 18]. In order to solve stationary Schrödinger equation in an unbounded region, self-energy term is usually added to the equation as open boundary condition in the framework of Green function. For transient problem, a proper boundary condition is also necessary because it is a requirement of such artificial boundary condition not to adversely affect the numerical calculation in the interior region [10]. Dirichlet boundary condition and Neumann boundary condition require an enough large computational region to avoid the wave to touch the boundary and produce unnecessary reflections [1, 22]. Non-reflecting boundary conditions of transient Schrödinger equation are proposed based on different physical backgrounds and methods. One is to add a negative imaginary potential outside of the device, which will absorb the wave that approaches the boundary. However, the negative imaginary potential is difficult to be determined previously [14]. Another kind of boundary condition can be derived based on the dispersion relationship between energy and wave vector [10]. This is a simple idea to derive corresponding boundary condition for different wave vector, but it will produce unexpected errors when the wave vector is relatively small [12, 19]. With the help of Laplace transform, an analytical boundary conditions can be derived based on different physical backgrounds, such as quantum mechanics [6, 13], electromagnetic [17] and underwater acoustics [4]. This precise boundary condition is a convolution integral with fractional-order derivative, which includes singularity leading to more computational techniques for numerical stimulation [3, 5]. The fast and accurate algorithms are focused on issues all the time [2, 21]. We will give the understanding of transparent boundary conditions from perspective of Green functions. The boundary conditions are introduced as self-energy terms in the framework of Green function. Usually, the understanding for Green functions in quantum transport is always based on physical assumption that the outgoing wave is meaningful solution [8]. How to understand Green functions in mathematics will help to improve the Green function theory in quantum mechanics and promote application of Green function method in quantum transport simulation. In this paper, we will clarify