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Local Discontinuous Galerkin Methods for the 2D Simulation of Quantum Transport Phenomena on Quantum Directional Coupler

Li Guo[1] and Yan Xu[1],*

[1] *School of Mathematical Sciences, University of Science and Technology of China, Hefei, Anhui 230026, P.R. China.*

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Abstract. In this paper, we present local discontinuous Galerkin methods (LDG) to simulate an important application of the 2D stationary Schrödinger equation called quantum transport phenomena on a typical quantum directional coupler, which frequency change mainly reflects in y-direction. We present the minimal dissipation LDG (MD-LDG) method with polynomial basis functions for the 2D stationary Schrödinger equation which can describe quantum transport phenomena. We also give the MD-LDG method with polynomial basis functions in x-direction and exponential basis functions in y-direction for the 2D stationary Schrödinger equation to reduce the computational cost. The numerical results are shown to demonstrate the accuracy and capability of these methods.

AMS subject classifications: 65N30, 35Q40

Key words: Local discontinuous Galerkin method, 2D stationary Schrödinger equation, quantum transport phenomena, quantum directional coupler.

1 Introduction

Schrödinger equation is used to describe the quantum mechanical wave function in the equation of motion proposed by the Austrian physicist Schrödinger in 1926 and is considered to be the theory which is one of the fundamental theories of quantum mechanics. Schrödinger equation is widely used in atomic physics, nuclear physics and solid state physics. Solutions to Schrödinger equation can clearly describe the statistical quantum behavior of the quantum size particles in quantum systems. So how to solve Schrödinger equation becomes very important.

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*Corresponding author. *Email addresses:* `lili2010@mail.ustc.edu.cn` (L. Guo), `yxu@ustc.edu.cn` (Y. Xu)

In this paper, we mainly discuss how to simulate numerical solutions of the 2D stationary Schrödinger equation (1.1) which can describe quantum transport phenomena

$$-\frac{1}{2}\varepsilon^2\triangle\varphi+V\varphi=E\varphi,\quad (x,y)\in\Omega, \tag{1.1}$$

where ε is the re-scaled Plank constant, E is the specified energy, $\varphi=\varphi(x,y)$ is a complex-valued function denoting the wave function, and $V=V(x,y)$ is the potential. The boundary conditions are given based on the specific issues. Many numerical methods have been developed to solve this equation. In [10, 11], the finite difference methods have been developed to simulate Schrödinger equations. Spectral method has been proposed in [8]. In [18, 19], the WKB scheme and finite element method have been used to compute this equation respectively. In addition, multi-mode approximation for resonant tunneling which can be described by the stationary Schrödinger equation is given to solve the equation in [1]. Also in [21], immersed interface method is used to compute the Schrödinger equation with discontinuous potential. In this paper, we mainly consider an important application of the 2D stationary Schrödinger equation called quantum transport phenomena on a typical quantum directional coupler shown in Fig. 1. Also various kinds of numerical methods can be found to simulate quantum transport phenomena in [4, 5, 9, 14–17, 20]. Moreover, many local discontinuous Galerkin methods have been developed to solve time dependent Schrödinger equations in [7, 12, 13, 22] but not simulate the stationary Schrödinger equation on the complicated computational domain.

We present local discontinuous Galerkin methods to solve the Schrödinger equation (1.1). Discontinuous Galerkin (DG) methods are a class of finite element methods using completely discontinuous basis functions, which are usually chosen as piecewise polynomials. The stability and convergence of LDG methods have been designed for elliptic equations in [3, 6]. DG method based on non-polynomial approximation spaces has been developed in [23]. The DG method has several advantages as follows. Firstly, it can be designed as any order of accuracy. Since the order of accuracy can be locally determined in each cell, it has efficient p adaptivity. Secondly, the allowance of arbitrary triangulation even with hanging nodes makes efficient h adaptivity come true. Moreover, the method has embarrassingly high parallel efficiency because the elements only communicate with immediate neighbors regardless of the order of the accuracy of the scheme.

In this paper, we mainly develop minimal dissipation local discontinuous Galerkin (MD-LDG) method based on the basis functions of polynomials for the Schrödinger equation (1.1). In addition, we choose polynomial basis functions in x-direction and the exponential basis functions in y-direction which is typical for the simulation of quantum transport phenomena. This choice is mainly based on the change of frequency of y-direction. This method not only maintains the advantages of the general LDG methods but also saves the computational cost.

This paper is organized as follows. In Subsection 2.1, we give the model problem which we are concerned about. We give the MD-LDG method and the MD-LDG method with different basis functions in different directions for the Schrödinger equation in Sub-