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CONSERVATIVE LOCAL DISCONTINUOUS GALERKIN METHODS FOR TIME DEPENDENT SCHRÖDINGER EQUATION

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Abstract. This paper presents a high order local discontinuous Galerkin time-domain method for solving time dependent Schrödinger equations. After rewriting the Schrödinger equation in terms of a first order system of equations, a numerical flux is constructed to preserve the conservative property for the density of the particle described. Numerical results for a model square potential scattering problem is included to demonstrate the high order accuracy of the proposed numerical method.

Key Words. Local discontinuous Galerkin (LDG) method, Schrödinger equation, quantum structures.

1. Introduction

Traditional analytic solutions of Schrödinger equations using plane wave analysis and perturbation technique can only handle simple planner structures or weak perturbations [1][2]. Direct numerical solution of the time dependent Schrödinger equation provides an efficient and flexible way to study quantum structures in complicated geometric configurations such as quantum wells, quantum wires and quantum dots embedded in layered media. It allows us to address the effect of impurities and scattering of rough interfaces and also different type of incident waves used to probe the quantum structures [2]. Finite element methods and boundary element methods have been used to solve Schrödinger equations [3].

In this paper, we will introduce a discontinuous Galerkin method for time dependent Schrödinger equations for hetero-structures with possible different effective masses. We will limit our consideration to one dimensional models though the basic numerical technique can be extended to multi-dimensional problems. An important property of the resulting numerical algorithms is the conservation for the probability density of the particles under consideration, which we will prove for the proposed numerical method. The basic numerical method follows closely with the discontinuous Galerkin methods proposed in [6] for the heat equation where an auxiliary flux variable was introduced to rewrite a second order partial differential diffusion equation in terms of a system of first order PDEs. For more references on the development of discontinuous Galerkin methods for other types of applications, we refer the readers to [4]-[8].

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The remaining of the paper is organized as follows. After introducing the basics of Schrödinger equation in Section 2, the local discontinuous Galerkin (LDG) method is proposed for an one-dimensional Schrödinger equation in Section 3. In Section 4, we will construct a numerical flux which is shown to keep the conservative property of the continuity equation for the density function. Numerical results are given in Section 5 to demonstrate the convergence of the proposed method for a model scattering problem of one square potential barrier. Finally, a conclusion and plan of future work is given in Section 6.

2. Time Dependent Schrödinger Equation

We consider the one-dimensional effective mass Schrödinger equation [2]

$$\frac{\partial u}{\partial t} - i\frac{\partial}{\partial x}\left(\frac{1}{m}\frac{\partial u}{\partial x}\right) = -iVu \quad \text{in} \quad (0,1)\times(0,T), \tag{1}$$

where m is the effective mass, V is the potential function, $i=\sqrt{-1}$, and u is the complex-valued wave function. Consider a single electron whose probability density is given by

$$n(x,t) = u^*(x,t)u(x,t) \tag{2}$$

and whose probability current density is given by

$$J(x,t) = -i\frac{1}{m}\left[\left(\frac{\partial u}{\partial x}\right)^* u - u^*\left(\frac{\partial u}{\partial x}\right)\right]. \tag{3}$$

If u obeys (1), probability density n and current density J satisfy the following continuity equation

$$\frac{\partial n}{\partial t} - \frac{\partial}{\partial x}J = 0. \tag{4}$$

3. Local Discontinuous Galerkin (LDG) Numerical Method

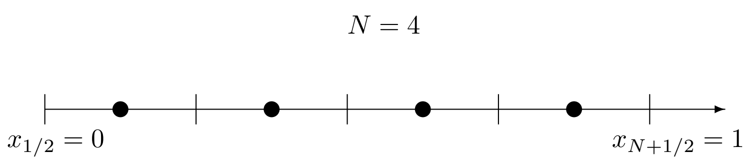

FIGURE 1. [0,1] is discretized into $N = 4$ segments. Black dots are the nodes x_j.

To define LDG method for (1), we introduce a variable

$$q = \frac{1}{m}\frac{\partial u}{\partial x}, \tag{5}$$

so we have (assuming that $V = 0$)

$$\frac{\partial u}{\partial t} - i\frac{\partial q}{\partial x} = 0 \qquad \text{in} \quad (0,1)\times(0,T), \tag{6}$$

$$q - \frac{1}{m}\frac{\partial u}{\partial x} = 0 \qquad \text{in} \quad (0,1)\times(0,T). \tag{7}$$