

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 planar 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]

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

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

$$(2) \quad n(x, t) = u^*(x, t)u(x, t)$$

and whose probability current density is given by

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

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

$$(4) \quad \frac{\partial n}{\partial t} - \frac{\partial}{\partial x} J = 0.$$

3. Local Discontinuous Galerkin (LDG) Numerical Method

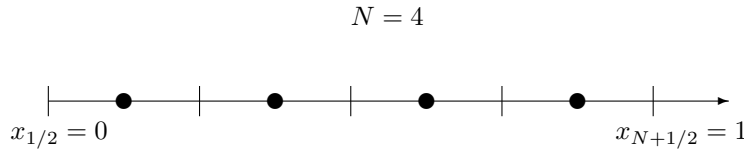


FIGURE 1. $[0, 1]$ is discretized into $N = 4$ segments. Black dots are the nodes x_j .

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

$$(5) \quad q = \frac{1}{m} \frac{\partial u}{\partial x},$$

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

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

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

The initial condition and the boundary condition are provided by the exact solution for simplicity. As illustrated in Fig. 1, the computational domain $[0,1]$ is divided into N segments, $0 = x_{1/2} < x_{3/2} < \dots < x_{N+1/2} = 1$, $j = 1, \dots, N$, $I_j = [x_{j-1/2}, x_{j+1/2}]$. The finite element space is

$$(8) \quad V_h = \left\{ v \in L^1(0,1) : v|_{I_j} \in P^k(I_j), j = 1, \dots, N \right\},$$

where $P^k(I)$ denotes the space of polynomials in I of degree at most k . The approximate solution (u_h, q_h) given by the LDG method is defined as the solution of the following weak formulation:

$$(9) \quad \begin{aligned} & \forall v_{h,u} \in P^k(I_j) : \\ & \int_{I_j} \frac{\partial u_h(x,t)}{\partial t} v_{h,u}(x) dx + i \int_{I_j} q_h(x,t) \frac{\partial v_{h,u}(x)}{\partial x} dx \\ & - h_{u,j+1/2}(t) v_{h,u}(x_{j+1/2}^-) + h_{u,j-1/2}(t) v_{h,u}(x_{j-1/2}^+) = 0, \end{aligned}$$

$$(10) \quad \begin{aligned} & \forall v_{h,q} \in P^k(I_j) : \\ & \int_{I_j} q_h(x,t) v_{h,q}(x) dx + \frac{1}{m_j} \int_{I_j} u_h(x,t) \frac{\partial v_{h,q}(x)}{\partial x} dx \\ & - \frac{1}{m_j} h_{q,j+1/2}(t) v_{h,q}(x_{j+1/2}^-) + \frac{1}{m_j} h_{q,j-1/2}(t) v_{h,q}(x_{j-1/2}^+) = 0, \end{aligned}$$

where $(h_{u,j+1/2}, h_{q,j+1/2})$ is the numerical flux which approximates (iq, u) at $x_{j+1/2}$, and m_j is the real constant effective mass in I_j .

4. Numerical Conservation for Probability Density

For simplicity, we rewrite the LDG formulation as

$$(11) \quad \begin{aligned} & \forall v_{h,u} \in P^k(I_j) : \\ & \int_{I_j} \frac{\partial u_h}{\partial t} v_{h,u} dx + i \int_{I_j} q_h \frac{\partial v_{h,u}}{\partial x} dx \\ & - h_{u,j+1/2} v_{h,u}(x_{j+1/2}^-) + h_{u,j-1/2} v_{h,u}(x_{j-1/2}^+) = 0, \end{aligned}$$

$$(12) \quad \begin{aligned} & \forall v_{h,q} \in P^k(I_j) : \\ & \int_{I_j} q_h v_{h,q} dx + \frac{1}{m_j} \int_{I_j} u_h \frac{\partial v_{h,q}}{\partial x} dx \\ & - \frac{1}{m_j} h_{q,j+1/2} v_{h,q}(x_{j+1/2}^-) + \frac{1}{m_j} h_{q,j-1/2} v_{h,q}(x_{j-1/2}^+) = 0. \end{aligned}$$

Setting $v_{h,u} = u_h^*$ in (11), we obtain

$$(13) \quad \begin{aligned} & \int_{I_j} \frac{\partial u_h}{\partial t} u_h^* dx + i \int_{I_j} q_h \frac{\partial u_h^*}{\partial x} dx \\ & - h_{u,j+1/2} u_h^*(x_{j+1/2}^-) + h_{u,j-1/2} u_h^*(x_{j-1/2}^+) = 0. \end{aligned}$$

From (13) and its complex conjugation, we obtain

$$\begin{aligned}
\int_{I_j} \frac{\partial n_h}{\partial t} dx &= \int_{I_j} \left(u_h^* \frac{\partial u_h}{\partial t} + u_h \frac{\partial u_h^*}{\partial t} \right) dx \\
&= -i \int_{I_j} \left(q_h \frac{\partial u_h^*}{\partial x} - q_h^* \frac{\partial u_h}{\partial x} \right) dx \\
&\quad + h_{u,j+1/2} u_h^*(x_{j+1/2}^-) - h_{u,j-1/2} u_h^*(x_{j-1/2}^+) \\
&\quad + h_{u,j+1/2}^* u_h(x_{j+1/2}^-) - h_{u,j-1/2}^* u_h(x_{j-1/2}^+).
\end{aligned} \tag{14}$$

Setting $v_{h,q} = \partial u_h^* / \partial x$ in (12), we obtain

$$\begin{aligned}
&\int_{I_j} q_h \frac{\partial u_h^*}{\partial x} dx + \frac{1}{m_j} \int_{I_j} u_h \frac{\partial^2 u_h^*}{\partial x^2} dx \\
&- \frac{1}{m_j} h_{q,j+1/2} \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) + \frac{1}{m_j} h_{q,j-1/2} \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) = 0.
\end{aligned} \tag{15}$$

Again, using (15) and its complex conjugation, we obtain

$$\begin{aligned}
&\int_{I_j} \left(q_h \frac{\partial u_h^*}{\partial x} - q_h^* \frac{\partial u_h}{\partial x} \right) dx \\
&= -\frac{1}{m_j} \int_{I_j} \left(u_h \frac{\partial^2 u_h^*}{\partial x^2} - u_h^* \frac{\partial^2 u_h}{\partial x^2} \right) dx \\
&\quad + \frac{1}{m_j} h_{q,j+1/2} \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) - \frac{1}{m_j} h_{q,j-1/2} \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) \\
&\quad - \frac{1}{m_j} h_{q,j+1/2}^* \frac{\partial u_h}{\partial x}(x_{j+1/2}^-) + \frac{1}{m_j} h_{q,j-1/2}^* \frac{\partial u_h}{\partial x}(x_{j-1/2}^+) \\
&= -\frac{1}{m_j} \int_{I_j} \frac{\partial}{\partial x} \left(u_h \frac{\partial u_h^*}{\partial x} - u_h^* \frac{\partial u_h}{\partial x} \right) dx \\
&\quad + \frac{1}{m_j} h_{q,j+1/2} \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) - \frac{1}{m_j} h_{q,j-1/2} \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) \\
&\quad - \frac{1}{m_j} h_{q,j+1/2}^* \frac{\partial u_h}{\partial x}(x_{j+1/2}^-) + \frac{1}{m_j} h_{q,j-1/2}^* \frac{\partial u_h}{\partial x}(x_{j-1/2}^+) \\
&= -\frac{1}{m_j} u_h(x_{j+1/2}^-) \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) + \frac{1}{m_j} u_h(x_{j-1/2}^+) \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) \\
&\quad + \frac{1}{m_j} u_h^*(x_{j+1/2}^-) \frac{\partial u_h}{\partial x}(x_{j+1/2}^-) - \frac{1}{m_j} u_h^*(x_{j-1/2}^+) \frac{\partial u_h}{\partial x}(x_{j-1/2}^+) \\
&\quad + \frac{1}{m_j} h_{q,j+1/2} \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) - \frac{1}{m_j} h_{q,j-1/2} \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) \\
&\quad - \frac{1}{m_j} h_{q,j+1/2}^* \frac{\partial u_h}{\partial x}(x_{j+1/2}^-) + \frac{1}{m_j} h_{q,j-1/2}^* \frac{\partial u_h}{\partial x}(x_{j-1/2}^+).
\end{aligned} \tag{16}$$

With (16) to replace $\int_{I_j} \left(q_h \frac{\partial u_h^*}{\partial x} - q_h^* \frac{\partial u_h}{\partial x} \right) dx$ in (14), we have

$$\begin{aligned}
 \int_{I_j} \frac{\partial n_h}{\partial t} dx &= -i \frac{1}{m_j} \left\{ -u_h(x_{j+1/2}^-) \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) + u_h(x_{j-1/2}^+) \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) \right. \\
 &\quad + u_h^*(x_{j+1/2}^-) \frac{\partial u_h}{\partial x}(x_{j+1/2}^-) - u_h^*(x_{j-1/2}^+) \frac{\partial u_h}{\partial x}(x_{j-1/2}^+) \\
 &\quad + h_{q,j+1/2} \frac{\partial u_h^*}{\partial x}(x_{j+1/2}^-) - h_{q,j-1/2} \frac{\partial u_h^*}{\partial x}(x_{j-1/2}^+) \\
 &\quad \left. - h_{q,j+1/2}^* \frac{\partial u_h}{\partial x}(x_{j+1/2}^-) + h_{q,j-1/2}^* \frac{\partial u_h}{\partial x}(x_{j-1/2}^+) \right\} \\
 &\quad + h_{u,j+1/2} u_h^*(x_{j+1/2}^-) - h_{u,j-1/2} u_h^*(x_{j-1/2}^+) \\
 (17) \quad &\quad + h_{u,j+1/2}^* u_h(x_{j+1/2}^-) - h_{u,j-1/2}^* u_h(x_{j-1/2}^+).
 \end{aligned}$$

- Periodic boundary condition

First let us consider periodic boundary condition. Summing (17) for j , we can obtain

$$\begin{aligned}
 \frac{\partial \bar{n}_h}{\partial t} &= \sum_{j=1}^N \int_{I_j} \frac{\partial n_h}{\partial t} dx \\
 &= -i \sum_{j=1}^N \left[u_h \frac{1}{m} \frac{\partial u_h^*}{\partial x} \right] \Big|_{j+1/2} + i \sum_{j=1}^N \left[u_h^* \frac{1}{m} \frac{\partial u_h}{\partial x} \right] \Big|_{j+1/2} \\
 &\quad + i \sum_{j=1}^N h_{q,j+1/2} \left[\frac{1}{m} \frac{\partial u_h^*}{\partial x} \right] \Big|_{j+1/2} - i \sum_{j=1}^N h_{q,j+1/2}^* \left[\frac{1}{m} \frac{\partial u_h}{\partial x} \right] \Big|_{j+1/2} \\
 (18) \quad &\quad - \sum_{j=1}^N h_{u,j+1/2} [u_h^*]_{j+1/2} - \sum_{j=1}^N h_{u,j+1/2}^* [u_h]_{j+1/2},
 \end{aligned}$$

where

$$[u]_{j+1/2} = u(x_{j+1/2}^+) - u(x_{j+1/2}^-), \quad m(x_{j+1/2}^+) = m_{j+1}, \quad m(x_{j+1/2}^-) = m_j.$$

Now substituting

$$h_{q,j+1/2} = \frac{u_h(x_{j+1/2}^-) + u_h(x_{j+1/2}^+)}{2}$$

into (18), we have

$$(19) \quad \frac{\partial \bar{n}_h}{\partial t} = \sum_{j=1}^N \int_{I_j} \frac{\partial n_h}{\partial t} dx = \frac{i}{2} \sum_{j=1}^N \left\{ [u_h^*]_{j+1/2} \text{TERM1} - [u_h]_{j+1/2} \text{TERM2} \right\},$$

where

$$\text{TERM1} = m(x_{j+1/2}^-) \frac{\partial u_h(x_{j+1/2}^-)}{\partial x} + m(x_{j+1/2}^+) \frac{\partial u_h(x_{j+1/2}^+)}{\partial x} + i2h_{u,j+1/2},$$

$$\text{TERM2} = m(x_{j+1/2}^-) \frac{\partial u_h^*(x_{j+1/2}^-)}{\partial x} + m(x_{j+1/2}^+) \frac{\partial u_h^*(x_{j+1/2}^+)}{\partial x} - i2h_{u,j+1/2}^*.$$

Observing the above equation, we can choose

$$h_{u,j+1/2} = \frac{i}{2} \left(m(x_{j+1/2}^-) \frac{\partial u_h(x_{j+1/2}^-)}{\partial x} + m(x_{j+1/2}^+) \frac{\partial u_h(x_{j+1/2}^+)}{\partial x} \right)$$

to keep the numerical conservation of the numerical probability density. Thus, we prove that if the numerical flux is defined as

$$(20a) \quad h_{u,j+1/2} = \frac{i}{2} \left(m(x_{j+1/2}^-) \frac{\partial u_h(x_{j+1/2}^-)}{\partial x} + m(x_{j+1/2}^+) \frac{\partial u_h(x_{j+1/2}^+)}{\partial x} \right),$$

$$(20b) \quad h_{q,j+1/2} = \frac{u_h(x_{j+1/2}^-) + u_h(x_{j+1/2}^+)}{2},$$

the numerical conservation of the probability density n holds.

- Nonperiodic boundary condition

The periodic boundary condition requires

$$(21) \quad \begin{aligned} u(x_{N+1/2}^+) &= u(x_{1/2}^+), & u(x_{N+1/2}^-) &= u(x_{1/2}^-), \\ \partial u(x_{N+1/2}^+)/\partial x &= \partial u(x_{1/2}^+)/\partial x, & \partial u(x_{N+1/2}^-)/\partial x &= \partial u(x_{1/2}^-)/\partial x. \end{aligned}$$

In the case of periodic boundary condition, we have (18) where the sum is taken for $j = 1, 2, \dots, N$. For nonperiodic boundary conditions, the sum is taken for $j = 1, 2, \dots, N - 1$, in addition, we have a boundary term

$$(22) \quad \begin{aligned} S_b &= \frac{1}{m(x_{1/2}^+)} \left(-iu_h(x_{1/2}^+) \frac{\partial u_h^*(x_{1/2}^+)}{\partial x} + iu_h^*(x_{1/2}^+) \frac{\partial u_h(x_{1/2}^+)}{\partial x} \right. \\ &\quad \left. + ih_{q,1/2} \frac{\partial u_h^*(x_{1/2}^+)}{\partial x} - ih_{q,1/2}^* \frac{\partial u_h(x_{1/2}^+)}{\partial x} \right) \\ &\quad - h_{u,1/2} u_h^*(x_{1/2}^+) - h_{u,1/2}^* u_h(x_{1/2}^+) \\ &\quad + \frac{1}{m(x_{N+1/2}^-)} \left(iu_h(x_{N+1/2}^-) \frac{\partial u_h^*(x_{N+1/2}^-)}{\partial x} - iu_h^*(x_{N+1/2}^-) \frac{\partial u_h(x_{N+1/2}^-)}{\partial x} \right. \\ &\quad \left. - ih_{q,N+1/2} \frac{\partial u_h^*(x_{N+1/2}^-)}{\partial x} + ih_{q,N+1/2}^* \frac{\partial u_h(x_{N+1/2}^-)}{\partial x} \right) \\ &\quad + h_{u,N+1/2} u_h^*(x_{N+1/2}^-) + h_{u,N+1/2}^* u_h(x_{N+1/2}^-). \end{aligned}$$

Also choosing the numerical flux (20a) and (20b), we have

$$(23) \quad \frac{\partial \bar{n}_h}{\partial t} = S_b,$$

where

$$\begin{aligned}
 S_b = \frac{i}{2} \left\{ & u_h(x_{1/2}^-) \frac{1}{m(x_{1/2}^+)} \frac{\partial u_h^*(x_{1/2}^+)}{\partial x} - u_h^*(x_{1/2}^-) \frac{1}{m(x_{1/2}^+)} \frac{\partial u_h(x_{1/2}^+)}{\partial x} \right. \\
 & - \frac{1}{m(x_{1/2}^-)} \frac{\partial u_h(x_{1/2}^-)}{\partial x} u_h^*(x_{1/2}^+) + u_h(x_{1/2}^+) \frac{1}{m(x_{1/2}^-)} \frac{\partial u_h^*(x_{1/2}^-)}{\partial x} \\
 & - u_h(x_{N+1/2}^+) \frac{1}{m(x_{N+1/2}^-)} \frac{\partial u_h^*(x_{N+1/2}^-)}{\partial x} \\
 & + u_h^*(x_{N+1/2}^+) \frac{1}{m(x_{N+1/2}^-)} \frac{\partial u_h(x_{N+1/2}^-)}{\partial x} \\
 & + \frac{1}{m(x_{N+1/2}^+)} \frac{\partial u_h(x_{N+1/2}^+)}{\partial x} u_h^*(x_{N+1/2}^-) \\
 & \left. - \frac{1}{m(x_{N+1/2}^+)} \frac{\partial u_h^*(x_{N+1/2}^+)}{\partial x} u_h(x_{N+1/2}^-) \right\}. \tag{24}
 \end{aligned}$$

If the periodic condition holds, it is obvious that $S_b = 0$. If m , u_h and $\partial u_h/\partial x$ are continuous at the boundary points, we have

$$\begin{aligned}
 S_b = & i \frac{1}{m(x_{1/2})} \left(\frac{\partial u_h^*(x_{1/2})}{\partial x} u_h(x_{1/2}) - \frac{\partial u_h(x_{1/2})}{\partial x} u_h^*(x_{1/2}) \right) \\
 & - i \frac{1}{m(x_{N+1/2})} \left(\frac{\partial u_h^*(x_{N+1/2})}{\partial x} u_h(x_{N+1/2}) - \frac{\partial u_h(x_{N+1/2})}{\partial x} u_h^*(x_{N+1/2}) \right). \tag{25}
 \end{aligned}$$

where

$$\begin{aligned}
 m(x_{1/2}) &= m(x_{1/2}^-) = m(x_{1/2}^+), \\
 u_h(x_{1/2}) &= u_h(x_{1/2}^-) = u_h(x_{1/2}^+), \\
 \frac{\partial u_h(x_{1/2})}{\partial x} &= \frac{\partial u_h(x_{1/2}^-)}{\partial x} = \frac{\partial u_h(x_{1/2}^+)}{\partial x}, \\
 m(x_{N+1/2}) &= m(x_{N+1/2}^-) = m(x_{N+1/2}^+), \\
 u_h(x_{N+1/2}) &= u_h(x_{N+1/2}^-) = u_h(x_{N+1/2}^+), \\
 \frac{\partial u_h(x_{N+1/2})}{\partial x} &= \frac{\partial u_h(x_{N+1/2}^-)}{\partial x} = \frac{\partial u_h(x_{N+1/2}^+)}{\partial x}.
 \end{aligned}$$

Using the definition of probability current (3), we have

$$S_b = J_h(x_{N+1/2}) - J_h(x_{1/2}) = J_h(1) - J_h(0). \tag{26}$$

5. Numerical Results

We consider the following one dimensional Schrödinger equation

$$\frac{\partial u}{\partial t} - i \frac{\partial^2 u}{\partial x^2} = -iVu \quad \text{in } (0, 1) \times (0, T). \tag{27}$$

Assuming that the time-dependent factor is $\exp(-iEt)$ (assuming that the Planck constant $\hbar = 1$), we have (here we denote the x -dependent part of u as u)

$$-u'' = (E - V)u \quad \text{in } (0, 1). \tag{28}$$

A simplest potential $V(x)$ shown in Fig. 2 is given by

$$(29) \quad V(x) = \begin{cases} V_0, & 0 \leq x \leq d, \\ 0, & \text{otherwise.} \end{cases}$$

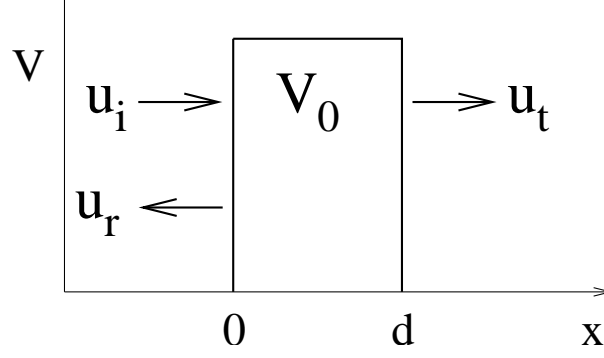


FIGURE 2. A simplest potential

Let the incident wave be

$$(30) \quad u_{inc} = \exp(ik_1x),$$

where $k_1 = \sqrt{E}$, and we can give the exact solution in two cases: $V_0 < E$ and $V_0 > E$.

- $V_0 < E$

we can obtain the wave function

$$(31) \quad u(x) = \begin{cases} \exp(ik_1x) + r \exp(-ik_1x), & x < 0, \\ C \exp(ik_2x) + D \exp(-ik_2x), & 0 < x < d, \\ t \exp(ik_1x), & x > d, \end{cases}$$

where $k_2 = \sqrt{E - V_0}$, r and t are the amplitudes of the reflected wave and transmitted wave, respectively, and

$$(32) \quad r = \frac{i(k_2^2 - k_1^2) \sin(k_2d)}{2k_1k_2 \cos(k_2d) - i(k_1^2 + k_2^2) \sin(k_2d)},$$

$$(33) \quad C = \frac{k_2(1+r) + k_1(1-r)}{2k_2},$$

$$(34) \quad D = \frac{k_2(1+r) - k_1(1-r)}{2k_2},$$

$$(35) \quad t = \frac{k_2(1+r) \cos(k_2d) + ik_1(1-r) \sin(k_2d)}{k_2 \exp(ik_1d)}.$$

- $V_0 > E$

we can obtain the wave function

$$(36) \quad u(x) = \begin{cases} \exp(ik_1x) + r \exp(-ik_1x), & x < 0, \\ C \exp(\kappa_2x) + D \exp(-\kappa_2x), & 0 < x < d, \\ t \exp(ik_1x), & x > d, \end{cases}$$

where $\kappa_2 = \sqrt{V_0 - E}$, and

$$(37) \quad r = \frac{(k_2^2 + k_1^2) \sinh(\kappa_2 d)}{2ik_1\kappa_2 \cosh(\kappa_2 d) + (k_1^2 - \kappa_2^2) \sinh(\kappa_2 d)},$$

$$(38) \quad C = \frac{\kappa_2(1+r) + ik_1(1-r)}{2\kappa_2},$$

$$(39) \quad D = \frac{\kappa_2(1+r) - ik_1(1-r)}{2\kappa_2},$$

$$(40) \quad t = \frac{\kappa_2(1+r) \cosh(\kappa_2 d) + ik_1(1-r) \sinh(\kappa_2 d)}{\kappa_2 \exp(ik_1 d)}.$$

In the numerical example, we set the parameters $E = 4\pi^2$, $V_0 = 2\pi$, $d = 0.2$. The computational domain is $[-0.5, 0.5]$. We use 4th-order basis functions and 4th-order Runge-Kutta method. Three different meshes with mesh sizes 0.1, 0.05 and 0.025 are used. The exact boundary condition and initial condition are used. We compute up to $T = 0.159$, which approximately equals one period.

While (20) is the numerical flux which maintains the numerical probability density conservation, another consistent numerical flux can be defined as

$$(41a) \quad h_{u,j+1/2} = \frac{i}{2} \left(q_h(x_{j+1/2}^-) + q_h(x_{j+1/2}^+) \right),$$

$$(41b) \quad h_{q,j+1/2} = \frac{1}{2} \left(u_h(x_{j+1/2}^-) + u_h(x_{j+1/2}^+) \right).$$

The L^2 errors with the flux (20) are listed in Table 1, and the L^2 errors with the flux (41) are listed in Table 2. It can be seen that the numerical results using the flux (41) are actually more accurate than that using the flux (20).

TABLE 1. L^2 errors with flux (20)

N	Δt	L^2 error of u	order	L^2 error of q	order
10	4e-6	1.209e-5		5.049e-4	
20	1e-6	4.037e-7	4.904	4.423e-5	3.513
40	2.5e-7	1.290e-8	4.968	3.300e-6	3.744

TABLE 2. L^2 errors with flux (41)

N	Δt	L^2 error of u	order	L^2 error of q	order
10	4e-6	1.988e-6		6.724e-5	
20	1e-6	7.507e-8	4.727	2.610e-6	4.687
40	2.5e-7	2.324e-9	5.014	1.031e-7	4.662

6. Conclusion

We have proposed and tested a LDG formulation for one-dimensional time dependent Schrödinger equation. The proposed numerical flux is shown to assure the numerical probability density conservation. However, alternative form of numerical flux using the mean value at the element interface, while not maintaining the conservative property of the density, yields better accuracy. Future work is planned to extend the proposed algorithms to multidimensional problems, also to include a Poisson equations to incorporate the effect of the charge on the potential in the Schrödinger equation self-consistently.

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