THE L^1-ERROR ESTIMATES FOR A HAMILTONIAN-PRESERVING SCHEME FOR THE LIOUVILLE EQUATION WITH PIECEWISE CONSTANT POTENTIALS *

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Abstract. We study the l^1-error of a Hamiltonian-preserving scheme, developed in [11], for the Liouville equation with a piecewise constant potential in one space dimension. This problem has important applications in computations of the semiclassical limit of the linear Schrödinger equation through barriers, and of the high frequency waves through interfaces. We use the l^1-error estimates established in [30, 28] for the immersed interface upwind scheme to the linear advection equations with piecewise constant coefficients. We prove that the scheme with the Dirichlet incoming boundary conditions is l^1-convergent for a class of bounded initial data, and derive the one-halfth order l^1-error bounds with *explicit* coefficients. The initial conditions can be satisfied by applying the decomposition technique proposed in [10] for solving the Liouville equation with measure-valued initial data, which arises in the semiclassical limit of the linear Schrödinger equation.

Key words. Liouville equations, Hamiltonian preserving schemes, piecewise constant potentials, error estimate, half order error bound, semiclassical limit

AMS subject classifications. 65M06, 65M12, 65M25, 35L45, 70H99

1. Introduction.

In [11], we constructed a class of numerical schemes for the d-dimensional Liouville equation in classical mechanics:

$$f_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{v}} f = 0\,, \quad t > 0, \quad \mathbf{x}, \mathbf{v} \in R^d\,, \tag{1.1}$$

where $f(t, \mathbf{x}, \mathbf{v})$ is the density distribution of a classical particle at position $\mathbf{x}$, time t and traveling with velocity $\mathbf{v}$. $V(\mathbf{x})$ is the potential. The main interest is in the case of a discontinuous potential $V(\mathbf{x})$, corresponding to a potential barrier. When V is discontinuous, the Liouville equation (1.1) is a linear hyperbolic equation with a measure-valued coefficient. Such a problem cannot be understood mathematically using the renormalized solution by DiPerna and Lions for linear advection equations with discontinuous coefficients [5] (see also [2]). Our approach in [11, 12] to such problems was to provide an interface condition to couple the Liouville equation (1.1) on both sides of the barrier or interface. The interface condition accounts for particle or wave transmission and reflection. Based on this notion of the solution, the so-called Hamiltonian-preserving schemes were constructed in [11, 12], which build this interface condition into the numerical flux. Schemes so constructed provide solutions that are physically relevant for particle or wave reflection and transmission through the barriers or interfaces.

The Liouville equation is the phase space representation of Newton's second law:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}\,, \quad \frac{d\mathbf{v}}{dt} = -\nabla_{\mathbf{x}} V\,,$$

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which is a Hamiltonian system with the Hamiltonian

$$H = \frac{1}{2}|\mathbf{v}|^2 + V(\mathbf{x}).$$

It is known from classical mechanics that the Hamiltonian remains constant across a potential barrier. This is one of the main ingredients in the Hamiltonian-preserving schemes developed in [11, 12]. The two schemes developed in [11]–one based on a finite difference formulation (called Scheme I) and the other on a finite volume formulation (called Scheme II) were proved, in one space dimension with a piecewise constant potential, to be positive, and l^1 and l^∞-stable for suitable initial value problems and under a hyperbolic CFL condition (see also [29]).

The more sophisticated issue of the l^1-stability of Scheme I was studied in [29]. We proved in [29] that, in the case of a step function potential, Scheme I with the homogeneous Dirichlet incoming boundary conditions is l^1-stable under a certain condition on the initial data. In particular, we showed that such an initial condition is satisfied when choosing the numerical initial data as the cell averages of a bounded analytical initial data. Since the exact solution, in the aforementioned notion using the interface condition, to the same problem is l^1-contracting, an l^1-convergent scheme should be l^1-stable. Thus the results established in [29] implies that Scheme I meets the necessary condition for the l^1-convergence in the case of the homogeneous Dirichlet boundary conditions and bounded initial data.

In this paper we will study the l^1-convergence of Scheme I in the case of a step function potential and the Dirichlet incoming boundary conditions. We will prove that in this case Scheme I is l^1-convergent for a class of bounded initial data. The initial conditions can be satisfied when applying the decomposition technique proposed in [10] for solving the Liouville equation with measure-valued initial data arising in the semiclassical limit of the linear Schrödinger equation.

The Liouville equation with a step function (or more generally piecewise constant) potential belongs to hyperbolic equations with singular (discontinuous or measure-valued) coefficients. For the discontinuous coefficient case, the convergence of numerical schemes were widely studied [6, 9, 14, 15, 4, 17, 25, 19, 21, 7, 26, 27, 16, 13, 1, 20]. However, in most cases the convergence rate estimates for numerical schemes were not studied. For the measure-valued coefficient case, recently we have obtained the halfth order l^1-error estimates for the immersed interface upwind scheme which builds the interface condition into the numerical flux, see [30, 28]. In this paper, we extend this result to the more interesting case of the Liouville equation with a step function potential. Since the Liouville equation is defined in the phase space, extra efforts are needed to deal with the discretization in the velocity space.

To derive the desired error estimates, we split the computational domain into several parts. In each subdomain, we will introduce a number of linear advection equations with step function coefficients. The immersed interface upwind schemes for these linear advection equations yield the same numerical solution as Scheme I for the Liouville equation with the step function potential. Then the l^1-error estimates for Scheme I can be achieved by applying the l^1-error estimates for the immersed interface upwind schemes and estimating the l^1-errors between the exact solutions of the linear advection equations with step function coefficients and that of the Liouville equation with the step function potential. The first part of the error estimates are obtained by applying the results established in [30, 28] with the aid of the condition on the initial data. The second part of the errors are analyzed also utilizing the condition on the initial data. With this approach, we can derive the halfth order l^1-error bound with *explicit* coefficients for Scheme I.

Our proof is based on the step function potential. This result clearly generates to piecewise constant potentials in a straightforward but tedious way. The same approach should also be applicable to analyze the l^1-error estimates for the finite volume Scheme II developed in [11]. But we will not pursue this in this paper.

This paper is organized as follows. In Section 2 we review the Hamiltonian-preserving scheme proposed in [11] for the Liouville equation with a discontinuous potential in one space dimension. In Section 3 we recall the l^1-error estimates for the immersed interface upwind scheme established in [30, 28] to the linear advection equation with a step function wave speed. In Section 4 we setup the problem and state the main Theorem of this paper which is proved in Section 5 using the results presented in Section 3. We conclude the paper in Section 6.

2. A Hamiltonian-preserving scheme. In this Section we review the Hamiltonian-preserving scheme proposed in [11] to the Liouville equation in one space dimension

$$f_t + \xi f_x - V_x f_\xi = 0 \tag{2.1}$$

with a discontinuous potential $V(x)$.

Consider a uniform mesh with grid points at $x_{i+\frac{1}{2}}, i \in \mathbb{Z}$ in the x-direction and $\xi_{j+\frac{1}{2}}, j \in \mathbb{Z}$ in the ξ-direction. The cells are centered at $(x_i, \xi_j), (i,j) \in \mathbb{Z}^2$ with $x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$ and $\xi_j = \frac{1}{2}(\xi_{j+\frac{1}{2}} + \xi_{j-\frac{1}{2}})$. The mesh size are denoted by $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}, \Delta\xi = \xi_{j+\frac{1}{2}} - \xi_{j-\frac{1}{2}}$. We also assume a uniform time step Δt and the discrete times are given by $t_n = n\Delta t, n \in \mathbb{N} \cup \{0\}$. We assume that the computation is performed in a bounded rectangular domain

$$\{(x,y)|x_{\frac{1}{2}} \le x \le x_{N+\frac{1}{2}},\ \xi_{\frac{1}{2}} \le \xi \le \xi_{M+\frac{1}{2}}\}. \tag{2.2}$$

Let the cell averages of f be

$$f_{ij} = \frac{1}{\Delta x \Delta\xi} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x,\xi,t) d\xi dx.$$

The 1-d average quantity $f_{i+1/2,j}$ is defined as

$$f_{i+1/2,j} = \frac{1}{\Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{i+1/2},\xi,t) d\xi\,.$$

$f_{i,j+1/2}$ is defined similarly.

In classical mechanics, a particle will either cross a potential barrier with a changing momentum, or be reflected, depending on its momentum and the strength of the potential barrier.

Figure 2.1 shows the typical situations when a particle moves from left to right at a potential barrier. If the potential is reduced, the particle will cross it with an accelerated speed. If the potential is increased, the particle is either reflected if its momentum is not big enough to overcome the barrier or transmitted otherwise with a reduced velocity. *The Hamiltonian* $H = \frac{1}{2}\xi^2 + V$ *is preserved across the potential barrier:*

$$\frac{1}{2}(\xi^+)^2 + V^+ = \frac{1}{2}(\xi^-)^2 + V^-, \tag{2.3}$$

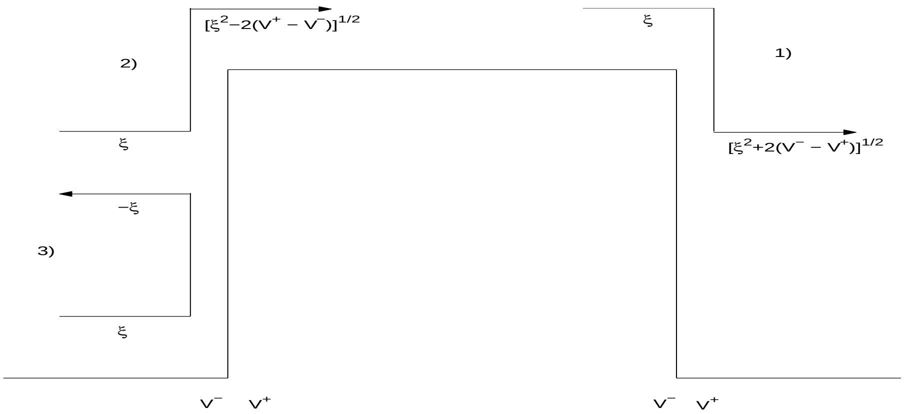

Figure 2.1 Transmission and reflection of a particle at a potential barrier.

where the superscripts $\pm$ indicate the right and left limits of the quantity at the potential barrier. This property was used in [11] to provide the interface condition for (2.1) at the barrier:

$$f(t, x^+, \xi^+) = f(t, x^-, \xi^-) \quad \text{for transmission} \tag{2.4}$$

$$f(t, x^\pm, \xi^\pm) = f(t, x^\pm, -\xi^\pm) \quad \text{for reflection} \tag{2.5}$$

where ξ^+ and ξ^- are related by the constant Hamiltonian condition (2.3) in the case of transmission. With such an interface condition, we established the well-posedness of the initial value problem to (1.1) with a piecewise constant potential in [12].

The main ingredient in the Hamiltonian-preserving schemes developed in [11], like the earlier work for shallow-water equations [22], was to build into the numerical flux the interface conditions (2.4), (2.5) at the barrier.

We now present the first Hamiltonian-preserving scheme, called *Scheme I* in [11].

Assume that the discontinuous points of the potential V are located at the grid points. Let the left and right limits of V at point $x_{i+1/2}$ be $V^-_{i+\frac{1}{2}}$ and $V^+_{i+\frac{1}{2}}$ respectively. Note that if V is continuous at $x_{j+1/2}$, then $V^-_{i+\frac{1}{2}} = V^+_{i+\frac{1}{2}}$. We approximate V by a piecewise linear function

$$V(x) \approx V^+_{i-1/2} + \frac{V^-_{i+1/2} - V^+_{i-1/2}}{\Delta x}(x - x_{i-1/2}) .$$

The flux-splitting, semidiscrete scheme (with time continuous) reads

$$\partial_t f_{ij} + \xi_j \frac{f^-_{i+\frac{1}{2},j} - f^+_{i-\frac{1}{2},j}}{\Delta x} - \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0,$$

where the numerical fluxes $f_{i,j+\frac{1}{2}}$ are defined using the upwind discretization. Since the characteristics of the Liouville equation may be different on the two sides of a barrier, the corresponding numerical fluxes should also be different. The essential part of the algorithm is to define the split numerical fluxes $f^-_{i+\frac{1}{2},j}, f^+_{i-\frac{1}{2},j}$ at each cell interface. (2.4) will be used to define these fluxes.

Assume V is discontinuous at $x_{i+1/2}$. Consider the case $\xi_j > 0$. Using upwind scheme, $f^-_{i+\frac{1}{2},j} = f_{ij}$. However,

$$f^+_{i+1/2,j} \equiv f(x^+_{i+1/2}, \xi^+) = f(x^-_{i+1/2}, \xi^-)$$

where ξ^- is obtained from $\xi^+ = \xi_j$ from (2.3). Since ξ^- may not be a grid point, we have to define it approximately. The first approach is to locate the two cell centers that bound this velocity, then use a linear interpolation to evaluate the needed numerical flux at ξ^-. The case of $\xi_j < 0$ is treated similarly. The algorithm to generate the numerical flux is given in [11]. Here we present the simplified algorithm for the case $V^-_{i+\frac{1}{2}} > V^+_{i+\frac{1}{2}}$ being discussed in this paper.

Algorithm I

- $\xi_j > 0$

  $f^-_{i+\frac{1}{2},j} = f_{ij}$,

  ❏ if $\xi_j > \sqrt{2\left(V^-_{i+\frac{1}{2}} - V^+_{i+\frac{1}{2}}\right)}$,

  $\xi^- = \sqrt{\xi_j^2 + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}$

  if $\xi_k \le \xi^- < \xi_{k+1}$ for some k

  then $f^+_{i+\frac{1}{2},j} = \frac{\xi_{k+1}-\xi^-}{\Delta\xi} f_{ik} + \frac{\xi^- - \xi_k}{\Delta\xi} f_{i,k+1}$

  ❏ else

  $f^+_{i+\frac{1}{2},j} = f_{i+1,k}$ where $\xi_k = -\xi_j$

  ❏ end
- $\xi_j < 0$

  $f^+_{i+\frac{1}{2},j} = f_{i+1,j}$,

  $\xi^+ = -\sqrt{\xi_j^2 + 2\left(V^-_{i+\frac{1}{2}} - V^+_{i+\frac{1}{2}}\right)}$

  if $\xi_k \le \xi^+ < \xi_{k+1}$ for some k

  then $f^-_{i+\frac{1}{2},j} = \frac{\xi_{k+1}-\xi^+}{\Delta\xi} f_{i+1,k} + \frac{\xi^+ - \xi_k}{\Delta\xi} f_{i+1,k+1}$

After the spatial discretization is specified, one can use any time discretization for the time derivative.

In [11] we proved that, when the first order upwind scheme is used spatially, and the forward Euler method is used in time, and the potential V has a single jump, Scheme I is positive and l^∞-contracting under the CFL condition:

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|}{\Delta \xi} \right] < 1. \tag{2.6}$$

In [29] we proved that when the potential is a step function, the same scheme is l^1-stable under the CFL condition (2.6) and a suitable condition on the numerical initial data.

Note that the quantity $\left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|$ represents the gradient of the potential at its *smooth* point, which has a *finite* upper bound. Thus the scheme satisfies a hyperbolic CFL condition.

3. The l^1-error estimates for the immersed interface upwind scheme. In this Section we present the l^1-error estimates for the immersed interface upwind scheme established in [30, 28] to the linear advection equation

$$\frac{\partial u}{\partial t} + c(x)\frac{\partial u}{\partial x} = 0, \qquad t > 0, x \in \mathbb{R}, \tag{3.1}$$

$$u|_{t=0} = u_0(x), \tag{3.2}$$

with a step function wave speed

$$c(x) = \begin{cases} c^- & x < 0 \\ c^+ & x > 0 \end{cases}. \tag{3.3}$$

We assume that $c(x)$ has a definite sign. This avoids the mathematical difficulties of dealing with non-uniqueness or measure-valued solutions, see for examples [3, 23]. Without loss of generality we assume $c(x) > 0$.

We consider the following interface condition for (3.1)-(3.3) requiring u being continuous across the interface

$$u(0^+, t) = u(0^-, t). \tag{3.4}$$

In [30] we have considered a more general class of interface conditions including (3.4). In this paper we only present the results corresponding to the interface condition (3.4), which will be used to derive the l^1-error estimates for Scheme I.

The exact solution of (3.1)-(3.3) with the interface condition (3.4) can be constructed using the method of characteristics:

$$u(x,t) = \begin{cases} u_0(x - c^- t) & x < 0 \\ u_0\left(\frac{c^-}{c^+} x - c^- t\right) & 0 < x < c^+ t \\ u_0(x - c^+ t) & x > c^+ t \end{cases}. \tag{3.5}$$

Consider the uniform mesh introduced in Section 2 in x and t-directions. We assume that the interface $x = 0$ is located at a grid point. We introduce quantities $\lambda^- = c^- \frac{\Delta t}{\Delta x}, \lambda^+ = c^+ \frac{\Delta t}{\Delta x}$. The condition $0 < \lambda^-, \lambda^+ < 1$ is the CFL condition.

The immersed interface upwind scheme which builds the interface condition (3.4) into the upwind difference scheme (with the forward Euler time discretization) for the equation (3.1)-(3.3) reads

$$v_i^{n+1} = (1 - \lambda^-) v_i^n + \lambda^- v_{i-1}^n, \quad \text{if } x_i < 0, \tag{3.6}$$

$$v_i^{n+1} = (1 - \lambda^+) v_i^n + \lambda^+ v_{i-1}^n, \quad \text{if } x_i > 0, \tag{3.7}$$

where

$$v_i^0 = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_0(x) dx. \tag{3.8}$$

To compare the numerical solution computed from (3.6)-(3.8) with the exact solution (3.5), we introduce

$$v(x,t) = v_i^n, \qquad \text{for } (x,t) \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}) \times [t_n, t_{n+1}).$$

The following Theorem was proven in [30]

THEOREM 3.1. *The upwind difference scheme (3.6)-(3.8), under the CFL condition* $0 < \lambda^-, \lambda^+ < 1$, *has the following* l^1*-error to the exact solution (3.5):*

$$\|v(\cdot, t_n) - u(\cdot, t_n)\|_{l^1(\mathbb{R})} \le \|u_0\|_{BV(\mathbb{R})} \left[\gamma_m \frac{c^M}{c^m} \sqrt{\Delta x} + \left(1 + \frac{c^M}{c^m} + \max\left\{\frac{c^+}{c^-}, 1\right\}\right) \Delta x\right], \tag{3.9}$$

where

$$c^m = \min\{c^-, c^+\}, \quad c^M = \max\{c^-, c^+\}, \quad \gamma_m = \sqrt{\frac{2}{e} c^m \left(1 - c^m \frac{\Delta t}{\Delta x}\right) t_{n+1}},$$

and the definition of the BV norm on $\mathbb{R}$ is given by

$$\|u_0\|_{BV(\mathbb{R})} = \sup_{|h| \neq 0} \frac{1}{|h|} \|u_0(\cdot + h) - u_0(\cdot)\|_{l^1(\mathbb{R})}. \tag{3.10}$$

REMARK 3.1. *In the case of $c^- = c^+$, namely a constant wave speed, the coefficient before Δx in* (3.9) *can be sharpened. In this paper we will also use* (3.9) *for the constant wave speed case since this will not affect the leading order coefficient in the l^1-error estimates for Scheme I.*

4. Setup of the problem and the main result. In this Section we establish the l^1-error estimates for Scheme I (with the first order numerical flux and the forward Euler method in time) under suitable conditions on the initial data. We consider the case when $V(x)$ is a step function, with a jump $-D, D > 0$ at $x = 0$. Namely

$$V(0^-) - V(0^+) = D.$$

Let the computational domain be confined in the rectangular domain (2.2). We employ the uniform mesh introduced in Section 2. Define mesh ratios $\lambda_x^t = \frac{\Delta t}{\Delta x}, \lambda_x^\xi = \frac{\Delta \xi}{\Delta x}$, assumed to be fixed. Let the potential barrier $x = 0$ be at a grid point $x_{m+\frac{1}{2}}$. Then the point-wise values of V satisfy

$$V^-_{m+\frac{1}{2}} - V^+_{m+\frac{1}{2}} = D, \quad V^\pm_{i+\frac{1}{2}} = V^-_{m+\frac{1}{2}}, i < m, \quad V^\pm_{i+\frac{1}{2}} = V^+_{m+\frac{1}{2}}, i > m,$$

where the superscripts $-, +$ represent the left and right limits at $x = 0$.

We consider the typical situation that $\xi_1 < -\sqrt{2D}, \xi_M > \sqrt{2D}$, so that all possible particle behaviors, including both transmission and reflection, are included. To simplify the discussion, we choose the mesh such that 0 and $\pm\sqrt{2D}$ are grid points in the ξ-direction. Define the indices I_0, I_+ satisfying

$$\xi_{I_0+\frac{1}{2}} = 0, \quad \xi_{I_++\frac{1}{2}} = \sqrt{2D}.$$

Define the domain

$$D_b = \left\{(x, y) | x < 0, \xi < -\sqrt{\left(\xi_{\frac{1}{2}}\right)^2 - 2D}\right\}.$$

Due to the velocity change across the barrier at $x = 0$, D_b represents the area where particles come from outside of the domain $[x_{\frac{1}{2}}, x_{N+\frac{1}{2}}] \times [\xi_{\frac{1}{2}}, \xi_{M+\frac{1}{2}}]$. In order to implement Scheme I conveniently, we need to exclude this domain from the computational domain. Define the index I_b satisfying

$$\xi_{I_b-\frac{3}{2}} < -\sqrt{\left(\xi_{\frac{1}{2}}\right)^2 - 2D} \leq \xi_{I_b-\frac{1}{2}}$$

and the domain

$$\widehat{D}_b = \left\{(x, \xi) | x < 0, \xi < \xi_{I_b-\frac{1}{2}}\right\}.$$

Then we choose the computational domain as

$$D_C = \{(x,\xi)|x_{\frac{1}{2}} \le x \le x_{N+\frac{1}{2}},\ \xi_{\frac{1}{2}} \le \xi \le \xi_{M+\frac{1}{2}}\} \setminus \widehat{D}_b.$$

Figure 4.1 depicts D_C and $\widehat{D}_b$.

We consider the Dirichlet boundary conditions at the incoming boundaries and assume that the initial data satisfy these boundary conditions:

$$f(x_{\frac{1}{2}},\xi,t) = f(x_{\frac{1}{2}},\xi,0), \quad 0 < \xi < \xi_{M+\frac{1}{2}}, \tag{4.1}$$

$$f(x_{N+\frac{1}{2}},\xi,t) = f(x_{N+\frac{1}{2}},\xi,0), \quad \xi_{\frac{1}{2}} < \xi < 0. \tag{4.2}$$

REMARK 4.1. *When V is a step function, (2.1) becomes*

$$f_t + \xi f_x = 0$$

where ξ only serves as a parameter. However, when implementing the interface conditions (2.4), (2.5) numerically, the mesh in ξ is needed. This is the main new difficulty when comparing with the problem presented in Section 3.

4.1. The initial data assumption. We now impose assumptions on the initial data. We assume the initial data are given on the rectangular domain (2.2). We have the following assumption:

ASSUMPTION 4.1.

The initial data $f(x,\xi,0)$ have bounded variation in the x-direction and is Lipschitz continuous in the ξ-direction. Namely

$$\|f(.,\xi,0)\|_{BV([x_{\frac{1}{2}},x_{N+\frac{1}{2}}])} \le A, \quad \forall \xi \in [\xi_{\frac{1}{2}},\xi_{M+\frac{1}{2}}], \tag{4.3}$$

$$|f(x,\xi',0) - f(x,\xi'',0)| \le B|\xi' - \xi''|, \quad \forall x \in \left[x_{\frac{1}{2}},x_{N+\frac{1}{2}}\right],\ \xi',\xi'' \in \left[\xi_{\frac{1}{2}},\xi_{M+\frac{1}{2}}\right]. \tag{4.4}$$

REMARK 4.2. *When arising in the semiclassical limit of the linear Schrödinger equation, the Liouville equation is supplied with the measure-valued initial data [8, 18], which does not satisfy Assumption 4.1. However, in [10], a decomposition of the initial data was introduced, which allows one to solve the semiclassical limit problem with bounded initial data which do satisfy Assumption 4.1. Specifically, if one needs to solve the Liouville equation (2.1) with the measure-valued initial data*

$$f(x,\xi,0) = \rho_0(x)\delta(\xi - v_0(x))\,, \tag{4.5}$$

the decomposition technique proposed in [10] suggests that one just solves two functions satisfying the same Liouville equation with initial data

$$\phi(x,\xi,0) = \rho_0(x)\,, \quad \psi(x,\xi,0) = \xi - v_0(x)\,. \tag{4.6}$$

Then the measure-valued solution to the Liouville equation with the initial data (4.5) is simply

$$f(x,\xi,t) = \phi(x,\xi,t)\delta(\psi(x,\xi,t)).$$

The evaluations of the moments of f then resort to the numerical approximations to the delta function integrals.

In solving for ϕ, ψ, the initial data (4.6) satisfy Assumption 4.1 if the initial density and velocity $\rho_0(x), v_0(x)$ have bounded variations. For this situation we have established the l^1-error estimates for Scheme I.

REMARK 4.3. *It can be checked that the initial data satisfying Assumption 4.1 is bounded in both l^∞ and l^1-norms on D_C. When the numerical initial data are chosen to be cell averages of such initial data, the l^1-stability of Scheme I with homogeneous Dirichlet boundary conditions was established in [29].*

4.2. The exact solution. For our proof, we need to introduce the partition of D_C as

$$D_l^+ = \Big\{(x,\xi) \mid x_{\frac12} < x < 0,\ 0 < \xi < \xi_{M+\frac12}\Big\}, \quad D_l^- = \Big\{(x,\xi) \mid x_{\frac12} < x < 0,\ \xi_{I_b-\frac12} < \xi < 0\Big\},$$
$$D_r^+ = \Big\{(x,\xi) \mid 0 < x < x_{N+\frac12},\ \sqrt{2D} < \xi < \xi_{M+\frac12}\Big\}, \quad D_r^- = \Big\{(x,\xi) \mid 0 < x < x_{N+\frac12},\ \xi_{\frac12} < \xi < -\sqrt{2D}\Big\},$$
$$D_r^r = \Big\{(x,\xi) \mid 0 < x < x_{N+\frac12},\ -\sqrt{2D} < \xi < \sqrt{2D}\Big\}$$

and the extension of the initial data

$$\widehat{f}_0(x,\xi) = \begin{cases} f(x,\xi,0) & x_{\frac12} \le x \le x_{N+\frac12} \\ f(x_{\frac12},\xi,0) & x < x_{\frac12} \\ f(x_{N+\frac12},\xi,0) & x > x_{N+\frac12} \end{cases} \quad \text{for } x \in \mathbb{R},\ \xi_{\frac12} \le \xi \le \xi_{M+\frac12}. \tag{4.7}$$

Figure 4.1 shows a sketch of the partition of D_C.

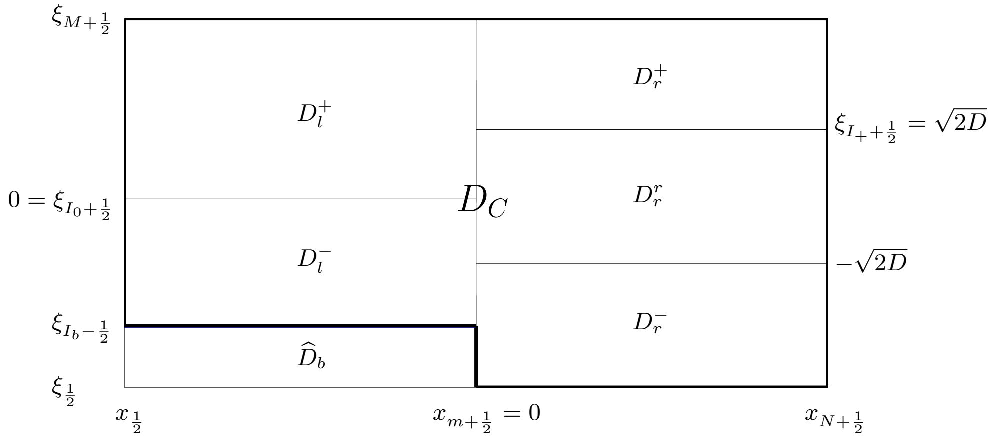

Figure 4.1 Sketch of partition of D_C and $\widehat{D}_b$.

The exact solution of (2.1) with the step function potential $V(x)$, when using the interface conditions (2.4) (2.5), can be obtained from the initial data $f(x,\xi,0)$ and boundary conditions (4.1), (4.2) by the method of characteristics:

1) for $(x,\xi) \in D_l^+ \cup D_r^-$,

$$f(x,\xi,t_n) = \widehat{f}_0(x - \xi t_n, \xi)\,; \tag{4.8}$$

2) for $(x,\xi) \in D_r^r$,

$$f(x,\xi,t_n) = \begin{cases} \widehat{f}_0(x-\xi t_n,\xi) & x > \xi t_n \\ \widehat{f}_0(-x+\xi t_n,-\xi) & x < \xi t_n \end{cases}\;; \tag{4.9}$$

3) for $(x,\xi) \in D_r^+$,

$$f(x,\xi,t_n) = \begin{cases} \widehat{f}_0\left(\frac{\sqrt{\xi^2-2D}}{\xi}x - \sqrt{\xi^2-2D}\,t_n, \sqrt{\xi^2-2D}\right) & 0 < x < \xi t_n \\ \widehat{f}_0\left(x-\xi t_n, \xi\right) & x > \xi t_n \end{cases}; \tag{4.10}$$

4) for $(x,\xi) \in D_l^-$,

$$f(x,\xi,t_n) = \begin{cases} \widehat{f}_0\left(-\frac{\sqrt{\xi^2+2D}}{\xi}x + \sqrt{\xi^2+2D}\,t_n, -\sqrt{\xi^2+2D}\right) & \xi t_n < x < 0 \\ \widehat{f}_0\left(x-\xi t_n, \xi\right) & x < \xi t_n \end{cases}. \tag{4.11}$$

4.3. The numerical solution. Denote

$$\mu_j = \lambda_x^t \left|\xi_j\right|, \qquad 1 \le j \le M. \tag{4.12}$$

Under the CFL condition (2.6), $\mu_j < 1$ for $1 \le j \le M$.

Since $V_x(x) = 0$ except at $x = x_{m+1/2}$, with the boundary conditions (4.1), (4.2), Scheme I on D_C is given by:

1) if $0 < \xi_j < \xi_{M+\frac{1}{2}}, i \neq m+1$,

$$g_{ij}^{n+1} = (1-\mu_j)g_{ij}^n + \mu_j g_{i-1,j}^n\,; \tag{4.13}$$

2) if $\xi_{I_b-\frac{1}{2}} < \xi_j < 0, i < m$ or $\xi_{\frac{1}{2}} < \xi_j < 0, i > m$,

$$g_{ij}^{n+1} = (1-\mu_j)g_{ij}^n + \mu_j g_{i+1,j}^n\,; \tag{4.14}$$

3) if $\sqrt{2D} < \xi_j < \xi_{M+\frac{1}{2}}$,

$$g_{m+1,j}^{n+1} = (1-\mu_j)g_{m+1,j}^n + \mu_j\left(c_{j,1}g_{m,d_j}^n + c_{j,2}g_{m,d_j+1}^n\right); \tag{4.15}$$

4) if $0 < \xi_j < \sqrt{2D}$,

$$g_{m+1,j}^{n+1} = (1-\mu_j)g_{m+1,j}^n + \mu_j g_{m+1,d_j}^n; \tag{4.16}$$

5) if $\xi_{I_b-\frac{1}{2}} < \xi_j < 0$,

$$g_{mj}^{n+1} = (1-\mu_j)g_{mj}^n + \mu_j\left(c_{j,1}g_{m+1,d_j}^n + c_{j,2}g_{m+1,d_j+1}^n\right), \tag{4.17}$$

where $0 \le c_{j,1}, c_{j,2} \le 1$ and $c_{j,1} + c_{j,2} = 1$. d_j's in (4.15)-(4.17) are determined according to Algorithm I by

$$\xi_{d_j} \le \sqrt{\left(\xi_j\right)^2 - 2D} < \xi_{d_j+1}, \qquad \text{for } d_j \text{ in (4.15)}, \tag{4.18}$$

$$\xi_{d_j} = -\xi_j, \qquad \text{for } d_j \text{ in (4.16)}, \tag{4.19}$$

$$\xi_{d_j} \le -\sqrt{\left(\xi_j\right)^2 + 2D} < \xi_{d_j+1}, \qquad \text{for } d_j \text{ in (4.17)}. \tag{4.20}$$

The initial and incoming boundary values of the numerical solution are given by

$$g_{ij}^0 = \frac{1}{\Delta x \Delta \xi}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x,\xi,0)\,d\xi dx, \quad (x_i,\xi_j) \in D_C, \tag{4.21}$$

$$g_{0,j}^n = \frac{1}{\Delta\xi}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{\frac{1}{2}},\xi,0)d\xi, \quad 0 < \xi_j < \xi_{M+\frac{1}{2}}, \tag{4.22}$$

$$g_{N+1,j}^n = \frac{1}{\Delta\xi}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{N+\frac{1}{2}},\xi,0)d\xi, \quad \xi_{\frac{1}{2}} < \xi_j < 0. \tag{4.23}$$

To compare the numerical solution computed from (4.13)-(4.23) with the exact solution (4.8)-(4.11), we introduce

$$g(x,\xi,t) = g_{ij}^n, \qquad \text{for } (x,\xi,t) \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})\times[\xi_{j-\frac{1}{2}},\xi_{j+\frac{1}{2}})\times[t_n,t_{n+1}), \quad (x_i,\xi_j)\in D_C.$$

We now state the main theorem of this paper:

THEOREM 4.1. *Under Assumption 4.1 on the initial data, the CFL condition (2.6) and the following mesh size restriction*

$$\Delta\xi \le \frac{3-2\sqrt{2}}{2}\sqrt{2D}, \tag{4.24}$$

Scheme I (4.13)-(4.23) has the following l^1-error bound compared to the exact solution (4.8)-(4.11)*:*

$$\begin{aligned}
&\|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_C)} \\
&\le \left[\left(\xi_{M+\frac{1}{2}} + \left|\xi_{\frac{1}{2}}\right| + \sqrt{2D}\right)A + 4DB\right]\sqrt{\frac{t_{n+1}}{2e\lambda_x^t}}\sqrt{\Delta x} \\
&\quad + \left(4A + 2\sqrt{2D}B\right)\sqrt{\frac{t_{n+1}}{2e}}\left(\frac{\xi_{M+\frac{1}{2}}}{(2D)^{\frac{1}{4}}}\sqrt{\frac{\xi_{M+\frac{1}{2}}-\sqrt{2D}}{\lambda_x^t}} + 2\left|\xi_{\frac{1}{2}}\right|\left[\left(\xi_{\frac{1}{2}}\right)^2 - 2D\right]^{\frac{1}{4}}\right)\sqrt{\Delta x} \\
&\quad + \left(2A + \sqrt{2D}B\right)\left[\frac{2\left(\xi_{M+\frac{1}{2}}\right)^2 t_n\lambda_x^\xi}{\sqrt{D}} + \left|\xi_{\frac{1}{2}}\right|\right]\ln\left(\frac{1}{\Delta x}\right)\Delta x + O(\Delta x).
\end{aligned} \tag{4.25}$$

5. The proof of Theorem 4.1.

This section is devoted to the proof of Theorem 4.1.

The l^1-error in (4.25) can be split according to the partition of D_C:

$$\begin{aligned}
&\|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_C)} \\
&= \|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_l^+)} + \|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_l^-)} \\
&\quad + \|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_r^+)} + \|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_r^r)} + \|g(\cdot,\cdot,t_n) - f(\cdot,\cdot,t_n)\|_{l^1(D_r^-)} \\
&\equiv E_l^+ + E_l^- + E_r^+ + E_r^r + E_r^-.
\end{aligned} \tag{5.1}$$

We will estimate the five terms in (5.1) respectively. As stated in Section 1, the strategy is to introduce a number of linear advection equations with step function coefficients in each partition whose immersed interface upwind schemes yield the same numerical solution as Scheme I. Then we apply the error estimates for the immersed interface upwind schemes given in Section 3 and compare the exact solutions of the linear advection equations and that of the Liouville equation to derive the desired estimates.

5.1. The upper bounds for E_l^+ and E_r^-. For E_l^+ one has

$$E_l^+ = \sum_{j=I_0+1}^{M} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \int_{x_{\frac{1}{2}}}^{0} |g(x,\xi,t_n) - f(x,\xi,t_n)| \, dx d\xi. \tag{5.2}$$

For $I_0 + 1 \le j \le M$, consider the linear advection equation

$$\frac{\partial u_{l,+}^j}{\partial t} + \xi_j \frac{\partial u_{l,+}^j}{\partial x} = 0, \qquad t > 0, x \in \mathbb{R}, \tag{5.3}$$

$$u_{l,+}^j|_{t=0} = \begin{cases} \frac{1}{\Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \widehat{f}_0(x,\xi) d\xi & x < 0 \\ \frac{1}{\Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \widehat{f}_0(0,\xi) d\xi & x \ge 0 \end{cases}. \tag{5.4}$$

The exact solution to (5.3),(5.4) is simply

$$u_{l,+}^j(x,t) = u_{l,+}^j(x - \xi_j t, 0). \tag{5.5}$$

Consider the upwind scheme for (5.3)

$$v_i^{n+1} = (1-\mu_j) v_i^n + \mu_j v_{i-1}^n, \tag{5.6}$$

$$v_i^0 = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_{l,+}^j(x,0) dx, \tag{5.7}$$

where μ_j is defined in (4.12).

Define

$$v_{l,+}^j(x,t) = v_i^n, \qquad \text{for } (x,t) \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}) \times [t_n, t_{n+1}).$$

Applying Theorem 3.1, the l^1-error between $v_{l,+}^j(x,t_n)$ and $u_{l,+}^j(x,t_n)$ is given by

$$\|v_{l,+}^j(\cdot,t_n) - u_{l,+}^j(\cdot,t_n)\|_{l^1(\mathbb{R})} \le \|u_{l,+}^j(\cdot,0)\|_{BV(\mathbb{R})} \left[\gamma_j \sqrt{\Delta x} + 3\Delta x\right], \tag{5.8}$$

where

$$\gamma_j = \sqrt{\frac{2}{e}\, \xi_j \left(1 - \xi_j \frac{\Delta t}{\Delta x}\right) t_{n+1}}. \tag{5.9}$$

From definition (4.7) and condition (4.3) one has

$$\|\widehat{f}_0(\cdot,\xi)\|_{BV(\mathbb{R})} \le A, \quad \xi_{\frac{1}{2}} \le \xi \le \xi_{M+\frac{1}{2}}. \tag{5.10}$$

Definition (5.4) and condition (5.10) imply

$$\|u_{l,+}^j(\cdot,0)\|_{BV(\mathbb{R})} \le A. \tag{5.11}$$

γ_j in (5.9) satisfies

$$\gamma_j \le \sqrt{\frac{t_{n+1}}{2e} \frac{\Delta x}{\Delta t}} \equiv \gamma. \tag{5.12}$$

Substituting (5.11), (5.12) into (5.8) gives

$$\|v^j_{l,+}(\cdot,t_n)-u^j_{l,+}(\cdot,t_n)\|_{l^1(\mathbb{R})}\le A\left[\gamma\sqrt{\Delta x}+3\Delta x\right]. \tag{5.13}$$

In comparison with schemes (4.13), (4.21), (4.22) and (5.6), (5.7), (5.4), (4.7), one can check that, for $I_0+1\le j\le M$,

$$g(x,\xi,t_n)=v^j_{l,+}(x,t_n),\quad \text{for } \xi_{j-\frac12}<\xi<\xi_{j+\frac12},\ x_{\frac12}<x<0. \tag{5.14}$$

From (5.2), (5.14), (5.13), (5.5), (5.4) and (4.8) one has, by the triangle inequality,

$$\begin{aligned} E^+_l \le & \sum_{j=I_0+1}^{M}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\int_{x_{\frac12}}^{0}\left|v^j_{l,+}(x,t_n)-u^j_{l,+}(x,t_n)\right|dxd\xi \\ & +\sum_{j=I_0+1}^{M}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\int_{x_{\frac12}}^{0}\left|u^j_{l,+}(x,t_n)-f(x,\xi,t_n)\right|dxd\xi \equiv E^{+,1}_l+E^{+,2}_l, \end{aligned} \tag{5.15}$$

where

$$E^{+,1}_l \le \xi_{M+\frac12}A\left[\gamma\sqrt{\Delta x}+3\Delta x\right], \tag{5.16}$$

$$\begin{aligned} E^{+,2}_l = & \sum_{j=I_0+1}^{M}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\int_{x_{\frac12}}^{0}\left|\frac{1}{\Delta\xi}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\widehat{f}_0(x-\xi_j t_n,\xi')d\xi'-\widehat{f}_0(x-\xi t_n,\xi)\right|dxd\xi \\ \le & \sum_{j=I_0+1}^{M}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\int_{x_{\frac12}}^{0}\left|\frac{1}{\Delta\xi}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\left[\widehat{f}_0(x-\xi_j t_n,\xi')-\widehat{f}_0(x-\xi_j t_n,\xi)\right]d\xi'\right|dxd\xi \\ & +\sum_{j=I_0+1}^{M}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\int_{x_{\frac12}}^{0}\left|\widehat{f}_0(x-\xi_j t_n,\xi)-\widehat{f}_0(x-\xi t_n,\xi)\right|dxd\xi. \end{aligned} \tag{5.17}$$

According to the definition of the BV norm (3.10) and condition (5.10), one has

$$\int_{x_{\frac12}}^{0}\left|\widehat{f}_0(x-\xi_j t_n,\xi)-\widehat{f}_0(x-\xi t_n,\xi)\right|dx\le\|\widehat{f}_0(\cdot,\xi)\|_{BV(\mathbb{R})}|\xi-\xi_j|t_n\le A|\xi-\xi_j|t_n. \tag{5.18}$$

Applying the Lipschitz condition (4.4) and (5.18) to (5.17) yields

$$E^{+,2}_l\le\xi_{M+\frac12}\left|x_{\frac12}\right|B\Delta\xi+\sum_{j=I_0+1}^{M}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}|\xi-\xi_j|\,t_nAd\xi\le\xi_{M+\frac12}\left[\left|x_{\frac12}\right|B+\frac{t_n}{2}A\right]\Delta\xi. \tag{5.19}$$

Combining (5.15), (5.16) and (5.19) leads to

$$E^+_l\le\xi_{M+\frac12}A\left[\gamma\sqrt{\Delta x}+3\Delta x\right]+\xi_{M+\frac12}\left[\left|x_{\frac12}\right|B+\frac{t_n}{2}A\right]\Delta\xi=\xi_{M+\frac12}A\gamma\sqrt{\Delta x}+O(\Delta x). \tag{5.20}$$

Similarly, for E^-_r one can deduce

$$\begin{aligned} E^-_r \le & \left|\xi_{\frac12}+\sqrt{2D}\right|A\left[\gamma\sqrt{\Delta x}+3\Delta x\right]+\left|\xi_{\frac12}+\sqrt{2D}\right|\left[x_{N+\frac12}B+\frac{t_n}{2}A\right]\Delta\xi \\ = & \left|\xi_{\frac12}+\sqrt{2D}\right|A\gamma\sqrt{\Delta x}+O(\Delta x). \end{aligned} \tag{5.21}$$

5.2. The upper bound for E_r^r. For E_r^r one has

$$E_r^r = \sum_{j=I_0+1}^{I_+} \int_0^{x_{N+\frac{1}{2}}} \left(\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} |g(x,\xi,t_n) - f(x,\xi,t_n)|\, d\xi + \int_{-\xi_{j+\frac{1}{2}}}^{-\xi_{j-\frac{1}{2}}} |g(x,\xi,t_n) - f(x,\xi,t_n)|\, d\xi \right) dx. \tag{5.22}$$

For $0 \le \xi \le \sqrt{2D}$, define the function

$$f_1(x,\xi) = \begin{cases} \widehat{f}_0(x,\xi) & x \ge 0 \\ \widehat{f}_0(-x,-\xi) & x < 0 \end{cases} \quad \text{for } x \in \mathbb{R},\ 0 \le \xi \le \sqrt{2D}. \tag{5.23}$$

For $I_0 + 1 \le j \le I_+$, consider the linear advection equation

$$\frac{\partial u^j_{r,r}}{\partial t} + \xi_j \frac{\partial u^j_{r,r}}{\partial x} = 0, \qquad t > 0, x \in \mathbb{R}, \tag{5.24}$$

$$u^j_{r,r}|_{t=0} = \frac{1}{\Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f_1(x,\xi) d\xi. \tag{5.25}$$

The exact solution to (5.24),(5.25) is simply

$$u^j_{r,r}(x,t) = u^j_{r,r}(x - \xi_j t, 0).$$

The upwind scheme for (5.24) is

$$v_i^{n+1} = (1-\mu_j) v_i^n + \mu_j v_{i-1}^n, \tag{5.26}$$

$$v_i^0 = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u^j_{r,r}(x,0) dx. \tag{5.27}$$

Define

$$v^j_{r,r}(x,t) = v_i^n, \qquad \text{for } (x,t) \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}) \times [t_n, t_{n+1}).$$

Applying Theorem 3.1, the l^1-error between $v^j_{r,r}(x,t_n)$ and $u^j_{r,r}(x,t_n)$ is given by

$$\|v^j_{r,r}(\cdot,t_n) - u^j_{r,r}(\cdot,t_n)\|_{l^1(\mathbb{R})} \le \|u^j_{r,r}(\cdot,0)\|_{BV(\mathbb{R})} \left[\gamma_j \sqrt{\Delta x} + \Delta x\right], \tag{5.28}$$

where γ_j is given by (5.9).

From definition (5.23) and conditions (4.3), (4.4) one has, for $0 \le \xi \le \sqrt{2D}$,

$$\begin{aligned} \|f_1(\cdot,\xi)\|_{BV(\mathbb{R})} &\le \|\widehat{f}_0(.,\xi)\|_{BV([0,x_{N+\frac{1}{2}}])} + \|\widehat{f}_0(.,-\xi)\|_{BV([0,x_{N+\frac{1}{2}}])} + \left|\widehat{f}_0(0,-\xi) - \widehat{f}_0(0,\xi)\right| \\ &\le 2A + 2\sqrt{2D}B. \end{aligned} \tag{5.29}$$

Therefore

$$\|u^j_{r,r}(\cdot,0)\|_{BV(\mathbb{R})} \le 2A + 2\sqrt{2D}B. \tag{5.30}$$

Combining (5.28), (5.30) and (5.12) gives

$$\|v^j_{r,r}(\cdot,t_n) - u^j_{r,r}(\cdot,t_n)\|_{l^1(\mathbb{R})} \le \left(2A + 2\sqrt{2D}B\right) \left[\gamma \sqrt{\Delta x} + \Delta x\right] \tag{5.31}$$

with γ defined in (5.12).

In comparison with schemes (4.13), (4.14), (4.16), (4.19), (4.21), (4.23) and (5.26), (5.27), (5.25), (5.23), (4.7), one can check that, for $I_0+1 \le j \le I_+$,

$$g(x,\xi,t_n) = \begin{cases} v^j_{r,r}(x,t_n), & \text{for } 0<x<x_{N+\frac12},\ \xi_{j-\frac12}<\xi<\xi_{j+\frac12} \\ v^j_{r,r}(-x,t_n), & \text{a.e. for } 0<x<x_{N+\frac12},\ -\xi_{j+\frac12}<\xi<-\xi_{j-\frac12} \end{cases}. \tag{5.32}$$

The second part of (5.32) holds except possibly at the cell interfaces.

From (5.22), (5.32), (4.9) and (5.23), one arrives at

$$\begin{aligned} E^r_r = & \sum_{j=I_0+1}^{I_+} \int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}} \int_0^{x_{N+\frac12}} \left| v^j_{r,r}(x,t_n) - f_1(x-\xi t_n,\xi)\right| dxd\xi \\ & + \sum_{j=I_0+1}^{I_+} \int_{-\xi_{j+\frac12}}^{-\xi_{j-\frac12}} \int_0^{x_{N+\frac12}} \left| v^j_{r,r}(-x,t_n) - f_1(-x+\xi t_n,-\xi)\right| dxd\xi \\ = & \sum_{j=I_0+1}^{I_+} \int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}} \int_{-x_{N+\frac12}}^{x_{N+\frac12}} \left| v^j_{r,r}(x,t_n) - f_1(x-\xi t_n,\xi)\right| dxd\xi. \end{aligned}$$

From definition (5.23) and condition (4.4), $f_1(x,\xi)$ satisfies the Lipschitz condition in ξ with the Lipschitz constant B. Utilizing this and (5.29), (5.31), similar to the deduction from (5.15) to (5.20), one obtains

$$\begin{aligned} E^r_r \le & \sqrt{2D}\left(2A+2\sqrt{2D}B\right)\left[\gamma\sqrt{\Delta x}+\Delta x\right] + \sqrt{2D}\left[2x_{N+\frac12}B + t_n\left(A+\sqrt{2D}B\right)\right]\Delta\xi \\ = & \sqrt{2D}\left(2A+2\sqrt{2D}B\right)\gamma\sqrt{\Delta x} + O(\Delta x). \end{aligned} \tag{5.33}$$

5.3. The upper bound for E^+_r. For E^+_r one has

$$E^+_r = \sum_{j=I_++1}^{M} \int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}} \int_0^{x_{N+\frac12}} |g(x,\xi,t_n) - f(x,\xi,t_n)|\, dxd\xi. \tag{5.34}$$

For $I_+ + 1 \le j \le M$, consider two linear advection equations

$$\frac{\partial u^j_{r,+,p}}{\partial t} + c_{+,p}\frac{\partial u^j_{r,+,p}}{\partial x} = 0, \qquad t>0, x\in\mathbb{R}, \tag{5.35}$$

$$c_{+,p}(x) = \begin{cases} \xi_{J_{j,p}} & x<0 \\ \xi_j & x>0 \end{cases}, \tag{5.36}$$

$$u^j_{r,+,p}|_{t=0} = \frac{1}{\Delta\xi}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}} f^j_{r,+,p}(x,\xi)d\xi, \tag{5.37}$$

$$f^j_{r,+,p}(x,\xi) = \begin{cases} \widehat{f}_0(x,\xi-\xi_j+\xi_{J_{j,p}}) & x<0 \\ \widehat{f}_0(x,\xi) & x\ge 0 \end{cases} \tag{5.38}$$

for $p=1,2$, where

$$J_{j,p} = d_j + p - 1, \quad p=1,2 \tag{5.39}$$

with d_j defined in (4.18).

The exact solutions to (5.35)-(5.38) are given by

$$u^j_{r,+,p}(x,t)=\begin{cases} u^j_{r,+,p}\left(x-\xi_{J_{j,p}}t,0\right) & x<0\\ u^j_{r,+,p}\left(\frac{\xi_{J_{j,p}}}{\xi_j}x-\xi_{J_{j,p}}t,0\right) & 0\le x<\xi_j t\\ u^j_{r,+,p}\left(x-\xi_j t,0\right) & x\ge \xi_j t\end{cases}, \quad p=1,2. \tag{5.40}$$

The upwind schemes for (5.35) are

$$v_i^{n+1,j,p}=\begin{cases}(1-\mu_{J_{j,p}})v_i^{n,j,p}+\mu_{J_{j,p}}v_{i-1}^{n,j,p}, & \text{if } x_i<0\\ (1-\mu_j)v_i^{n,j,p}+\mu_j v_{i-1}^{n,j,p}, & \text{if } x_i>0\end{cases}, \tag{5.41}$$

$$v_i^{0,j,p}=\frac{1}{\Delta x}\int_{x_{i-\frac12}}^{x_{i+\frac12}}u^j_{r,+,p}(x,0)dx \tag{5.42}$$

for $p=1,2$.

Define

$$v^j_{r,+,p}(x,t)=v_i^{n,j,p}, \qquad \text{for } (x,t)\in[x_{i-\frac12},x_{i+\frac12})\times[t_n,t_{n+1}), \quad p=1,2.$$

We present some Lemmas before giving estimates for E_r^+.

Lemma 5.1. *If the mesh size satisfies* (4.24), *then*

$$\frac{\xi_j}{\xi_{J_{j,p}}}\le\frac{\xi_{M+\frac12}}{(2D)^{\frac14}\sqrt{(j-I_+-\frac12)\Delta\xi}}, \quad p=1,2, \tag{5.43}$$

$$\frac{\xi_j}{\sqrt{(\xi_j)^2-2D}}\le\frac{\xi_{M+\frac12}}{\sqrt{2}(2D)^{\frac14}\sqrt{(j-I_+-\frac12)\Delta\xi}} \tag{5.44}$$

for $I_++1\le j\le M$.

Proof. We give proof for (5.43), the proof for (5.44)is similar. One has for $I_++1\le j\le M$

$$\frac{\xi_j}{\xi_{J_{j,p}}}\le\frac{\sqrt{2D}+(j-I_+-\frac12)\Delta\xi}{\sqrt{2\sqrt{2D}(j-I_+-\frac12)\Delta\xi+\left[(j-I_+-\frac12)\Delta\xi\right]^2}-\Delta\xi}\le\frac{\xi_{M+\frac12}}{\sqrt{2\sqrt{2D}(j-I_+-\frac12)\Delta\xi}-\Delta\xi}.$$

Utilizing the mesh size condition (4.24) then obtains (5.43). ∎

Lemma 5.2.

$$\left|\sqrt{\xi^2-2D}-\xi'\right|\le\frac{\xi_j\Delta\xi}{\sqrt{(\xi_j)^2-2D}}+\frac32\Delta\xi, \quad \forall\xi_{j-\frac12}\le\xi\le\xi_{j+\frac12},\ \xi_{d_j-\frac12}\le\xi'\le\xi_{d_j+\frac32} \tag{5.45}$$

for $I_++1\le j\le M$.

Proof. Observe that $\forall\xi$, $\xi_{j-\frac12}\le\xi\le\xi_{j+\frac12}$

$$\left|\sqrt{\xi^2-2D}-\sqrt{(\xi_j)^2-2D}\right|\le\sqrt{(\xi_j)^2-2D}-\sqrt{\left(\xi_{j-\frac12}\right)^2-2D}\le\frac{(\xi_j)^2-\left(\xi_j-\frac12\Delta\xi\right)^2}{\sqrt{(\xi_j)^2-2D}}\le\frac{\xi_j\Delta\xi}{\sqrt{(\xi_j)^2-2D}}.$$

Therefore

$$\left|\sqrt{\xi^2-2D}-\xi_{J_{j,p}}\right| \le \frac{\xi_j\Delta\xi}{\sqrt{\left(\xi_j\right)^2-2D}}+\Delta\xi, \quad p=1,2. \tag{5.46}$$

Thus (5.45) can be deduced. □

LEMMA 5.3.

Define functions

$$H_{\xi}^{+,j,p}(x)=\begin{cases} \left(\frac{\sqrt{\xi^2-2D}}{\xi}x-\sqrt{\xi^2-2D}\,t_n+\xi_{J_{j,p}}t_n\right)\frac{\xi_j}{\xi_{J_{j,p}}} & x<\xi t_n \\ x-\xi t_n+\xi_j t_n & x\ge \xi t_n \end{cases}.$$

Then

$$\left|H_{\xi}^{+,j,p}(x)-x\right|\le E_H^j \tag{5.47}$$

for $x\ge 0$, $\xi_{j-\frac12}\le\xi\le\xi_{j+\frac12}, I_+ +1\le j\le M, p=1,2,$ *where*

$$E_H^j=\frac52\frac{t_n\xi_{M+\frac12}}{(2D)^{\frac14}}\frac{\Delta\xi}{\sqrt{(j-I_+-\frac12)\Delta\xi}}+\frac{\sqrt2\left(\xi_{M+\frac12}\right)^2t_n}{\sqrt{2D}}\frac{\Delta\xi}{(j-I_+-\frac12)\Delta\xi}. \tag{5.48}$$

Proof. Clearly,

$$\left|H_{\xi}^{+,j,p}(x)-x\right|\le\frac{\Delta\xi}{2}t_n,\quad \text{for } x\ge\xi t_n,\ \xi_{j-\frac12}\le\xi\le\xi_{j+\frac12}. \tag{5.49}$$

For $0\le x<\xi t_n$,

$$\begin{aligned}\left|H_{\xi}^{+,j,p}(x)-x\right| &= \left|\frac{\sqrt{\xi^2-2D}}{\xi}x-\frac{\xi_{J_{j,p}}}{\xi_j}x+\left(\xi_{J_{j,p}}-\sqrt{\xi^2-2D}\right)t_n\right|\frac{\xi_j}{\xi_{J_{j,p}}}\\
&\le\left[\left(\frac{\xi_{J_{j,p}}\left|\xi-\xi_j\right|}{\xi\xi_j}+\frac{\left|\sqrt{\xi^2-2D}-\xi_{J_{j,p}}\right|}{\xi}\right)x+\left|\sqrt{\xi^2-2D}-\xi_{J_{j,p}}\right|t_n\right]\frac{\xi_j}{\xi_{J_{j,p}}}\\
&\le\left(2\left|\sqrt{\xi^2-2D}-\xi_{J_{j,p}}\right|+\left|\xi-\xi_j\right|\right)t_n\frac{\xi_j}{\xi_{J_{j,p}}}.\end{aligned} \tag{5.50}$$

Combining (5.49) and (5.50), applying (5.46) and Lemma 5.1 to (5.50) then leads to the estimates (5.47). □

LEMMA 5.4.

Define functions

$$F_p^j(\xi)=\int_0^{x_{N+\frac12}}\left|\widetilde{f}_{r,+,p}^j(x,\xi,t_n)-\widehat{f}_{r,+}(x,\xi,t_n)\right|dx, \tag{5.51}$$

for $\xi_{j-\frac12}\le\xi\le\xi_{j+\frac12}, I_+ +1\le j\le M, p=1,2,$ *where*

$$\widetilde{f}_{r,+,p}^j(x,\xi,t)=\begin{cases}\widehat{f}_0\left(\frac{\xi_{J_{j,p}}}{\xi_j}x-\xi_{J_{j,p}}t,\sqrt{\xi^2-2D}\right) & x<\xi_j t\\ \widehat{f}_0\left(x-\xi_j t,\xi\right) & x\ge\xi_j t\end{cases}, \tag{5.52}$$

$$\widehat{f}_{r,+}(x,\xi,t) = \begin{cases} \widehat{f}_0\left(\frac{\sqrt{\xi^2-2D}}{\xi}x - \sqrt{\xi^2-2D}\,t, \sqrt{\xi^2-2D}\right) & x < \xi t \\ \widehat{f}_0\left(x-\xi t, \xi\right) & x \geq \xi t \end{cases}. \quad (5.53)$$

Then

$$F_p^j(\xi) \leq 2\left(2A + \sqrt{2D}B\right)E_H^j. \quad (5.54)$$

with E_H^j *defined in* (5.48).

Proof. From the definition (5.52) and the conditions (4.3), (4.4), one obtains

$$\|\widetilde{f}^j_{r,+,p}(\cdot,\xi,t)\|_{BV(\mathbb{R})} \leq 2A + \sqrt{2D}B. \quad (5.55)$$

We use the fact that

$$\widehat{f}_{r,+}(x,\xi,t_n) = \widetilde{f}^j_{r,+,p}\left(H_\xi^{+,j,p}(x),\xi,t_n\right), \quad x\in\mathbb{R},\ p=1,2. \quad (5.56)$$

From (5.51), (5.56) and (5.55), applying Lemma 5.3 and Lemma A.1 in the Appendix then leads to (5.54). □

We now give estimates for E_r^+. In comparison with schemes (4.13), (4.15), (4.18), (4.21), (4.22) and (5.41), (5.42), (5.37), (5.38), (4.7) one can check that, for $I_+ + 1 \leq j \leq M$,

$$g(x,\xi,t_n) = \sum_{p=1}^{2} c_{j,p} v^j_{r,+,p}(x,t_n), \quad \text{for } \xi_{j-\frac{1}{2}} < \xi < \xi_{j+\frac{1}{2}},\ 0 < x < x_{N+\frac{1}{2}}. \quad (5.57)$$

Together with (5.34), (5.57) and the expression (4.10) of $f(x,\xi,t_n)$ in D_r^+, one obtains by triangle inequality

$$E_r^+ \leq E_r^{+,1} + E_r^{+,2} + E_r^{+,3}, \quad (5.58)$$

where

$$E_r^{+,1} = \sum_{j=I_++1}^{M}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}}\int_0^{x_{N+\frac{1}{2}}}\sum_{p=1}^{2} c_{j,p}\left|v^j_{r,+,p}(x,t_n) - u^j_{r,+,p}(x,t_n)\right| dx d\xi, \quad (5.59)$$

$$E_r^{+,2} = \sum_{j=I_++1}^{M}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}}\int_0^{x_{N+\frac{1}{2}}}\sum_{p=1}^{2} c_{j,p}\left|u^j_{r,+,p}(x,t_n) - \widetilde{f}^j_{r,+,p}(x,\xi,t_n)\right| dx d\xi, \quad (5.60)$$

$$E_r^{+,3} = \sum_{j=I_++1}^{M}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}}\int_0^{x_{N+\frac{1}{2}}}\sum_{p=1}^{2} c_{j,p}\left|\widetilde{f}^j_{r,+,p}(x,\xi,t_n) - \widehat{f}_{r,+}(x,\xi,t_n)\right| dx d\xi. \quad (5.61)$$

We then estimate these three terms respectively.

Applying Theorem 3.1, the l^1-error between $v^j_{r,+,p}$ and $u^j_{r,+,p}$, $p=1,2$ are given by

$$\|v^j_{r,+,p}(\cdot,t_n) - u^j_{r,+,p}(\cdot,t_n)\|_{l^1(\mathbb{R})} \leq \|u^j_{r,+,p}(\cdot,0)\|_{BV(\mathbb{R})}\left[\Delta x + \left(\gamma\sqrt{\Delta x} + 2\Delta x\right)\frac{\xi_j}{\xi_{J_{j,p}}}\right], \quad (5.62)$$

where γ is given by (5.12).

For $I_+ + 1 \le j \le M$, the index d_j defined in (4.18) satisfies

$$\xi_j - \sqrt{2D} \le \xi_{d_j} < \xi_{d_j+1} \le \xi_j. \tag{5.63}$$

From definitions (5.38) and conditions (4.3), (4.4), (5.63) one has, for $p = 1, 2$,

$$\|f^j_{r,+,p}(\cdot, \xi)\|_{BV(\mathbb{R})} \le 2A + \sqrt{2D}B, \qquad \xi_{j-\frac{1}{2}} \le \xi \le \xi_{j+\frac{1}{2}}.$$

Therefore

$$\|u^j_{r,+,p}(\cdot, 0)\|_{BV(\mathbb{R})} \le 2A + \sqrt{2D}B. \tag{5.64}$$

Utilizing (5.62), (5.64) and (5.43) for (5.59), by summation of j and using the inequality

$$\sum_{j=I_++1}^{M} \frac{\Delta\xi}{\sqrt{(j - I_+ - \frac{1}{2})\Delta\xi}} \le 2\sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}}, \tag{5.65}$$

one obtains

$$E^{+,1}_r \le \left(4A + 2\sqrt{2D}B\right) \frac{\xi_{M+\frac{1}{2}}}{(2D)^{\frac{1}{4}}} \sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}}\gamma\sqrt{\Delta x} + O(\Delta x). \tag{5.66}$$

Using Lemma 5.2 and the fact that

$$|\xi - \xi'| \le \Delta\xi \quad \forall \xi_{j-\frac{1}{2}} \le \xi, \xi' \le \xi_{j+\frac{1}{2}}, \tag{5.67}$$

and condition (4.4), from definitions (5.37), (5.38), (5.40) and (5.52) one has

$$\left|u^j_{r,+,p}(x, t_n) - \widetilde{f}^j_{r,+,p}(x, \xi, t_n)\right| \le B\left[\frac{\xi_j \Delta\xi}{\sqrt{(\xi_j)^2 - 2D}} + \frac{3}{2}\Delta\xi\right] \tag{5.68}$$

for $x \ge 0, \xi_{j-\frac{1}{2}} \le \xi \le \xi_{j+\frac{1}{2}}$.

Utilizing (5.68) and (5.44) for (5.60) and using the inequality (5.65) one obtains

$$E^{+,2}_r \le x_{N+\frac{1}{2}} B\left[\left(\xi_{M+\frac{1}{2}} - \sqrt{2D}\right)\frac{3}{2} + \frac{\xi_{M+\frac{1}{2}}}{\sqrt{2}(2D)^{\frac{1}{4}}} 2\sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}}\right]\Delta\xi. \tag{5.69}$$

Applying Lemma 5.4 to (5.61), using the inequality (5.65) and

$$\sum_{j=I_++1}^{M} \frac{\Delta\xi}{(j - I_+ - \frac{1}{2})\Delta\xi} \le 2 + \ln\left(\xi_{M+\frac{1}{2}} - \sqrt{2D}\right) + \ln\left(\frac{1}{\Delta\xi}\right), \tag{5.70}$$

one obtains

$$E^{+,3}_r \le \left(4A + 2\sqrt{2D}B\right) \frac{\left(\xi_{M+\frac{1}{2}}\right)^2 t_n \lambda^\xi_x}{\sqrt{D}} \ln\left(\frac{1}{\Delta x}\right)\Delta x + O(\Delta x). \tag{5.71}$$

The inequalities (5.65) and (5.70) are obtained using the fact that the midpoint rule is less than the exact integral when the integrand is convex. The right hand side of the inequality (5.70) contains the ln(·) term which results in the ln(·) term appearing in the estimate (4.25) in Theorem 4.1.

Combining (5.58), (5.66), (5.69), (5.71) gives

$$E_r^+ \leq \left(4A + 2\sqrt{2D}B\right) \frac{\xi_{M+\frac{1}{2}}}{(2D)^{\frac{1}{4}}} \sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}\gamma\sqrt{\Delta x}}$$
$$+ \left(4A + 2\sqrt{2D}B\right) \frac{\left(\xi_{M+\frac{1}{2}}\right)^2 t_n \lambda_x^\xi}{\sqrt{D}} \ln\left(\frac{1}{\Delta x}\right)\Delta x + O(\Delta x). \qquad (5.72)$$

5.4. The upper bound for E_l^-. For E_l^- one has

$$E_l^- = \sum_{j=I_b}^{I_0} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \int_{x_{\frac{1}{2}}}^{0} |g(x,\xi,t_n) - f(x,\xi,t_n)|\, dx d\xi. \qquad (5.73)$$

For $I_b \leq j \leq I_0$, consider two linear advection equations

$$\frac{\partial u_{l,-,p}^j}{\partial t} + c_{-,p}\frac{\partial u_{l,-,p}^j}{\partial x} = 0, \qquad t > 0, x \in \mathbb{R}, \qquad (5.74)$$

$$c_{-,p}(x) = \begin{cases} \left|\xi_{J_{j,p}}\right| & x < 0 \\ |\xi_j| & x > 0 \end{cases}, \qquad (5.75)$$

$$u_{l,-,p}^j|_{t=0} = \frac{1}{\Delta\xi}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f_{l,-,p}^j(x,\xi)d\xi, \qquad (5.76)$$

$$f_{l,-,p}^j(x,\xi) = \begin{cases} \widehat{f}_0(-x, \xi - \xi_j + \xi_{J_{j,p}}) & x < 0 \\ \widehat{f}_0(-x,\xi) & x \geq 0 \end{cases} \qquad (5.77)$$

for $p = 1,2$, where $J_{j,p}$ is defined in (5.39) with d_j defined in (4.20).

The exact solutions to (5.74)-(5.77) are given by

$$u_{l,-,p}^j(x,t) = \begin{cases} u_{l,-,p}^j\left(x - \left|\xi_{J_{j,p}}\right| t, 0\right) & x < 0 \\ u_{l,-,p}^j\left(\left|\frac{\xi_{J_{j,p}}}{\xi_j}\right| x - \left|\xi_{J_{j,p}}\right| t, 0\right) & 0 \leq x < |\xi_j|\, t \\ u_{l,-,p}^j\left(x - |\xi_j|\, t, 0\right) & x \geq |\xi_j|\, t \end{cases}, \quad p = 1,2. \qquad (5.78)$$

The upwind schemes for (5.74) are

$$v_i^{n+1,j,p} = \begin{cases} (1-\mu_{J_{j,p}})v_i^{n,j,p} + \mu_{J_{j,p}}v_{i-1}^{n,j,p}, & \text{if } x_i < 0 \\ (1-\mu_j)v_i^{n,j,p} + \mu_j v_{i-1}^{n,j,p}, & \text{if } x_i > 0 \end{cases}, \qquad (5.79)$$

$$v_i^{0,j,p} = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_{l,-,p}^j(x,0)dx \qquad (5.80)$$

for $p = 1,2$.

Define

$$v_{l,-,p}^j(x,t) = v_i^{n,j,p}, \qquad \text{for } (x,t) \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}) \times [t_n, t_{n+1}), \;\; p = 1,2.$$

We have the following Lemmas

LEMMA 5.5.

$$\left|\sqrt{\xi^2+2D}+\xi'\right| \le 2\Delta\xi, \quad \forall \xi_{j-\frac{1}{2}} \le \xi \le \xi_{j+\frac{1}{2}},\ \xi_{d_j-\frac{1}{2}} \le \xi' \le \xi_{d_j+\frac{3}{2}} \tag{5.81}$$

for $I_b \le j \le I_0$.

This Lemma can be directly checked and the proof is omitted.

LEMMA 5.6.

Define functions

$$H_\xi^{-,j,p}(x) = \begin{cases} -\left(\frac{\xi_{J_{j,p}}}{\xi_j}x - \xi_{J_{j,p}}t_n - \sqrt{\xi^2+2D}\,t_n\right)\frac{\xi}{\sqrt{\xi^2+2D}} & x > \xi_j t_n \\ x - \xi_j t_n + \xi t_n & x \le \xi_j t_n \end{cases}.$$

Then

$$\left|H_\xi^{-,j,p}(x) - x\right| \le \frac{7}{2}\Delta\xi t_n \tag{5.82}$$

for $x \le 0$, $\xi_{j-\frac{1}{2}} \le \xi \le \xi_{j+\frac{1}{2}}, I_b \le j \le I_0, p = 1,2$.

This Lemma can be proved using similar technique for proving Lemma 5.3 and we omit the detailed proof.

LEMMA 5.7.

Define functions

$$G_p^j(\xi) = \int_{x_{\frac{1}{2}}}^0 \left|\widetilde{f}_{l,-,p}^j(x,\xi,t_n) - \widehat{f}_{l,-}(x,\xi,t_n)\right| dx, \tag{5.83}$$

for $\xi_{j-\frac{1}{2}} \le \xi \le \xi_{j+\frac{1}{2}}, I_b \le j \le I_0, p = 1,2,$ *where*

$$\widetilde{f}_{l,-,p}^j(x,\xi,t) = \begin{cases} \widehat{f}_0\left(\frac{\xi_{J_{j,p}}}{\xi_j}x - \xi_{J_{j,p}}t, -\sqrt{\xi^2+2D}\right) & x > \xi_j t \\ \widehat{f}_0\left(x - \xi_j t, \xi\right) & x \le \xi_j t \end{cases}, \tag{5.84}$$

$$\widehat{f}_{l,-}(x,\xi,t) = \begin{cases} \widehat{f}_0\left(-\frac{\sqrt{\xi^2+2D}}{\xi}x + \sqrt{\xi^2+2D}\,t, -\sqrt{\xi^2+2D}\right) & x > \xi t \\ \widehat{f}_0\left(x - \xi t, \xi\right) & x \le \xi t \end{cases}. \tag{5.85}$$

Then

$$G_p^j(\xi) \le \left(2A + \sqrt{2D}B\right) 7\Delta\xi t_n. \tag{5.86}$$

Proof. From definition (5.85) and conditions (4.3), (4.4) one obtains

$$\|\widehat{f}_{l,-}(\cdot,\xi,t)\|_{BV(\mathbb{R})} \le 2A + \sqrt{2D}B. \tag{5.87}$$

We use the fact that

$$\widetilde{f}_{l,-,p}^j(x,\xi,t_n) = \widehat{f}_{l,-}\left(H_\xi^{-,j,p}(x),\xi,t_n\right), \quad x \in \mathbb{R},\ p = 1,2. \tag{5.88}$$

From (5.83), (5.88) and (5.87), applying Lemma 5.6 and Lemma A.1 in the Appendix gives (5.86). ∎

We now give estimates for E_l^-. In comparison with schemes (4.14), (4.17), (4.20), (4.21), (4.23) and (5.79), (5.80), (5.76), (5.77), (4.7), one can check that for $I_b \le j \le I_0$

$$g(x,\xi,t_n) = \sum_{p=1}^{2} c_{j,p} v_{l,-,p}^j(-x,t_n), \quad \text{a.e. for } \xi_{j-\frac{1}{2}} < \xi < \xi_{j+\frac{1}{2}},\ x_{\frac{1}{2}} < x < 0. \tag{5.89}$$

Together with (5.73), (5.89) and the expression (4.11) of $f(x,\xi,t_n)$ in D_l^-, one obtains

$$E_l^- \le E_l^{-,1} + E_l^{-,2} + E_l^{-,3}, \tag{5.90}$$

where

$$E_l^{-,1} = \sum_{j=I_b}^{I_0} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \int_{x_{\frac{1}{2}}}^{0} \sum_{p=1}^{2} c_{j,p} \left| v_{l,-,p}^j(-x,t_n) - u_{l,-,p}^j(-x,t_n) \right| dx d\xi, \tag{5.91}$$

$$E_l^{-,2} = \sum_{j=I_b}^{I_0} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \int_{x_{\frac{1}{2}}}^{0} \sum_{p=1}^{2} c_{j,p} \left| u_{l,-,p}^j(-x,t_n) - \widetilde{f}_{l,-,p}^j(x,\xi,t_n) \right| dx d\xi, \tag{5.92}$$

$$E_l^{-,3} = \sum_{j=I_b}^{I_0} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \int_{x_{\frac{1}{2}}}^{0} \sum_{p=1}^{2} c_{j,p} \left| \widetilde{f}_{l,-,p}^j(x,\xi,t_n) - \widehat{f}_{l,-}(x,\xi,t_n) \right| dx d\xi. \tag{5.93}$$

Applying Theorem 3.1, the l^1-error between $v_{l,-,p}^j$ and $u_{l,-,p}^j$, $p = 1,2$ are given by

$$\|v_{l,-,p}^j(\cdot,t_n) - u_{l,-,p}^j(\cdot,t_n)\|_{l^1(\mathbb{R})} \le \|u_{l,-,p}^j(\cdot,0)\|_{BV(\mathbb{R})} \left[\sqrt{\frac{2t_{n+1}}{e}} \frac{|\xi_{J_{j,p}}|}{\sqrt{|\xi_j|}} \sqrt{\Delta x} + \left(2 + \left|\frac{\xi_{J_{j,p}}}{\xi_j}\right|\right) \Delta x \right]. \tag{5.94}$$

Similar to the derivation of (5.64), one has

$$\|u_{l,-,p}^j(\cdot,0)\|_{BV(\mathbb{R})} \le 2A + \sqrt{2D}B. \tag{5.95}$$

Applying (5.94) and (5.95) to (5.91), by summation of j and using the inequalities (5.65) and (5.70) one obtains

$$\begin{aligned} E_l^{-,1} \le & \left(4A + 2\sqrt{2D}B\right) \sqrt{\frac{2t_{n+1}}{e}} \left|\xi_{\frac{1}{2}}\right| \left[\left(\xi_{\frac{1}{2}}\right)^2 - 2D \right]^{\frac{1}{4}} \sqrt{\Delta x} \\ & + \left(2A + \sqrt{2D}B\right) \left|\xi_{\frac{1}{2}}\right| \ln\left(\frac{1}{\Delta x}\right) \Delta x + O(\Delta x). \end{aligned} \tag{5.96}$$

Using Lemma 5.5, (5.67) and condition (4.4), from the definitions (5.76), (5.77), (5.78) and (5.84), one has

$$\left| u_{l,-,p}^j(-x,t_n) - \widetilde{f}_{l,-,p}^j(x,\xi,t_n) \right| \le 2B\Delta\xi,$$

for $x \le 0, \xi_{j-\frac{1}{2}} \le \xi \le \xi_{j+\frac{1}{2}}$.

Thus one has

$$E_l^{-,2} \le \left|\xi_{I_b-\frac{1}{2}}\right| \left|x_{\frac{1}{2}}\right| 2B\Delta\xi. \tag{5.97}$$

Applying Lemma 5.7 to (5.93) yields

$$E_l^{-,3} \le 7\left(2A + \sqrt{2D}B\right)\left|\xi_{I_b-\frac{1}{2}}\right| t_n \Delta\xi. \tag{5.98}$$

Combining (5.90), (5.96), (5.97), (5.98) leads to

$$\begin{aligned} E_l^- \le & \left(4A + 2\sqrt{2D}B\right)\sqrt{\frac{2t_{n+1}}{e}}\left|\xi_{\frac{1}{2}}\right|\left[\left(\xi_{\frac{1}{2}}\right)^2 - 2D\right]^{\frac{1}{4}}\sqrt{\Delta x} \\ & + \left(2A + \sqrt{2D}B\right)\left|\xi_{\frac{1}{2}}\right| \ln\left(\frac{1}{\Delta x}\right)\Delta x + O(\Delta x). \end{aligned} \tag{5.99}$$

Finally combining (5.1), (5.20), (5.21), (5.33), (5.72), (5.99), (5.12) completes the proof for Theorem 4.1.

REMARK 5.1. *The error terms derived in* (4.25) *include the halfth order terms and the* $\ln\left(\frac{1}{\Delta x}\right)\Delta x$ *terms. Thus the leading error terms are of halfth order and Scheme I has a halfth order convergence rate. Note that this is sharp, since even for the discontinuous solution to linear hyperbolic equation with a smooth coefficient, one cannot expect a better convergence order in the* l^1*-norm [24].*

6. Conclusion. In this paper we derived the l^1-error estimates for a Hamiltonian-preserving scheme, developed in [11], for the Liouville equation with a piecewise constant potential in one space dimension. The Hamiltonian-preserving scheme is designed by incorporating into the numerical fluxes the particle behavior–transmission and reflection– at the potential barrier. We proved that, with the Dirichlet incoming boundary conditions and for a class of bounded initial data, the numerical solution by the Hamiltonian-preserving scheme converges in l^1-norm to the solution of the Liouville equation–defined by using the interface condition that accounts for particle transmission and reflection. The initial data conditions can be satisfied by applying the decomposition technique proposed in [10] for solving the Liouville equation with measure-valued initial data arising in the semiclassical limit of the linear Schrödinger equation.

The strategy for the error analysis in this paper is to apply the l^1-error estimates established in [30, 28] for the immersed interface upwind scheme to the linear advection equations with piecewise constant coefficients. This is a natural approach since the solution of the Liouville equation with a step function potential satisfies linear advection equations with piecewise constant coefficients on the bicharacteristics. To apply this strategy, we split the computational domain into several parts. In each subdomain, we introduced a number of linear advection equations with step function coefficients to which the immersed interface upwind schemes yield the same numerical solution as the Hamiltonian-preserving scheme for the Liouville equation with the step function potential. Then the l^1-error estimates for the Hamiltonian-preserving scheme were derived by applying the l^1-error estimates for the immersed interface upwind schemes and comparing the exact solutions of the linear advection equations and that of the Liouville equation in each of these subdomains. The condition on the initial data were used in deriving these estimates. As a result, we obtained the half order l^1-error bound with explicit coefficients for the Hamiltonian-preserving scheme.

The problem under study has important applications in the computation of the semiclassical limit of the linear Schrödinger equation through barriers, and more generally, in the computation of high frequency waves through interfaces.

Appendix

In this Appendix we prove a property of BV functions on $\mathbb{R}$.

LEMMA A.1. *Let $f(x)$ be a BV function on $\mathbb{R}$, $H(x)$ be a function on $[a,b]$ satisfying*

$$|H(x) - x| \le H_C, \quad \text{for } x \in [a,b],$$

where H_C is a positive constant. Then

$$\|f(\cdot) - f(H(\cdot))\|_{L^1([a,b])} \le 2H_C \|f\|_{BV(\mathbb{R})}. \tag{A.1}$$

Proof. $\forall x \in [a,b]$, one has

$$|f(x) - f(H(x))| \le \|f\|_{BV([x-H_C, x+H_C])}.$$

Since $f(x)$ has a bounded variation on $\mathbb{R}$, $f'(x)$ exists a.e., and

$$\|f\|_{BV([x-H_C, x+H_C])} = \int_{x-H_C}^{x+H_C} |f'(y)|\, dy.$$

Thus

$$\|f(\cdot) - f(H(\cdot))\|_{L^1([a,b])} \le \int_a^b \int_{x-H_C}^{x+H_C} |f'(y)|\, dy dx. \tag{A.2}$$

Introduce the function

$$g(x,y) = \begin{cases} |f'(y)| & \text{if } |x-y| \le H_C \\ 0 & \text{else} \end{cases}.$$

Then $g(x,y) \in L^1([a,b] \times [a - H_C, b + H_C])$. Applying Fubini Theorem gives

$$\begin{aligned} &\int_a^b \int_{x-H_C}^{x+H_C} |f'(y)|\, dy dx = \int_a^b \int_{a-H_C}^{b+H_C} g(x,y) dy dx \\ &= \int_{a-H_C}^{b+H_C} \int_a^b g(x,y) dx dy \le \int_{a-H_C}^{b+H_C} \int_{y-H_C}^{y+H_C} |f'(y)|\, dx dy \\ &= 2H_C \int_{a-H_C}^{b+H_C} |f'(y)|\, dy \le 2H_C \|f\|_{BV(\mathbb{R})}. \end{aligned} \tag{A.3}$$

Combining (A.2) and (A.3) gives (A.1). □

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