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ℓ^1-ERROR ESTIMATES ON THE HAMILTONIAN-PRESERVING SCHEME FOR THE LIOUVILLE EQUATION WITH PIECEWISE CONSTANT POTENTIALS: A SIMPLE PROOF*

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Abstract

This work is concerned with ℓ^1-error estimates on a Hamiltonian-preserving scheme for the Liouville equation with piecewise constant potentials in one space dimension. We provide an analysis much simpler than these in literature and obtain the same half-order convergence rate. We formulate the Liouville equation with discretized velocities into a series of linear convection equations with piecewise constant coefficients, and rewrite the numerical scheme into some immersed interface upwind schemes. The ℓ^1-error estimates are then evaluated by comparing the derived equations and schemes.

Mathematics subject classification: 65M06, 65M12, 35L45, 70H99.
Key words: Liouville equations, Hamiltonian-preserving schemes, Piecewise constant potentials, ℓ^1-error estimate, Half-order error bound, Semiclassical limit.

1. Introduction

The Liouville equation with discontinuous potential functions is the semiclassical approximation of the linear Schrödinger equation with quantum barriers [1]. It has many applications in quantum mechanics [2,3] and wave propagation in heterogeneous media [4,5]. In this paper, we consider a one-dimensional Liouville equation:

$$f_t + \xi f_x - V_x f_\xi = 0, \quad t > 0, \quad x \in \mathbb{R}, \tag{1.1}$$

with a discontinuous potential $V(x)$. Such a problem cannot be analyzed using the method of renormalized solutions proposed in [6] for linear transport equations with discontinuous coefficients (see also [7]). In [5,8] Jin and Wen developed interface conditions coupling the Liouville equation (1.1) on both sides of the barrier and Hamiltonian-preserving schemes building the interface conditions into the numerical flux for such problems. They also studied ℓ^1-error estimates on these schemes in [9], and the ℓ^1-stability in [10].

The Liouville equation with piecewise constant potentials belongs to hyperbolic equations with singular coefficients. For conservation laws with discontinuous flux functions, there have been extensive theoretical and numerical results. Temple and his co-workers employed the *singular mapping* to study the Glimm's scheme and Godunov's method for 2×2 resonant systems of conservation laws in [11, 12]. Front tracking is also used as a method of analysis in [13–16]. Towers [17,18] developed appropriate scalar versions of the Godunov and Engquist-Osher methods and used the *singular mapping* approach to deduce convergence of these methods

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(see also [19, 20]). Karlsen applied the compensated compactness method to study some scalar approximation schemes in [21, 22].

However, limited work has been done on the convergence rate of these schemes until an half-order ℓ^1-error estimate was established in [23]. Both of the proof in [9, 23] rely on the expression of the exact solution at later time derived from the initial data by the method of characteristics, which is not naturally available for a complicated potential barrier or interface condition.

Compared with [23], Jin and Qi avoided finding the exact solutions, but obtained the same convergence rate with larger constants in a much simpler proof in [24]. Their work motivated us to deduce a simple analysis on the ℓ^1-error estimates for the Hamiltonian-preserving scheme (named Scheme I) for the Liouville equation with discontinuous potentials [9]. Our main idea is: 1) introducing linear convection equations with piecewise constant coefficients for (1.1) with fixed velocities on each partition of the computational domain, 2) rewriting Scheme I into a composition of immersed interface upwind schemes, and 3) deriving consistent convection equations for these upwind schemes. Then we use some theorems and inequalities in [9, 24, 25] to estimate the ℓ^1-error between the equations and numerical schemes.

The paper is organized as follows. In Section 2 we review the setup of the problem and Scheme I. In Section 3 we present the main result and recall some theorems and inequalities in [9, 24, 25]. We present the proof on each partition of the computational domain in Section 4. Finally, we conclude the paper in Section 5.

2. Setup of the Problem

We will employ the same interface condition, computational domain and numerical solution for Scheme I in [9]. For reader's convenience, we will restate some important setups.

In classical mechanics, a particle's momentum and the strength of the potential barrier decide whether it will cross the potential barrier or be reflected. Nevertheless, the Hamiltonian $H = \frac{1}{2}\xi^2 + V$ is preserved across the potential barrier:

$$\frac{1}{2}(\xi^+)^2 + V^+ = \frac{1}{2}(\xi^-)^2 + V^-, \tag{2.1}$$

where the superscripts $\pm$ stand for the right and left limits of the quantity respectively at the potential barrier. This property was used in [8] to provide the interface condition for (1.1) at the barrier :

$$f(x^+, \xi^+, t) = f(x^-, \xi^-, t) \qquad \text{for transmission}, \tag{2.2}$$

$$f(x^\pm, \xi^\pm, t) = f(x^\pm, -\xi^\pm, t) \qquad \text{for reflection}, \tag{2.3}$$

where $\xi^\pm$ is determined from the constant Hamiltonian condition (2.1) from $\xi^\mp$ in the case of transmission. Typical situations when a particle moves from left to right at a potential barrier are shown in Figure 2.1.

Let us consider the case when $V(x)$ is piecewise constant, with a jump $-D$ ($D > 0$) at $x = 0$. Namely

$$V(0^-) - V(0^+) = D > 0. \tag{2.4}$$

Therefore, (1.1) becomes

$$f_t + \xi f_x = 0, \quad \text{for} \quad x \neq 0, \tag{2.5}$$

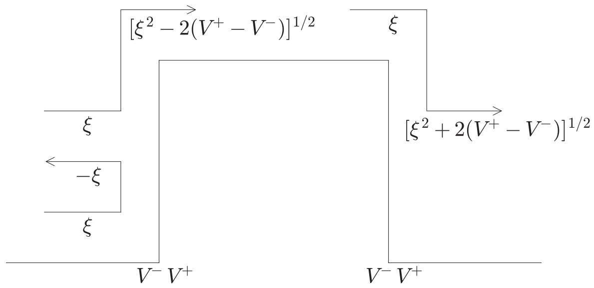

Fig. 2.1. Transmission and reflection of a particle at a potential barrier.

where ξ only serves as a parameter.

The computational domain is confined in a rectangular domain:

$$D_{\text{Main}} = \Big\{(x,\xi) \mid x_{\frac{1}{2}} \le x \le x_{N+\frac{1}{2}}, \quad \xi_{\frac{1}{2}} \le \xi \le \xi_{M+\frac{1}{2}}\Big\}.$$

We employ a uniform mesh in this domain. Let $x_{i+\frac{1}{2}} = x_{\frac{1}{2}} + i\Delta x$, $0 \le i \le N$, $\xi_{j+\frac{1}{2}} = \xi_{\frac{1}{2}} + j\Delta\xi$, $0 \le j \le M$, Δx is the mesh size in x-direction and $\Delta\xi$ is the mesh size in ξ-direction. Let Δt be the time step. Define fixed mesh ratios $\lambda_x^t = \frac{\Delta t}{\Delta x}$, $\lambda_x^\xi = \frac{\Delta \xi}{\Delta x}$. Let the potential barrier $x = 0$ be at a grid point $x_{m+\frac{1}{2}}$. And $\xi_{I_0+\frac{1}{2}} = 0$, $\xi_{I_+ + \frac{1}{2}} = \sqrt{2D}$ are grid points in the ξ-direction.

Define the domain

$$D_b = \Big\{(x,\xi) \mid x < 0, \quad \xi < -\sqrt{\xi_{\frac{1}{2}}^2 - 2D}\Big\},$$

which represents the area where particles come from outside of D_{Main}. For convenience, we need to exclude D_b from D_{Main}. Define the index I_b satisfying

$$\xi_{I_b - \frac{3}{2}} < -\sqrt{\xi_{\frac{1}{2}}^2 - 2D} \le \xi_{I_b - \frac{1}{2}}$$

and the domain

$$\hat{D}_b = \Big\{(x,\xi) \mid x < 0, \quad \xi < \xi_{I_b - \frac{1}{2}}\Big\}.$$

Then we choose the computational domain as $D_C = D_{Main} \setminus \hat{D}_b$.

We employ the Dirichlet boundary conditions at the incoming boundaries,

$$f(x_{\frac{1}{2}}, \xi, t) = f(x_{\frac{1}{2}}, \xi, 0), \qquad 0 < \xi < \xi_{M+\frac{1}{2}}, \tag{2.6}$$

$$f(x_{N+\frac{1}{2}}, \xi, t) = f(x_{N+\frac{1}{2}}, \xi, 0), \qquad \xi_{\frac{1}{2}} < \xi < 0, \tag{2.7}$$

and an extension of the initial data

$$\hat{f}_0(x,\xi) = \begin{cases} f(x,\xi,0), & x_{\frac{1}{2}} \le x \le x_{N+\frac{1}{2}}, \\ f(x_{\frac{1}{2}},\xi,0), & x < x_{\frac{1}{2}}, \\ f(x_{N+\frac{1}{2}},\xi,0), & x > x_{N+\frac{1}{2}}, \end{cases} \qquad \xi_{\frac{1}{2}} < \xi < \xi_{M+\frac{1}{2}}. \tag{2.8}$$

Now we introduce the Hamiltonian-preserving scheme. Denote

$$\mu_j = \lambda_x^t |\xi_j|, \quad 1 \le j \le M. \tag{2.9}$$

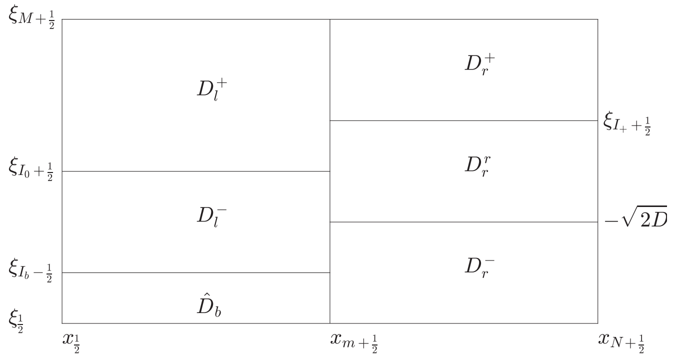

Fig. 2.2. Sketch of partition of D_C and $\hat{D}_b$.

Under the CFL condition:

$$\Delta t \left(\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|}{\Delta \xi} \right) < 1, \tag{2.10}$$

$\mu_j < 1$, for $1 \le j \le M$. Let $g^n_{i,j} = g(x_i, \xi_j, t^n)$ be the numerical approximation of $f(x_i, \xi_j, t^n)$. Scheme I on D_C proposed in [8] is given by:

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

$$g^{n+1}_{i,j} = (1-\mu_j) g^n_{i,j} + \mu_j g^n_{i-1,j}; \tag{2.11}$$

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

$$g^{n+1}_{i,j} = (1-\mu_j) g^n_{i,j} + \mu_j g^n_{i+1,j}; \tag{2.12}$$

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

$$g^{n+1}_{m+1,j} = (1-\mu_j) g^n_{m+1,j} + \mu_j \Big(\theta^j_0 g^n_{m,d_j} + \theta^j_1 g^n_{m,d_{j+1}} \Big); \tag{2.13}$$

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

$$g^{n+1}_{m+1,j} = (1-\mu_j) g^n_{m+1,j} + \mu_j g^n_{m+1,d_j}; \tag{2.14}$$

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

$$g^{n+1}_{m,j} = (1-\mu_j) g^n_{m,j} + \mu_j \Big(\theta^j_0 g^n_{m+1,d_j} + \theta^j_1 g^n_{m+1,d_{j+1}} \Big), \tag{2.15}$$

where $0 \le \theta^j_0$, $\theta^j_1 \le 1$ and $\theta^j_0 + \theta^j_1 = 1$. And d_js are determined by

$$\xi_{d_j} \le \sqrt{\xi_j^2 - 2D} < \xi_{d_{j+1}}, \qquad \text{for } d_j \text{ in (2.13)}, \tag{2.16}$$

$$\xi_{d_j} = -\xi_j, \qquad \text{for } d_j \text{ in (2.14)}, \tag{2.17}$$

$$\xi_{d_j} \le -\sqrt{\xi_j^2 + 2D} < \xi_{d_j+1}, \qquad \text{for } d_j \text{ in (2.15)}. \tag{2.18}$$

The initial and incoming boundary values are given by

$$\begin{cases} g_{i,j}^0 = \hat{f}_0(x_i, \xi_j), & (x_i, \xi_j) \in D_C, \\ g_{0,j}^n = \hat{f}_0(x_{\frac{1}{2}}, \xi_j), & 0 < \xi_j < \xi_{M+\frac{1}{2}}, \\ g_{N+1,j}^n = \hat{f}_0(x_{N+\frac{1}{2}}, \xi_j), & \xi_{\frac{1}{2}} < \xi_j < 0. \end{cases} \tag{2.19}$$

Criteria of different cases in Scheme I and the potential barrier naturally form a partition of D_C:

$$\begin{aligned} D_l^+ &= \{(x,\xi) \mid x_{\frac{1}{2}} < x < 0, \quad 0 < \xi < \xi_{M+\frac{1}{2}}\}, \\ D_l^- &= \{(x,\xi) \mid x_{\frac{1}{2}} < x < 0, \quad \xi_{I_b-\frac{1}{2}} < \xi < 0\}, \\ D_r^+ &= \{(x,\xi) \mid 0 < x < x_{N+\frac{1}{2}}, \quad \sqrt{2D} < \xi < \xi_{M+\frac{1}{2}}\}, \\ D_r^- &= \{(x,\xi) \mid 0 < x < x_{N+\frac{1}{2}}, \quad \xi_{\frac{1}{2}} < \xi < -\sqrt{2D}\}, \\ D_r^r &= \{(x,\xi) \mid 0 < x < x_{N+\frac{1}{2}}, \quad -\sqrt{2D} < \xi < \sqrt{2D}\}. \end{aligned}$$

A sketch of the partition of D_C is shown in Figure 2.2.

3. The Main Theorem and Previous Results

We assume the initial data are given on the computational domain D_C. Our main result is summarized in the following theorem.

Theorem 3.1. *Let the initial data $f(x,\xi,0)$ have bounded variation in the x-direction and is Lipschitz continuous in the ξ-direction. Namely, $\exists$ constants $A, B > 0$,*

$$\|f(\cdot,\xi,0)\|_{BV([x_{\frac{1}{2}},x_{N+\frac{1}{2}}])} \le A, \qquad \forall \xi \in [\xi_{\frac{1}{2}}, \xi_{M+\frac{1}{2}}], \tag{3.1}$$

$$|f(\cdot,\xi',0) - f(\cdot,\xi'',0)| \le B\left|\xi'^{\xi} - \xi''\right|, \qquad \forall x \in [x_{\frac{1}{2}}, x_{N+\frac{1}{2}}], \xi', \xi'' \in [\xi_{\frac{1}{2}}, \xi_{M+\frac{1}{2}}]. \tag{3.2}$$

Under the the CFL condition (2.10) *and the following mesh size restriction*

$$\Delta\xi \le \frac{3-2\sqrt{2}}{2}\sqrt{2D}, \tag{3.3}$$

the numerical solution (2.11)-(2.15) *has the following ℓ^1-error bound:*

$$\begin{aligned} &\left\|g_{\cdot,\cdot}^n - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_C)} \\ \le& \Big[\big(4\xi_{M_{\frac{1}{2}}} + 4|\xi_{\frac{1}{2}}| + \sqrt{2D}\big)A + 4DB\Big]\sqrt{\frac{t_n}{\lambda_x^t}}\sqrt{\Delta x} \\ &+ \frac{(4A + 2\sqrt{2D}B)}{(2D)^{\frac{1}{4}}}\Big[\xi_{M+\frac{1}{2}}\sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}} + 2|\xi_{\frac{1}{2}}|(\xi_{\frac{1}{2}}^2 - 2D)^{\frac{1}{4}}\Big]\sqrt{\frac{t_n}{\lambda_x^t}}\sqrt{\Delta x} + O(\Delta x). \end{aligned} \tag{3.4}$$

This error bound has the same leading $O(\sqrt{\Delta x})$ convergence rate as the result of [9] with a larger coefficient. But we make a much simpler proof than that of [9] which relies on a complex analytical solution and tedious inequalities. The slightly larger coefficient in (3.4) is caused by applying Theorem 1 in [24] instead of Theorem 3.1 in [9].

Our proof will use the ℓ^1-error estimates on the immersed interface upwind scheme for linear convection equations with piecewise constant coefficients proved in [24]:

Lemma 3.1. ([24]) *Consider a linear convection equation*

$$\begin{cases} u_t + (c(x)u)_x = 0, & t > 0, \quad x \in \mathbb{R}, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{3.5}$$

with a piecewise constant coefficient

$$c(x,t) = \begin{cases} c^- > 0, & x < 0, \\ c^+ > 0, & x > 0, \end{cases} \tag{3.6}$$

and an interface condition given at $x = 0$:

$$u(0^+, t) = \rho u(0^-, t), \tag{3.7}$$

where $\rho = 1$ corresponds to conservation of mass (u) or $\rho = c^-/c^+$ for the conservation of flux. The immersed upwind scheme proposed in [23] *for* (3.5)-(3.7) *is*

$$\begin{cases} (U)_i^{n+1} = (1-\lambda^-)(U)_i^n + \lambda^-(U)_{i-1}^n, & i \le 0, \\ (U)_i^{n+1} = (1-\lambda^+)(U)_i^n + \lambda^+\rho(U)_{i-1}^n, & i = 1, \\ (U)_i^{n+1} = (1-\lambda^+)(U)_i^n + \lambda^+(U)_{i-1}^n, & i \ge 2, \end{cases} \tag{3.8}$$

where $\lambda^\pm = c^\pm \frac{\Delta t}{\Delta x}$, Δx is the mesh size, and Δt is the time step.

Let $u_0(x)$ be a function of bounded variation. Then $\forall \rho > 0$ in the interface condition (3.7)*, the immersed interface upwind difference scheme* (3.8)*, under the CFL condition $0 < \lambda^\pm < 1$, has the following ℓ^1-error bound:*

$$\begin{aligned} &\|U^n - u(\cdot, t_n; u_0)\|_{\ell^1} \\ \le &\Big[\|u_0\|_{BV(\mathbb{R}^- \cup \{0\})} + \Big(2\rho \|u_0\|_{BV(\mathbb{R}^- \cup \{0\})} + L\Big)\Big(\frac{c^+}{c^-}\Big)\Big]\Gamma(c^-) \\ &+ \Big[\rho \|u_0\|_{BV(\mathbb{R}^- \cup \{0\})} + \|u_0\|_{BV(\mathbb{R}^+)}\Big]\Gamma(c^+), \end{aligned} \tag{3.9}$$

where $L = |\rho u_0(0^+) - u_0(0^-)|$ and

$$\Gamma(\xi) \triangleq 2\sqrt{\xi(1 - \xi\frac{\Delta t}{\Delta x})t_n \Delta x} + \Delta x. \tag{3.10}$$

For (3.5) with a general $c(x)$ on indefinite sign changes, Gosse established the convergence of a class of finite difference schemes to the duality solutions in [26] (see also [27,28] for some related theoretical frameworks).

Our proof will also use the ℓ^1-error estimate proved in [25], for linear convection equations with constant $c(x)$:

Lemma 3.2. ([25]) *The ℓ^1-error of the upwind scheme for solving* (3.5) *with $c(x) \equiv a > 0$ is*

$$\|U^n - u(\cdot, t_n; u_0)\|_{\ell^1} \le \|u_0(x)\|_{BV} \Gamma(a). \tag{3.11}$$

The following result proved in [9] will also be used:

Lemma 3.3. ([9]) *Let $f(x)$ be a BV function on $\mathbb{R}$, $H(x)$ be a function on $[a,b]$ satisfying*

$$|H(x) - x| \le H_C, \quad \forall x \in [a,b], \tag{3.12}$$

where H_C is a positive constant. Then

$$\|f(\cdot) - f(H(\cdot))\|_{L^1([a,b])} \le 2H_C \|f\|_{BV(\mathbb{R})}. \tag{3.13}$$

For convenience, we also employ the following inequalities proved in [9]:

$$\Gamma(\xi) \le \gamma\sqrt{\Delta x} + \Delta x, \quad \gamma = \sqrt{t_n/\lambda_x^t}, \qquad \forall \xi_{\frac{1}{2}} < \xi < \xi_{M+\frac{1}{2}}, \tag{3.14}$$

$$\frac{\xi_j}{\xi_{d_j+p}} \le \frac{\xi_{M+\frac{1}{2}}}{(2D)^{\frac{1}{4}}\sqrt{(j-I_+-\frac{1}{2})\Delta\xi}}, \qquad \forall I_+ + 1 \le j \le M, \quad p=0,1, \tag{3.15}$$

$$\Delta\xi \sum_{j=I_++1}^{M} \frac{1}{\sqrt{(j-I_+-\frac{1}{2})\Delta\xi}} \le 2\sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}}. \tag{3.16}$$

4. Proof of the Main Theorem

The ℓ^1-error in Theorem 3.1 can be split according to the partition of D_C:

$$\begin{aligned}
&\left\|g^n_{\cdot,\cdot} - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_C)} \\
=&\left\|g^n_{\cdot,\cdot} - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_l^+)} + \left\|g^n_{\cdot,\cdot} - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_r^+)} + \left\|g^n_{\cdot,\cdot} - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_l^-)} \\
&+ \left\|g^n_{\cdot,\cdot} - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_r^-)} + \left\|g^n_{\cdot,\cdot} - f(\cdot,\cdot,t_n)\right\|_{\ell^1(D_r^r)} \\
=:&E_l^+ + E_r^+ + E_l^- + E_r^- + E_r^r.
\end{aligned} \tag{4.1}$$

The five terms in (4.1) will be estimated respectively.

4.1. The upper bound for E_r^+ and E_l^-.

We start the proof with E_r^+, which is the most representative part. Note that E_r^+ is defined as

$$E_r^+ = \Delta\xi \sum_{j=I_++1}^{M} \mathcal{E}(j), \tag{4.2}$$

where

$$\mathcal{E}(j) \triangleq \left\|g^n_{i,j} - f(x_i,\xi_j,t_n)\right\|_{\ell^1(m<i\le N)}, \quad I_+ + 1 \le j \le M.$$

For a fixed j, we define a linear convection equation satisfying (2.2), (2.5) and (2.8) restricted on D_r^+ and omit the subscript j for convenience. Namely,

$$\begin{cases} u_t + c^+ u_x = 0, & t>0, \quad x>0, \\ u(0^+,t) = f(0^-,c^-,t), & t>0, \\ u(x,0) = u_0(x) \triangleq \hat{f}_0(x,c^+), & x>0, \end{cases} \tag{4.3}$$

where $c^+ = \xi_j$, and $c^- = \sqrt{(\xi_j)^2 - 2D}$ which is deduced from (2.1) and (2.4). We extend the definition of (4.3) to the left half plane by setting $u(x,t)$ satisfying (2.5) and (2.8) restricted on D_l^+,

$$\begin{cases} u_t + c^- u_x = 0, & t>0, \quad x<0, \\ u(x,0) = u_0(x) \triangleq \hat{f}_0(x,c^-), & x \le 0, \end{cases} \tag{4.4}$$

then one can check that $f(0^-,c^-,t) = u(0^-,t)$ and $f(x,\xi_j,t) = u(x,t)$ on D_r^+. Combining (4.3) and (4.4) gives a linear convection equation with a piecewise constant coefficient:

$$\begin{cases} u_t + c^- u_x = 0, & t>0, \quad x<0, \\ u_t + c^+ u_x = 0, & t>0, \quad x>0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{4.5}$$

with an interface condition given at $x = 0$:

$$u(0^+, t) = u(0^-, t), \quad t > 0. \tag{4.6}$$

Now we rewrite $g^n_{i,j}$ into a composition of solutions of immersed interface upwind schemes. Define $(G^p)^n_i$ for the fixed j and $p = 0, 1$,

$$\begin{cases} (G^p)^{n+1}_i = (1-\mu^p)(G^p)^n_i + \mu^p (G^p)^n_{i-1}, & i \le m, \\ (G^p)^{n+1}_i = (1-\mu^+)(G^p)^n_i + \mu^+ (G^p)^n_{i-1}, & i > m, \end{cases} \tag{4.7}$$

with initial condition

$$(G^p)^0_i = \begin{cases} \hat{f}_0(x_i, c^p), & i \le m, \\ \hat{f}_0(x_i, c^+), & i > m, \end{cases} \tag{4.8}$$

where $c^p = \xi_{d_j+p}$, $\mu^p = \lambda^t_x c^p$, and $\mu^+ = \lambda^t_x c^+$ with ξ_{d_j+p} defined in (2.16). In comparison with (2.11), (2.13), (2.16) and (2.19), for the fixed j one has

$$g^n_{i,j} = \sum_{p=0}^{1} \theta^j_p (G^p)^n_i, \quad \forall 0 < i \le N, \quad n \ge 0. \tag{4.9}$$

It is easy to check that $(G^p)^n_i$ are consistent with the following convection equations with discontinuous coefficients,

$$\begin{cases} \tilde{u}^p_t + c^p \tilde{u}^p_x = 0, & t > 0, \quad x < 0, \\ \tilde{u}^p_t + c^+ \tilde{u}^p_x = 0, & t > 0, \quad x > 0, \\ \tilde{u}^p(x, 0) = \tilde{u}^p_0(x), & x \in \mathbb{R}, \\ \tilde{u}^p(0^+, t) = \tilde{u}^p(0^-, t), & t > 0, \end{cases} \tag{4.10}$$

with, for $p = 0, 1$,

$$\tilde{u}^p_0(x) = \begin{cases} \hat{f}_0(x, c^p), & x \le 0, \\ \hat{f}_0(x, c^+), & x > 0. \end{cases} \tag{4.11}$$

For the ℓ^1-error between $u(x,t)$ and $\tilde{u}^p(x,t)$, we use the main idea in [24] (see also [29] for variable mesh problems) and convert $u(x,t)$ and $\tilde{u}^p(x,t)$ into convection equations with constant coefficients. We can write $u(x,t)$ as the sum of $v(x,t)$ and $w(x,t)$, where

$$\begin{cases} v_t + c^+ v_x = 0, & t > 0, \quad x \in \mathbb{R}, \\ v(x, 0) = v_0(x), & x \in \mathbb{R}, \\ v_0(x) = \begin{cases} u_0(\frac{c^-}{c^+} x), & x \le 0, \\ u_0(0^+), & x > 0, \end{cases} \end{cases} \tag{4.12}$$

$$\begin{cases} w_t + c^+ w_x = 0, & t > 0, \quad x \in \mathbb{R}, \\ w(x, 0) = w_0(x), & x \in \mathbb{R}, \\ w_0(x) = \begin{cases} 0, & x \le 0, \\ u_0(x) - u_0(0^+), & x > 0. \end{cases} \end{cases} \tag{4.13}$$

Then the relationship between $u(x,t)$, $v(x,t)$ and $w(x,t)$ is

$$u(x,t) = \begin{cases} v(\frac{c^+}{c^-} x, t), & x \le 0, \\ v(x,t) + w(x,t), & x > 0. \end{cases} \tag{4.14}$$

Similarly, we can write $\tilde{u}^p(x,t)$ as the sum of $\tilde{v}^p(x,t)$ and $w(x,t)$, where

$$\begin{cases} \tilde{v}^p_t + c^+ \tilde{v}^p_x = 0, & t>0, \quad x\in\mathbb{R}, \\ \tilde{v}^p(x,0) = \tilde{v}^p_0(x), & x\in\mathbb{R}, \\ \tilde{v}^p_0(x) = \begin{cases} \tilde{u}^p_0(\frac{c^p}{c^+}x), & x\le 0, \\ u_0(0^+), & x>0. \end{cases} \end{cases} \tag{4.15}$$

One can verify that the relationship between $\tilde{u}^p(x,t)$, $\tilde{v}^p(x,t)$ and $w(x,t)$ is

$$\tilde{u}^p(x,t) = \begin{cases} \tilde{v}^p(\frac{c^+}{c^p}x,t), & x\le 0, \\ \tilde{v}^p(x,t) + w(x,t), & x>0, \end{cases} \tag{4.16}$$

for $p=0,1$.

Utilizing (4.14) and (4.16), for $p=0$ and 1, one obtains

$$\begin{aligned} &\|\tilde{u}^p(x_i,t_n) - u(x_i,t_n)\|_{\ell^1(m<i\le N)} \le \|\tilde{v}^p(x_i,t_n) - v(x_i,t_n)\|_{\ell^1(m<i\le N)} \\ \le &\left\| \tilde{u}^p_0\left(\frac{c^p}{c^+}x_i\right) - u_0\left(\frac{c^-}{c^+}x_i\right) \right\|_{\ell^1(0<i\le m)}, \end{aligned} \tag{4.17}$$

since (4.12) and (4.15) have the same equation but different initial conditions.

Together with (4.9) and (4.17) and the definitions of $\mathcal{E}(j)$, $u(x,t)$ and $\tilde{u}^p(x,t)$, one obtains by triangle inequality

$$\mathcal{E}(j) \le \mathcal{E}_1(j) + \mathcal{E}_2(j) + \mathcal{E}_3(j), \tag{4.18}$$

where

$$\mathcal{E}_1(j) = \sum_{p=0}^{1} \theta^j_p \left\| (G^p)^n_i - \tilde{u}^p(x_i,t_n) \right\|_{\ell^1(m<i\le N)}, \tag{4.19}$$

$$\mathcal{E}_2(j) = \sum_{p=0}^{1} \theta^j_p \left\| \tilde{u}^p_0\left(\frac{c^p}{c^+}x_i\right) - u_0\left(\frac{c^p}{c^+}x_i\right) \right\|_{\ell^1(0<i\le m)}, \tag{4.20}$$

$$\mathcal{E}_3(j) = \sum_{p=0}^{1} \theta^j_p \left\| u_0\left(\frac{c^p}{c^+}x_i\right) - u_0\left(\frac{c^-}{c^+}x_i\right) \right\|_{\ell^1(0<i\le m)}. \tag{4.21}$$

Using assumptions (3.1) and (3.2) and definitions (2.8) and (4.11), one obtains the following bounded variation conditions:

$$\|\tilde{u}^p_0(x)\|_{BV(\mathbb{R}^-)} \le A, \tag{4.22}$$

$$\|\tilde{u}^p_0(x)\|_{BV(\mathbb{R}^+)} \le A, \tag{4.23}$$

for $p=0,1$, and the Lipschitz continuous conditions:

$$\left|\tilde{u}^p_0(0^+) - \tilde{u}^p_0(0^-)\right| \le B\left|c^+ - c^p\right| \le B(\left|c^+ - c^-\right| + \left|c^- - c^p\right|), \tag{4.24}$$

$$\left|\tilde{u}^p_0(\frac{c^p}{c^+}x) - u_0(\frac{c^p}{c^+}x)\right| \le B\left|c^p - c^-\right|, \quad x\in\mathbb{R}^-, \tag{4.25}$$

where $|c^+ - c^-| \le \sqrt{2D}$ and $|c^- - c^p| \le \Delta\xi$. Similarly one has

$$\|u_0(x)\|_{BV(\mathbb{R})} \le 2A + \sqrt{2D}B. \tag{4.26}$$

Utilizing (4.22)-(4.24) and applying Lemma 3.1 to $\mathcal{E}_1(j)$ lead to

$$\begin{aligned}\mathcal{E}_1(j) \leq &\sum_{p=0}^{1} \theta_p^j \Big[\Big(A + \big(2A + B(\sqrt{2D} + \Delta\xi)\big)\frac{c^+}{c^p}\Big)\Gamma(c^p) + 2A\Gamma(c^+)\Big] \\ = &\sum_{p=0}^{1} \theta_p^j \Big[\big(A + (2A + B\sqrt{2D})\frac{c^+}{c^p}\big)\Gamma(c^p) + 2A\Gamma(c^+)\Big] + \sum_{p=0}^{1} \theta_p^j B \frac{c^+}{c^p}\Gamma(c^p)\Delta\xi. \qquad (4.27)\end{aligned}$$

From (4.25), one has

$$\mathcal{E}_2(j) \leq \sum_{p=0}^{1} \theta_p^j B\Delta\xi |x_{\frac{1}{2}}| = B|x_{\frac{1}{2}}|\Delta\xi. \qquad (4.28)$$

Because of (4.26), $u_0'(x)$ exists a.e. on $[x_{\frac{1}{2}}, 0]$. Then applying Lemma 3.3 to $\mathcal{E}_3(j)$ gives

$$\begin{aligned}\mathcal{E}_3(j) \leq &\sum_{p=0}^{1} \theta_p^j \left\| u_0\Big(\frac{c^p}{c^+}x_i\Big) - u_0\Big(\frac{c^-}{c^+}x_i\Big)\right\|_{L^1(x_{\frac{1}{2}} < x \leq 0)} + O(\Delta x) \\ \leq &\, 2(2A + \sqrt{2D}B)|x_{\frac{1}{2}}| \sum_{p=0}^{1} \theta_p^j \frac{|c^p - c^-|}{c^p} + O(\Delta x) \\ \leq &\, 2(2A + \sqrt{2D}B)|x_{\frac{1}{2}}| \sum_{p=0}^{1} \theta_p^j \frac{\Delta\xi}{c^p} + O(\Delta x). \qquad (4.29)\end{aligned}$$

Combining (4.27)-(4.29) gives an estimate for $\mathcal{E}(j)$. Summing these estimates over j and using the inequalities (3.14)-(3.16) yield

$$E_r^+ \leq \Big(3A\xi_{M+\frac{1}{2}} + 2(2A + \sqrt{2D}B)\frac{\xi_{M+\frac{1}{2}}}{(2D)^{\frac{1}{4}}}\sqrt{\xi_{M+\frac{1}{2}} - \sqrt{2D}}\Big)\gamma\sqrt{\Delta x} + O(\Delta x), \qquad (4.30)$$

where we used $\Delta\xi = \lambda_x^\xi \Delta x$. Note that E_l^- is defined as

$$E_l^- = \Delta\xi \sum_{j=I_b}^{I_0} \left\| g_{i,j}^n - f(x_i, \xi_j, t_n)\right\|_{\ell^1(0<i\leq m)}. \qquad (4.31)$$

For a fixed j, we give the linear convection equation for $f(x, \xi_j, t)$ on D_l^-:

$$\begin{cases} u_t + c^- u_x = 0, & t > 0, \quad x < 0, \\ u_t + c_+ u_x = 0, & t > 0, \quad x > 0, \\ u(x, 0) = u_0(x), & x \in \mathbb{R}, \end{cases} \qquad (4.32)$$

with

$$u_0(x) = \begin{cases} \hat{f}_0(-x, -c^-), & x \leq 0, \\ \hat{f}_0(-x, -c^+), & x > 0, \end{cases} \qquad (4.33)$$

and an interface condition given at $x = 0$:

$$u(0^+, t) = u(0^-, t), \quad t > 0. \qquad (4.34)$$

where $c^+ = |\xi_j|$, and $c^- = \sqrt{(\xi_j)^2 + 2D}$ which is deduced from (2.1) and (2.4). Similar to (3.15), we can prove the following inequality on D_l^-,

$$\frac{\xi_j}{\xi_{d_j+p}} \leq \frac{|\xi_{\frac{1}{2}}|}{\sqrt{2\,|\xi_j|\,\sqrt{2D} - \Delta\xi}} \leq \frac{2|\xi_{\frac{1}{2}}|}{(2D)^{\frac{1}{4}}\sqrt{|\xi_j|}}, \quad \forall I_b \leq j \leq I_0, \quad p = 0, 1, \tag{4.35}$$

where $|\xi_{d_j+p}|$ is defined in (2.18). Then one can follow the estimate of E_r^+ to complete the proof for E_l^- and obtain

$$E_l^- \leq \Big(3A|\xi_{\frac{1}{2}}| + 4(2A + \sqrt{2D}B)\frac{|\xi_{\frac{1}{2}}|}{(2D)^{\frac{1}{4}}}(\xi_{\frac{1}{2}}^2 - 2D)^{\frac{1}{4}}\Big)\gamma\sqrt{\Delta x} + O(\Delta x). \tag{4.36}$$

4.2. The upper bounds for E_l^+, E_r^- and E_r^r

Note that E_l^+ is defined as

$$E_l^+ = \Delta\xi \sum_{j=I_0+1}^{M} \left\| g_{i,j}^n - f(x_i, \xi_j, t_n) \right\|_{l^1(0<i\leq m)}. \tag{4.37}$$

For a fixed j, (2.5) restricted on D_l^+ is a linear convection equation with a constant coefficient. One can check that (2.11) and (2.19) constitute an upwind scheme for it. Then by assumption (3.1) and applying Lemma 3.2 to E_l^+ one obtains

$$E_l^+ \leq \Delta\xi \sum_{j=I_0+1}^{M} A\Gamma(\xi_j) \leq \xi_{M+\frac{1}{2}} A\gamma\sqrt{\Delta x} + O(\Delta x). \tag{4.38}$$

Similarly, for E_r^- one can deduce

$$E_r^- \leq \left|\xi_{\frac{1}{2}} + \sqrt{2D}\right| A\gamma\sqrt{\Delta x} + O(\Delta x). \tag{4.39}$$

Note that E_r^r is defined as

$$\begin{aligned} E_r^r =& \Delta\xi \sum_{j=I_0+1}^{I_+} \left\| g_{i,j}^n - f(x_i, \xi_j, t_n) \right\|_{l^1(m<i\leq N)} \\ &+ \Delta\xi \sum_{j=I_0+1}^{I_+} \left\| g_{i,2I_0+1-j}^n - f(x_i, -\xi_j, t_n) \right\|_{l^1(m<i\leq N)}. \end{aligned} \tag{4.40}$$

For a fixed j, we can define a linear convection equation satisfying (2.3) and (2.5) restricted on D_r^r and extend it to the whole x-t plane,

$$\begin{cases} u_t + cu_x = 0, & t > 0, \quad x \in \mathbb{R}, \\ u(x,0) = u_0(x) \triangleq \begin{cases} \hat{f}_0(x, c), & x > 0, \\ \hat{f}_0(-x, -c, 0), & x \leq 0, \end{cases} \end{cases} \tag{4.41}$$

where $c = \xi_j$ and $|c| \leq \sqrt{2D}$. One can check that on D_r^r,

$$u(x,t) = \begin{cases} f(x, \xi_j, t), & 0 < x < x_{N+\frac{1}{2}}, \\ f(-x, -\xi_j, t), & -x_{N+\frac{1}{2}} < x \leq 0. \end{cases} \tag{4.42}$$

And assumptions (3.1) and (3.2) imply,

$$\begin{aligned}\|u_0(\cdot)\|_{BV(\mathbb{R})} \leq& \|u_0(\cdot)\|_{BV(\mathbb{R}^+)} + \|u_0(\cdot)\|_{BV(\mathbb{R}^-)} + \left|u_0(0^+) - u_0(0^-)\right| \\ \leq& 2A + 2B\sqrt{2D}. \end{aligned} \tag{4.43}$$

Introduce an upwind scheme G_i^n for $u(x,t)$,

$$G_i^{n+1} = (1-\mu)G_i^n + \mu G_{i-1}^n, \quad i \in \mathbb{Z}, \tag{4.44}$$

with initial condition

$$G_i^0 = u_0(x), \quad i \in \mathbb{Z}, \tag{4.45}$$

where $\mu = \lambda_x^t c$. In comparison with (2.11), (2.12), (2.14), (2.17), (2.19), (4.44) and (4.45) for the fixed j, one has

$$G_i^n = \begin{cases} g_{i,j}^n, & m < i \leq N, \\ g_{2m+1-i,2I_0+1-j}^n, & 0 < i \leq m. \end{cases} \tag{4.46}$$

Using (4.42) and (4.46), one obtains

$$E_r^r = \Delta\xi \sum_{j=I_0+1}^{I_+} \|G_i^n - u(x_i,t_n)\|_{l^1(0<i\leq N)}. \tag{4.47}$$

Utilizing (3.14) and (4.43) and applying Lemma 3.1 to (4.47) one deduces

$$\begin{aligned} E_r^r \leq& \Delta\xi \sum_{j=I_0+1}^{I_+} (2A + 2\sqrt{2D}B)\Gamma(\xi_j) \\ \leq& \sqrt{2D}(2A + 2\sqrt{2D}B)\gamma\sqrt{\Delta x} + O(\Delta x). \end{aligned} \tag{4.48}$$

Finally, combining (4.30), (4.36), (4.38), (4.39) and (4.48) completes the proof for Theorem 3.1.

Remark 4.1. For a general piecewise smooth potential, one can introduce the piecewise constant approximation to it and then use the estimate of the paper. Since piecewise constant approximation is first order, and the overall scheme has only half-order accuracy due to contact discontinuity, so despite of the approximation of the potential by piecewise constant, the scheme will still have the same rate of the convergence for the numerical method.

5. Conclusion

In this paper, we studied the ℓ^1-error bound of the Hamilton-preserving scheme, developed in [8], for the Liouville equation with a piecewise constant potential. Compared with [9], we obtained the same leading $O(\sqrt{\Delta x})$ convergence rate with larger coefficients in a much simpler method of proof. Our proof employs the main idea and theorems in [24] to derive the ℓ^1-error bound in each subdomain. The simplicity of this approach makes it potential application to more complicated problems in computational high frequency waves in heterogeneous media and semiclassical modeling of quantum dynamics with potential barriers, see [2, 3].

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