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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

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