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

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Abstract

We study the L^1-error of a Hamiltonian-preserving scheme, developed in [19], for the Liouville equation with a piecewise constant potential in one space dimension when the initial data is given with perturbation errors. We extend the l^1-stability analysis in [46] and apply the L^1-error estimates with exact initial data established in [45] for the same scheme. We prove that the scheme with the Dirichlet incoming boundary conditions and for a class of bounded initial data is L^1-convergent when the initial data is given with a wide class of perturbation errors, and derive the L^1-error bounds with *explicit* coefficients. The convergence rate of the scheme is shown to be less than the order of the initial perturbation error, matching with the fact that the perturbation solution can be l^1-unstable.

Mathematics subject classification: 65M06, 65M12, 65M25, 35L45, 70H99.
Key words: Liouville equations, Hamiltonian preserving schemes, Piecewise constant potentials, Error estimate, Perturbed initial data, Semiclassical limit.

1. Introduction

In [19], 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. Such problem has applications in computational high frequency waves [3,6,12,13,17,23,33,42,43]. 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 [19–21] 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. An important property of the interface condition is that the Hamiltonian is preserved on particle trajectory in case of either transmission or reflection. By using this property to determine the particle trajectory for constructing numerical fluxes,

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the so-called Hamiltonian-preserving schemes were constructed in [19–21]. See also the related work on Hamiltonian-preserving schemes [10, 11, 14–16, 18, 22–25, 40]. 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:

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

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 [19–21]. The two schemes developed in [19]–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 except the l^1-stability of Scheme I.

The more difficult issue of the l^1-stability and error estimates for Scheme I was further established in the recent work [45, 46]. We proved in [46] 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. We also presented counter examples showing that Scheme I can be l^1-unstable if the initial data condition is violated. In [45] we proved that in the case of a step function potential and the Dirichlet incoming boundary conditions, Scheme I is L^1-convergent for a class of bounded initial data by utilizing the L^1-error estimates developed in [41,44] for the immersed interface upwind scheme to the linear advection equations with piecewise constant coefficients. We presented the halfth order L^1-error bound with explicit coefficients. The halfth order convergence rate is sharp, since even for the discontinuous solution to linear hyperbolic equation with a smooth coefficient, the halfth order convergence rate is already optimal for a monotone difference scheme [36]. The Liouville equation with a step function potential belongs to hyperbolic equations with measure-valued coefficients. For the discontinuous coefficient case, one can refer to [1, 4, 7–9, 26–32, 34, 37–39] for the wide study of the convergence of numerical schemes. The initial conditions considered in [45] can be satisfied when applying the decomposition technique proposed in [12] for solving the Liouville equation with measure-valued initial data arisen in the semiclassical limit of the linear Schrödinger equation. In particular, the initial data condition in [46] is more general than that in [45], which implies that the stability results established in [46] is in consistent with the convergence results established in [45] since a convergent scheme for the Liouville equation with the homogeneous Dirichlet boundary condition should be l^1-stable.

The error estimates for Scheme I in [45] was established under the condition that the initial data is exactly given. In practical computation, however it is common that the initial data is given with errors. Therefore an interesting issue is to further investigate error estimates for Scheme I when the initial data is given with perturbation errors. In this paper we will study this issue. Due to the linearity of Scheme I, these error estimates can be obtained by applying the error estimates for Scheme I with exact initial data established in [45] and the l^1-norm estimates for the perturbation solutions. Therefore in this paper we will investigate the