Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Computational Physics 214 (2006) 672–697
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

Hamiltonian-preserving schemes for the Liouville equation of geometrical optics with discontinuous local wave speeds

Shi Jin [a,b,*], Xin Wen [b,1]

[a] Department of Mathematics, University of Wisconsin – Madison, Van Vleck Hall, 480 Lincoln Drive, Madison, WI 53706-1388, USA
[b] Department of Mathematical Sciences, Tsinghua University, Beijing 100084, PR China

Received 8 June 2005; received in revised form 11 October 2005; accepted 12 October 2005
Available online 6 December 2005

Abstract

In this paper, we construct two classes of Hamiltonian-preserving numerical schemes for a Liouville equation with discontinuous local wave speed. This equation arises in the phase space description of geometrical optics, and has been the foundation of the recently developed level set methods for multivalued solution in geometrical optics. We extend our previous work in [S. Jin, X. Wen, Hamiltonian-preserving schemes for the Liouville equation with discontinuous potentials, Commun. Math. Sci. 3 (2005) 285–315] for the semiclassical limit of the Schrödinger equation into this system. The designing principle of the Hamiltonian preservation by building in the particle behavior at the interface into the numerical flux is used here, and as a consequence we obtain two classes of schemes that allow a hyperbolic stability condition. When a plane wave hits a flat interface, the Hamiltonian preservation is shown to be equivalent to Snell's law of refraction in the case when the ratio of wave length over the width of the interface goes to zero, when both length scales go to zero. Positivity, and stabilities in both l^1 and l^∞ norms, are established for both schemes. The approach also provides a selection criterion for a unique solution of the underlying linear hyperbolic equation with singular (discontinuous and measure-valued) coefficients. Benchmark numerical examples are given, with analytic solution constructed, to study the numerical accuracy of these schemes.

Keywords: Geometrical optics; Liouville equation; Level set method; Hamiltonian-preserving schemes; Snell's law of refraction

1. Introduction

In this paper, we construct and study numerical schemes for the Liouville equation in d-dimension:

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

* Corresponding author. Tel.: +1 608 263 3302; fax: +1 608 263 8891.
E-mail addresses: jin@math.wisc.edu (S. Jin), wenxin@amss.ac.cn (X. Wen).
1 Present address: Institute of Computational Mathematics and Scientific and Engineering Computing, Chinese Academy of Science, Beijing 100080, China.

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2005.10.012

where the Hamiltonian H is given by

$$H(\mathbf{x},\mathbf{v},t) = c(\mathbf{x})|\mathbf{v}| = c(\mathbf{x})\sqrt{v_1^2 + v_2^2 + \cdots + v_d^2} \tag{1.2}$$

with $c(\mathbf{x}) > 0$ being the local wave speed. $f(t,\mathbf{x},\mathbf{v})$ is the density distribution of particles depending on position $\mathbf{x}$, time t and the slowness vector $\mathbf{v}$. In this paper, we are interested in the case when $c(\mathbf{x})$ contains *discontinuities* corresponding to different indices of refraction at different media. This discontinuity will generate an *interface* at the point of discontinuity of $c(\mathbf{x})$, and as a consequence waves crossing this interface will undergo transmissions and reflections. The incident and transmitted waves obey Snell's law of refraction.

The bicharacteristics of the Liouville equation (1.1) satisfy the Hamiltonian system:

$$\frac{d\mathbf{x}}{dt} = c(\mathbf{x})\frac{\mathbf{v}}{|\mathbf{v}|}, \quad \frac{d\mathbf{v}}{dt} = -|\mathbf{v}|\nabla_{\mathbf{x}}c. \tag{1.3}$$

In classical mechanics the Hamiltonian (1.2) of a particle remains a constant along particle trajectory, even across an interface.

This Liouville equation arises in the phase space description of geometrical optics. It is the high frequency limit of the wave equation

$$u_{tt} - c(\mathbf{x})^2\Delta u = 0, \quad t > 0, \ \ \mathbf{x} \in R^d. \tag{1.4}$$

Recently, several phase space based level set methods are based on this equation, see [13,16,22,31]. High frequency limit of wave equations with transmissions and reflections at the interfaces was studied in [1,30,39]. A Liouville equation based level set method for the wave front, but with only reflection, was introduced in [7]. It was also suggested to smooth out the local wave speed in [31].

The Liouville equation (1.1) is a linear wave equation, with the characteristic speed determined by bicharacteristic (1.3). If $c(\mathbf{x})$ is smooth, then the standard numerical methods (for example, the upwind scheme and its higher order extensions) for linear wave equations give satisfactory results. However, if $c(\mathbf{x})$ is discontinuous, then the conventional numerical schemes suffer from two problems. Firstly, the characteristic speed $c_{\mathbf{x}}$ of the Liouville equation is *infinity* at the discontinuous point of wave speed. When numerically approximating $c_{\mathbf{x}}$ crossing the interface (for example by smoothing out $c(\mathbf{x})$ [31]), the numerical derivative of c is of $O(1/\Delta x)$, with Δx the mesh size in the physical space. Thus an explicit scheme needs time step $\Delta t = O(\Delta x \Delta v)$ with Δv the mesh size in particle slowness space. This is very expensive. Moreover, a conventional numerical scheme in general does not preserve a *constant Hamiltonian* across the interface, usually leading to poor or even incorrect numerical resolutions by ignoring the discontinuities of $c(\mathbf{x})$. Theoretically, there is a uniqueness issue for weak solutions to these linear hyperbolic equations with singular wave speeds [6,9,19,34,35]. It is not clear which weak solution a standard numerical discretization that ignores the discontinuity of $c(\mathbf{x})$ will select.

We also remark that Hamiltonian or sympletic schemes have been introduced for Hamiltonian ODEs and PDEs in order to preserve the Hamiltonian or sympletic structures, see for example [15,28]. To our knowledge, no such schemes have been constructed for Hamiltonian systems with discontinuous Hamiltonians.

In this paper, we construct a class of numerical schemes that are suitable for the Liouville equation (1.1) with a discontinuous local wave speed $c(\mathbf{x})$. An important feature of our schemes is that they are consistent with the constant Hamiltonian across the interface. This gives a selection criterion for a unique solution to the governing equation. As done in [24] for the Liouville equation for the semiclassical limit of the linear Schrödinger equation, we call such schemes *Hamiltonian-preserving schemes*. A key idea of these schemes is to build the behavior of a particle at the interface – either cross over with a changed velocity or be reflected with a negative velocity – into the numerical flux. This idea was formerly used by Perthame and Semioni in their work [33] to construct a well-balanced kinetic scheme for the shallow water equations with a (discontinuous) bottom topography which can capture the steady state solutions – corresponding to a constant energy – of the shallow water equations when the water velocity is zero. As a consequence, these new schemes allow a typical hyperbolic stability condition $\Delta t = O(\Delta x, \Delta v)$.

We extend both classes of the Hamiltonian-preserving schemes developed in [24] here. One (called *Scheme I*) is based on a finite difference approach, and involves interpolation in the slowness space. The second (called *Scheme II*) uses a finite volume approach, and numerical quadrature rule in the slowness space is needed. These new schemes allow a typical hyperbolic stability condition $\Delta t = O(\Delta x, \Delta v)$. We will also establish the