

Hamiltonian-preserving schemes for the Liouville equation with discontinuous potentials ^{*}

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Abstract

When numerically solving the Liouville equation with a discontinuous potential, one faces the problem of selecting a unique, physically relevant solution across the potential barrier, and the problem of a severe time step constraint due to the CFL condition. In this paper, We introduce two classes of Hamiltonian-preserving schemes for such problems. By using the constant Hamiltonian across the potential barrier, we introduced a selection criterion for a unique, physically relevant solution to the underlying linear hyperbolic equation with singular coefficients. These scheme have a hyperbolic CFL condition, which is a significant improvement over a conventional discretization. We also establish the positivity, and stability in both l^1 and l^∞ norms, of these discretizations, and conducted numerical experiments to study the numerical accuracy.

This work is motivated by the well-balanced kinetic schemes by Perthame and Simeoni for the shallow water equations with a discontinuous bottom topography, and has applications to the level set methods for the computations of multivalued physical observables in the semiclassical limit of the linear Schrödinger equation with a discontinuous potential, among other applications.

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1 Introduction

In this paper, we construct and study a class of numerical schemes for the d -dimensional Liouville equation in classical mechanics:

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

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 Liouville equation is a different formulation of Newton's second law:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}}{dt} = -\nabla_{\mathbf{x}} V, \quad (1.2)$$

which is a Hamiltonian system with the Hamiltonian

$$H = \frac{1}{2}|\mathbf{v}|^2 + V(\mathbf{x}) \quad (1.3)$$

It is known from classical mechanics that the Hamiltonian remains constant across a potential barrier.

The Liouville equation is a linear wave equation, with the characteristic speed determined by the Newton's equation (1.2)—which is usually called the bicharacteristic. If $V(\mathbf{x})$ is smooth, then the initial value problem to (1.2) is well-posed, and a standard numerical method (for example, the upwind scheme and its higher order extensions) for linear wave equation gives satisfactory results. However, if $V(\mathbf{x})$ is discontinuous—which corresponding to a potential barrier—then the characteristic speed of the Liouville equation given by (1.2) is *infinity* at the discontinuous point. When numerically approximating V_x across the interface, the numerical derivative of V is of $O(1/\Delta x)$, with Δx the mesh size in the physical space. Thus an explicit scheme needs time step $\Delta t = O(\Delta x \Delta \xi)$ with $\Delta \xi$ the mesh size in particle velocity space. This is very expensive. Moreover, a conventional numerical scheme in general does not preserve a *constant Hamiltonian* across the interface, usually leads to poor or even incorrect numerical resolutions by ignoring the discontinuities of $V(x)$. Theoretically, there is a uniqueness issue for weak solutions to these linear hyperbolic equations with singular wave speeds [2, 4, 7, 20, 21]. It is not clear which weak solution a standard numerical discretization that ignores the discontinuity of $V(x)$ will select.

Potential barriers appear in many important physical problems, such as the quantum tunneling (and quantum dots) in semiconductor device modeling, plasmas, and geometrical optics through different materials. Liouville or Vlasov equations describes the density distribution of particles in such a heterogeneous medium. For some recent mathematical study of discontinuous potentials in high frequency waves see [1, 17, 22].

In this paper, we construct a class of numerical schemes that are suitable for the Liouville equation (1.1) with a discontinuous potential. An important feature of

these schemes is that they are consistent to the constant Hamiltonian across a potential barrier for the Liouville equation (1.1). We call such schemes **Hamiltonian-preserving schemes**. A key idea in this paper is to use the behavior of a classical particle at the potential barrier—either cross over if its kinetic energy is sufficiently large— or be reflected with a negative velocity. We build this mechanics into the numerical scheme to construct the Hamiltonian-preserving schemes. This work is motivated by the well-balanced kinetic scheme of Perthame and Simeoni [19] for the shallow water equations with a (discontinuous) bottom topography, in which the similar mechanics was built into a hydrodynamic scheme for the shallow water equations in order to capture the steady state solutions—corresponding to a constant energy— of the shallow water equations. However, the work of Perthame and Simeoni was focused on a kinetic scheme for the shallow water equations defined in the physical space, thus the numerical discretization in the phase space was not studied. The phase space discretization is an important issue for the Liouville equation with a discontinuous potential. As shown by this work, if designed properly, the explicit Hamiltonian-preserving schemes allow a standard hyperbolic CFL condition $\Delta t = O(\Delta x, \Delta \xi)$. More importantly, by using the a constant Hamiltonian condition across the potential barrier, these schemes select a unique, and physically relevant, solutions for the underlying linear hyperbolic equation with singular coefficients.

Another application of the Liouville equation like (1.1) is the level set method for the computation of multivalued solutions to quasilinear PDEs, see [12, 3]. Such problem arises in the semiclassical limit of the linear Schrödinger equation, which yields the Liouville equation (1.1) with the initial data

$$f(\mathbf{x}, \mathbf{v}, 0) = \rho_0(\mathbf{x})\delta(\mathbf{v} - \mathbf{u}_0(\mathbf{x})), \quad (1.4)$$

see for example [16, 9]. In the physical space, the moments of f :

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}, \quad (1.5)$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x}, t)} \int f(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v} \quad (1.6)$$

may become *multivalued*, see [10, 25] and the relevant numerical methods [8, 6]. The level set method proposed in [11] solves the Liouville equation (1.1) with the initial data (1.4) by decomposing f into ϕ and $\psi_i (i = 1, \dots, d)$ where ϕ and ψ_i solve the same Liouville equation (1.1) with initial data

$$\phi(\mathbf{x}, \mathbf{v}, 0) = \rho_0(\mathbf{x}), \quad \psi_i(\mathbf{x}, \mathbf{v}, 0) = v_i - u_{i0}(\mathbf{x}), \quad (1.7)$$

respectively. This allows the numerical computations for a bounded solution rather than measure-valued solution of the Liouville equation with singular initial data (1.4), which greatly enhancing the numerical resolution. The moments can be recovered through

$$\rho(\mathbf{x}, t) = \int \phi(\mathbf{x}, \mathbf{v}, t) \prod_{i=1}^d \delta(\psi_i) d\mathbf{v}, \quad (1.8)$$

$$\mathbf{u}(\mathbf{x}, t) = \int \phi(\mathbf{x}, \mathbf{v}, t) \mathbf{v} \prod_{i=1}^d \delta(\psi_i) d\mathbf{v} / \rho(\mathbf{x}, t) \quad (1.9)$$

Numerical computations of multivalued solution for smooth potential using this technique were given in [11] for smooth potentials. In this article we will also apply the Hamiltonian-preserving schemes for the level set computations of multivalued solution of the physical observables ρ , \mathbf{u} , etc.

In Sections 2, we first point out the problems with the usual finite difference scheme to solve the Liouville equation with discontinuous potentials. We then present the designing principle of our Hamiltonian-preserving schemes using the behavior of classical particles at a potential barrier. In Section 3, a 1d Hamiltonian-preserving scheme based on a finite difference approach (called Scheme I) is given, and its positivity and l^∞ are established. In Section 4, a 1D Hamiltonian-preserving scheme based on a finite volume approach (called Scheme II) is given. We extend these schemes to higher dimension in Section 5. In Section 6, we study the l^1 -stability of Scheme I. We prove that the scheme is l^1 -stable for suitable initial data, while for other (such as the measure-valued (1.4)) initial data the solution may become unbounded. In Section 7, we prove that Scheme II is positive, l^∞ -stable, and l^1 -contracting (for more general l^1 initial data than Scheme I). In Section 8, we show that even for smooth initial data, the solution to the Liouville equation (1.1) could become discontinuous in the downstream part of the potential barrier. This contributes to the reduced numerical convergence rate to 1/2 for a formally first order scheme, as in any shock capturing method for a linear wave equation with discontinuous initial data. Numerical examples are given in Section 9 to verify the accuracy of the two schemes constructed in this paper. We conclude the paper in Section 10.

2 The designing principle of the Hamiltonian-preserving schemes

2.1 Deficiency of the usual finite difference schemes

We consider the numerical solution of the 1D Liouville equation

$$f_t + \xi f_x - V_x f_\xi = 0 \quad (2.1)$$

with a discontinuous potential $V(x)$.

Without loss of generality, we employ an uniform mesh with grid points at $x_{i+\frac{1}{2}}, i = 0, \dots, N$, in the x -direction and $\xi_{j+\frac{1}{2}}, j = 0, \dots, M$ in the ξ -direction. The cells are centered at $(x_i, \xi_j), i = 1, \dots, N, j = 1, \dots, M$ 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 is 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 time is given by

$0 = t_0 < t_1 < \dots < t_L = T$. We introduce mesh ratios $\lambda_x^t = \frac{\Delta t}{\Delta x}$, $\lambda_\xi^t = \frac{\Delta t}{\Delta \xi}$, $\lambda_x^\xi = \frac{\Delta \xi}{\Delta x}$, assumed to be fixed. We define the cell averages of f as

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

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

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

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

A typical semi-discrete finite difference method for this equation is

$$\partial_t f_{ij} + \xi_j \frac{f_{i+\frac{1}{2},j} - f_{i-\frac{1}{2},j}}{\Delta x} - DV_i \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0, \quad (2.2)$$

where the numerical fluxes $f_{i+\frac{1}{2},j}$, $f_{i,j+\frac{1}{2}}$ are defined by the upwind scheme, and DV_i is some numerical approximation of V_x at $x = x_i$.

Such a discretization suffers from at least two problems:

- The above discretization in general does not preserve a constant Hamiltonian $H = \frac{1}{2}\xi^2 + V$ across the discontinuities of V . Such a numerical approximation may lead to unphysical problem or poor numerical resolution.
- If an explicit time discretization is used, the CFL condition for this scheme requires the time step to satisfy

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i |DV_i|}{\Delta \xi} \right] \leq 1. \quad (2.3)$$

Since the potential $V(x)$ is discontinuous at some points, $\max_i |DV_i| = O(1/\Delta x)$, so the CFL condition (2.3) requires $\Delta t = O(\Delta x \Delta \xi)$.

2.2 Behavior of a classical particle at a potential barrier

In classical mechanics, a particle will either cross a potential barrier with a changing momentum, or be reflected, depending on its momentum and on the strength of the potential barrier. *The Hamiltonian $H = \frac{1}{2}\xi^2 + V$ should be preserved across the potential barrier:*

$$\frac{1}{2}(\xi^+)^2 + V^+ = \frac{1}{2}(\xi^-)^2 + V^- \quad (2.4)$$

where the superscripts \pm indicate the right and left limits of the quantity at the potential barrier.

For example, consider the case when, at a potential discontinuity, the characteristic on the left of the potential discontinuity is given as a constant velocity $\xi^- > 0$. There are three possibilities (see Figure 2.1) :

- 1) $V^- > V^+$. In this case, the potential decreases, so the particle will cross the potential barrier and gain momentum in order to maintain a constant Hamiltonian. (2.4) implies

$$\xi^+ = \sqrt{(\xi^-)^2 + 2(V^- - V^+)}.$$

- 2) $V^- < V^+$ and $\frac{1}{2}(\xi^-)^2 > V^+ - V^-$. If the kinetic energy of the particle is bigger than the potential jump then the particle will cross the barrier with a reduced momentum. (2.4) implies

$$\xi^+ = \sqrt{(\xi^-)^2 - 2(V^+ - V^-)}$$

- 3) $V^- < V^+$ and $\frac{1}{2}(\xi^-)^2 < V^+ - V^-$. In this case, the kinetic energy is not large enough for the particle to cross the potential barrier, so the particle will be reflected with a negative velocity $-\xi^-$.

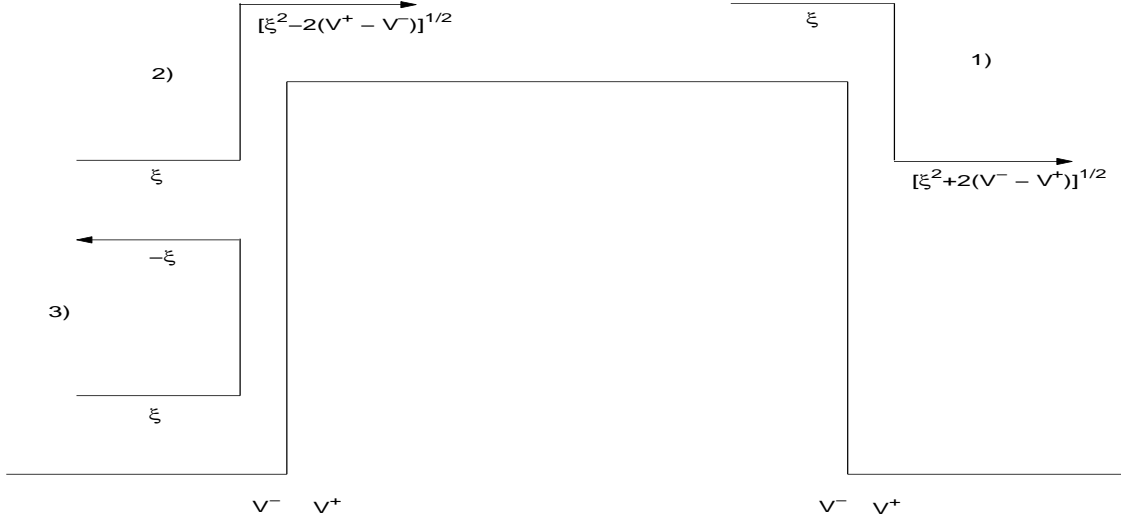


Figure 2.1 Change of particle momentum across a potential barrier for the case when $\xi^- > 0$.

If $\xi^- < 0$, similar behavior can also be analyzed using the constant Hamiltonian condition (2.4). See Fig.2.1.

The main ingredient in the *well-balanced* kinetic scheme by Perthame and Simeoni [19] for the shallow water equations with topography was to build in the above mechanism into the numerical scheme in order to preserve the steady state solution of the shallow water equations when the water velocity is zero. Note that the density distribution f remains unchanged across the potential barrier, thus

$$f(t, x^+, \xi^+) = f(t, x_-, \xi^-) \quad (2.5)$$

at a discontinuous point x of $V(x)$, where ξ^+ and ξ^- are related by the constant Hamiltonian condition (2.4). This was used in constructing the numerical flux in [19].

In this paper, we use this mechanism for the numerical approximation to the Liouville equation with a discontinuous potential. This approximation, by its design, maintains a constant Hamiltonian up to approximation error across the potential barrier. The new issue faced here, not explored in [19], is the discretization in the ξ -direction. Given ξ^- as a grid point, the ξ^+ constructed from the constant Hamiltonian condition (2.4) may not be a grid point, thus some appropriate interpolations in the ξ -direction is needed here. The approximation in the ξ -direction, and its consequent numerical properties, constitutes the main body of this paper.

3 Scheme I: a finite difference approach

3.1 The Hamiltonian-preserving numerical flux

We now describe our first finite difference scheme for the Liouville equation with a discontinuous potential. We call this scheme as *Scheme I*.

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

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

We will adopt the flux splitting technique used in [19]. The semidiscrete scheme (with time continuous) reads

$$\partial_t f_{ij} + \xi_j \frac{f_{i+1/2,j}^- - f_{i-1/2,j}^+}{\Delta x} - \frac{V_{i+1/2}^- - V_{i-1/2}^+}{\Delta x} \frac{f_{i,j+1/2} - f_{i,j-1/2}}{\Delta \xi} = 0, \quad (3.1)$$

where the numerical fluxes $f_{i,j+1/2}$ are defined using the upwind discretization. Since the characteristics of the Liouville equation may be different on the two sides of a potential discontinuity, the corresponding numerical fluxes should also be different. The essential part of our algorithm is to define the split numerical fluxes $f_{i+1/2,j}^-$, $f_{i-1/2,j}^+$ at each cell interface. We will use (2.5) to define these fluxes.

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

$$f_{i+1/2,j}^+ = f(x_{i+1/2}^+, \xi_j^+) = f(x_{i+1/2}^-, \xi_j^-)$$

while ξ^- is obtained from $\xi_j^+ = \xi_j$ from (2.4). 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 detailed algorithm to generate the numerical flux is given below.

Algorithm I

- $\xi_j > 0$

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

- if $V_{i+\frac{1}{2}}^- > V_{i+\frac{1}{2}}^+$,

$$\star \text{ if } \xi_j > \sqrt{2 \left(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+ \right)},$$

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

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

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

☆ else

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

☆ end

- if $V_{i+\frac{1}{2}}^- < V_{i+\frac{1}{2}}^+$

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

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

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

- if $V_{i+\frac{1}{2}}^- = V_{i+\frac{1}{2}}^+$

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

- end

- $\xi_j < 0$

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

- if $V_{i+\frac{1}{2}}^- < V_{i+\frac{1}{2}}^+$,

$$\star \text{ if } |\xi_j| > \sqrt{2 \left(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^- \right)},$$

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

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

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

☆ else

$$f_{i+\frac{1}{2},j}^- = f_{ik} \text{ where } \xi_k = -\xi_j$$

☆ end

□ if $V_{i+\frac{1}{2}}^- > V_{i+\frac{1}{2}}^+$

$$\xi^+ = -\sqrt{\xi_j^2 + 2(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+)}$$

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

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

□ if $V_{i+\frac{1}{2}}^- = V_{i+\frac{1}{2}}^+$

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

□ end

The above algorithm for evaluating numerical fluxes is of first order. One can obtain a second order flux by incorporating the slope limiter, such as van Leer or minmod slope limiter [15, 26], into the above algorithm. This can be achieved by replacing f_{ik} by $f_{ik} + \frac{\Delta x}{2} s_{ik}$, and replacing $f_{i+1,k}$ by $f_{i+1,k} - \frac{\Delta x}{2} s_{i+1,k}$ in the above algorithm for all the possible index k , where s_{ik} is the slope limiter in the x -direction.

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

3.2 Positivity and l^∞ contraction

Since the exact solution of the Liouville equation is positive when the initial profile is, it is important that the numerical solution inherits this property.

We only consider the scheme using the first order numerical flux, and the forward Euler method in time. Without loss of generality, we consider the case $\xi_j > 0$ and $V_{i+\frac{1}{2}}^- < V_{i-\frac{1}{2}}^+$ for all i (the other cases can be treated similarly with the same conclusion). The scheme reads

$$\frac{f_{ij}^{n+1} - f_{ij}}{\Delta t} + \xi_j \frac{f_{ij} - (c_1 f_{i-1,k} + c_2 f_{i-1,k+1})}{\Delta x} - \frac{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+}{\Delta x} \frac{f_{ij} - f_{i,j-1}}{\Delta \xi} = 0,$$

where c_1, c_2 are positive and $c_1 + c_2 = 1$. We omit the possible superscript n of f . The above scheme can be rewritten as

$$\begin{aligned} f_{ij}^{n+1} &= \left(1 - |\xi_j| \lambda_x^t - \frac{|V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+|}{\Delta x} \lambda_\xi^t \right) f_{ij} + |\xi_j| \lambda_x^t (c_1 f_{i-1,k} + c_2 f_{i-1,k+1}) \\ &+ \frac{|V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+|}{\Delta x} \lambda_\xi^t f_{i,j-1}. \end{aligned} \quad (3.2)$$

Now we investigate the positivity of scheme (3.2). This is to prove that if $f_{ij}^n \geq 0$ for all (i, j) , then this is also true for f^{n+1} . Clearly one just needs to show that all the coefficients before f^n are non-negative. A sufficient condition for this is clearly

$$1 - |\xi_j| \lambda_x^t - \frac{|V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+|}{\Delta x} \lambda_\xi^t \geq 0,$$

or

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \frac{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+}{\Delta x} \right|}{\Delta \xi} \right] \leq 1. \quad (3.3)$$

This CFL condition is similar to the CFL condition (2.3) of the usual finite difference scheme *except* that the quantity $\left| \frac{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+}{\Delta x} \right|$ now represents the gradient of potential at its *smooth* point, which has a *finite* upper bound. Thus our new scheme has a hyperbolic CFL condition.

According to the study in [18], our second order scheme, which incorporates slope limiter into the first order scheme, is positive under the half CFL condition, namely, the constant on the right hand side of (3.3) is 1/2.

The above conclusion are analyzed based on forward Euler time discretization. One can draw the same conclusion for the second order TVD Runge-Kutta time discretization [24].

The l^∞ -contracting property of this scheme follows easily with the same hyperbolic CFL condition, because the coefficients in (3.2) are positive and the sum of them is 1.

4 Scheme II: a finite volume approach

In this section another flux which results in an l^1 -contracting scheme is proposed. We call this scheme *Scheme II*.

By integrating the Liouville equation (2.1) over the cell $[x_{i-1/2}, x_{i+1/2}] \times [\xi_{j-1/2}, \xi_{j+1/2}]$, one gets the following equation

$$\partial_t f_{ij} + \xi_j \frac{f_{i+\frac{1}{2},j}^- - f_{i-\frac{1}{2},j}^+}{\Delta x} - \frac{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+}{\Delta x} \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0. \quad (4.1)$$

The upwind discretization depends on the sign of ξ_j and $\frac{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+}{\Delta x}$. To illustrate the basic idea, we assume $\xi_j > 0$, $\frac{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+}{\Delta x} < 0$ and $V_{i+\frac{1}{2}}^- < V_{i+\frac{1}{2}}^+$ (this is the case

when the particle loses momentum from left to right at the barrier). In this case

$$\begin{aligned} f_{i+\frac{1}{2},j}^- &= \frac{1}{\xi_j \Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi f \left(x_{i+\frac{1}{2}}^-, \xi, t \right) d\xi, \\ f_{i,j+\frac{1}{2}} &= \frac{1}{V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} V_x f \left(x, \xi_{j+\frac{1}{2}}^-, t \right) dx \end{aligned}$$

By using the condition (2.5):

$$f_{i+\frac{1}{2},j}^+ = \frac{1}{\xi_j \Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi f \left(x_{i+\frac{1}{2}}^+, \xi, t \right) d\xi, = \frac{1}{\xi_j \Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi \bar{f} \left(x_{i+\frac{1}{2}}^-, \xi, t \right) d\xi, \quad (4.2)$$

where \bar{f} is defined as

$$\bar{f} \left(x_{i+\frac{1}{2}}^-, \xi, t \right) = f \left(x_{i+\frac{1}{2}}^-, \sqrt{\xi^2 + 2 \left(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^- \right)}, t \right).$$

Using a change of variable on (4.2) leads to

$$\begin{aligned} f_{i+\frac{1}{2},j}^+ &= \frac{1}{\xi_j \Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi f \left(x_{i+\frac{1}{2}}^-, \sqrt{\xi^2 + 2 \left(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^- \right)}, t \right) d\xi \\ &= \frac{1}{\xi_j \Delta \xi} \int_{\xi'_1}^{\xi'_2} \xi f \left(x_{i+\frac{1}{2}}^-, \xi, t \right) d\xi. \end{aligned} \quad (4.3)$$

where

$$\xi'_1 = \sqrt{\xi_{j-\frac{1}{2}}^2 + 2(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^-)}, \quad \xi'_2 = \sqrt{\xi_{j+\frac{1}{2}}^2 + 2(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^-)}. \quad (4.4)$$

The integral in (4.3) will be approximated by a quadrature rule. Since the end point ξ'_1 and ξ'_2 may not be grid points in the ξ -direction. We first need to locate the grid points that bound ξ'_1 and ξ'_2 . There are two possibilities, namely, either ξ'_1 and ξ'_2 fall into the same cell, or they are in separate cells. In the former case, we use the midpoint rule. In the second case, the composite midpoint rule is used.

We propose the following evaluation of the split fluxes $f_{i+\frac{1}{2},j}^\pm$ in (4.1)

Algorithm II

- if $\xi_j > 0$

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

- if $V_{i+\frac{1}{2}}^- > V_{i+\frac{1}{2}}^+$,

$$\star \text{ if } \xi_{j-\frac{1}{2}} \geq \sqrt{2 \left(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+ \right)},$$

$$\xi'_1 = \sqrt{\xi_{j-\frac{1}{2}}^2 - 2 \left(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+ \right)}$$

$$\xi'_2 = \sqrt{\xi_{j+\frac{1}{2}}^2 - 2 \left(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+ \right)}$$

* if $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi'_2 \leq \xi_{k+\frac{1}{2}}$ for some k

$$f_{i+\frac{1}{2},j}^+ = \frac{1}{\xi_j} \frac{\xi'_2 - \xi'_1}{\Delta \xi} \xi_k f_{ik}$$

* else $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi_{k+\frac{1}{2}} < \dots < \xi_{k+s-\frac{1}{2}} < \xi'_2 \leq \xi_{k+s+\frac{1}{2}}$ for some k, s

$$f_{i+\frac{1}{2},j}^+ = \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta \xi} \xi_k f_{ik} + \xi_{k+1} f_{i,k+1} + \dots \right. \\ \left. + \xi_{k+s-1} f_{i,k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta \xi} \xi_{k+s} f_{i,k+s} \right\}$$

* end

☆ else

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

☆ end

□ if $V_{i+\frac{1}{2}}^- < V_{i+\frac{1}{2}}^+$

$$\xi'_1 = \sqrt{\xi_{j-\frac{1}{2}}^2 + 2 \left(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^- \right)}$$

$$\xi'_2 = \sqrt{\xi_{j+\frac{1}{2}}^2 + 2 \left(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^- \right)}$$

* if $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi'_2 \leq \xi_{k+\frac{1}{2}}$ for some k

$$f_{i+\frac{1}{2},j}^+ = \frac{1}{\xi_j} \frac{\xi'_2 - \xi'_1}{\Delta \xi} \xi_k f_{ik}$$

* else $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi_{k+\frac{1}{2}} < \dots < \xi_{k+s-\frac{1}{2}} < \xi'_2 \leq \xi_{k+s+\frac{1}{2}}$ for some k, s

$$f_{i+\frac{1}{2},j}^+ = \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta \xi} \xi_k f_{ik} + \xi_{k+1} f_{i,k+1} + \dots \right. \\ \left. + \xi_{k+s-1} f_{i,k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta \xi} \xi_{k+s} f_{i,k+s} \right\}$$

* end

□ if $V_{i+\frac{1}{2}}^- = V_{i+\frac{1}{2}}^+$

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

□ end

• if $\xi_j < 0$

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

□ if $V_{i+\frac{1}{2}}^- < V_{i+\frac{1}{2}}^+$,

☆ if $|\xi_{j+\frac{1}{2}}| > \sqrt{2(V_{i+\frac{1}{2}}^+ - V_{i+\frac{1}{2}}^-)}$,

$$\xi'_1 = -\sqrt{\xi_{j-\frac{1}{2}}^2 + 2(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+)}$$

$$\xi'_2 = -\sqrt{\xi_{j+\frac{1}{2}}^2 + 2(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+)}$$

* if $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi'_2 \leq \xi_{k+\frac{1}{2}}$ for some k

$$f_{i+\frac{1}{2},j}^- = \frac{1}{\xi_j} \frac{\xi'_2 - \xi'_1}{\Delta\xi} \xi_k f_{i+1,k}$$

* else $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi_{k+\frac{1}{2}} < \dots < \xi_{k+s-\frac{1}{2}} < \xi'_2 \leq \xi_{k+s+\frac{1}{2}}$ for some k, s

$$f_{i+\frac{1}{2},j}^- = \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k f_{i+1,k} + \xi_{k+1} f_{i+1,k+1} + \dots \right. \\ \left. + \xi_{k+s-1} f_{i+1,k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s} f_{i+1,k+s} \right\}$$

* end

☆ else

$$f_{i+\frac{1}{2},j}^- = f_{ik} \text{ where } \xi_k = -\xi_j$$

☆ end

□ if $V_{i+\frac{1}{2}}^- > V_{i+\frac{1}{2}}^+$

$$\xi'_1 = -\sqrt{\xi_{j-\frac{1}{2}}^2 + 2(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+)}$$

$$\xi'_2 = -\sqrt{\xi_{j+\frac{1}{2}}^2 + 2(V_{i+\frac{1}{2}}^- - V_{i+\frac{1}{2}}^+)}$$

* if $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi'_2 \leq \xi_{k+\frac{1}{2}}$ for some k

$$f_{i+\frac{1}{2},j}^- = \frac{1}{\xi_j} \frac{\xi'_2 - \xi'_1}{\Delta\xi} \xi_k f_{i+1,k}$$

* else $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi_{k+\frac{1}{2}} < \dots < \xi_{k+s-\frac{1}{2}} < \xi'_2 \leq \xi_{k+s+\frac{1}{2}}$ for some k, s

$$f_{i+\frac{1}{2},j}^- = \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k f_{i+1,k} + \xi_{k+1} f_{i+1,k+1} + \dots \right. \\ \left. + \xi_{k+s-1} f_{i+1,k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s} f_{i+1,k+s} \right\}$$

* end

□ if $V_{i+\frac{1}{2}}^- = V_{i+\frac{1}{2}}^+$

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

□ end

- end

Remark 4.1. The above Algorithm uses a first order quadrature rule at the ends of the interval (4.3), thus it is of first order even if the slope limiters in x -direction are incorporated into the algorithm. One can also use a second order quadrature rule at the ends of intervals (4.3).

5 The schemes in higher dimensions

Our 1D schemes can be easily extended to higher dimension using a dimension-by-dimension approach. For example, consider the 2D Liouville equation

$$f_t + \xi f_x + \eta f_y - V_x f_\xi - V_y f_\eta = 0. \quad (5.1)$$

We employ a uniform mesh with grid points at $x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, \xi_{k+\frac{1}{2}}, \eta_{l+\frac{1}{2}}$ in each direction. The cells are centered at $(x_i, y_j, \xi_k, \eta_l)$ with $x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$, $y_j = \frac{1}{2}(y_{j+\frac{1}{2}} + y_{j-\frac{1}{2}})$, $\xi_k = \frac{1}{2}(\xi_{k+\frac{1}{2}} + \xi_{k-\frac{1}{2}})$, $\eta_l = \frac{1}{2}(\eta_{l+\frac{1}{2}} + \eta_{l-\frac{1}{2}})$. The mesh size is denoted by $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$, $\Delta y = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}$, $\Delta \xi = \xi_{k+\frac{1}{2}} - \xi_{k-\frac{1}{2}}$, $\Delta \eta = \eta_{l+\frac{1}{2}} - \eta_{l-\frac{1}{2}}$. We define the cell average of f as

$$f_{ijkl} = \frac{1}{\Delta x \Delta y \Delta \xi \Delta \eta} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{\xi_{k-\frac{1}{2}}}^{\xi_{k+\frac{1}{2}}} \int_{\eta_{l-\frac{1}{2}}}^{\eta_{l+\frac{1}{2}}} f(x, y, \xi, \eta, t) d\eta d\xi dy dx.$$

Similarly to the 1D case, we approximate the potential by a piecewise bilinear function, and for convenience, we always provide two interface values of potential at each cell interface. When the potential is smooth at a cell interface, the two potential interface values are identical.

The 2D Liouville equation (5.1) can be semi-discretized as

$$\begin{aligned} \partial_t f_{ijkl} &+ \xi_k \frac{f_{i+\frac{1}{2},jkl}^- - f_{i-\frac{1}{2},jkl}^+}{\Delta x} + \eta_l \frac{f_{i,j+\frac{1}{2},kl}^- - f_{i,j-\frac{1}{2},kl}^+}{\Delta y} \\ &- \frac{V_{i+\frac{1}{2},j}^- - V_{i-\frac{1}{2},j}^+}{\Delta x} \frac{f_{ij,k+\frac{1}{2},l} - f_{ij,k-\frac{1}{2},l}}{\Delta \xi} - \frac{V_{i,j+\frac{1}{2}}^- - V_{i,j-\frac{1}{2}}^+}{\Delta y} \frac{f_{ijk,l+\frac{1}{2}} - f_{ijk,l-\frac{1}{2}}}{\Delta \eta} = 0, \end{aligned}$$

where the interface values $f_{ij,k+\frac{1}{2},l}, f_{ijk,l+\frac{1}{2}}$ are provided by the upwind approximation, and the split interface values $f_{i+\frac{1}{2},jkl}^-, f_{i-\frac{1}{2},jkl}^+, f_{i,j+\frac{1}{2},kl}^-, f_{i,j-\frac{1}{2},kl}^+$ can be obtained using essentially the same algorithm described in subsection 2.3 or 2.5 for the 1D case. Since the gradient of the potential at its smooth points are bounded, this scheme similar to the 1D scheme, is also subject to a hyperbolic CFL condition under which the scheme is positive, and Hamiltonian preserving (if the discontinuity of V aligns with the grids).

6 The l^1 -stability theory of Scheme I

In this section we prove the l^1 -stability of Scheme I (with the first order numerical flux and the forward Euler method in time) under a suitable assumption on the initial data. We also show that if this assumption does not hold, the numerical solution can grow unbounded in l^1 . We consider the simple case when $V(x)$ is a step function, with a jump $-D, D > 0$ at $x_{m+\frac{1}{2}}$. Namely

$$V_{m+\frac{1}{2}}^- - V_{m+\frac{1}{2}}^+ = D, \quad V_{i+\frac{1}{2}}^\pm = V_{m+\frac{1}{2}}^-, i < m, \quad V_{i+\frac{1}{2}}^\pm = V_{m+\frac{1}{2}}^+, i > m.$$

We consider the typical situation that $\xi_1 < -\sqrt{2D}, \xi_M > \sqrt{2D}$, so that all the three situations discussed in Section 2 are included. We also choose the mesh such that 0 is a grid point in the ξ -direction.

Define an index set

$$D_l^4 = \{(i, j) | x_i \leq x_m, \xi_j < -\sqrt{\xi_1^2 - 2D}\}.$$

Due to velocity change across the potential jump at $x_{m+\frac{1}{2}}$, D_l^4 represents the area where particles come from outside of the domain $[x_1, x_N] \times [\xi_1, \xi_M]$. In order to implement Scheme I conveniently, we need to choose the computational domain as

$$E_d = \{(i, j) | i = 1, \dots, N, j = 1, \dots, M\} \setminus D_l^4. \quad (6.1)$$

Figure 6.1 depicts E_d and D_l^4 .

We define the l^1 -norm of a numerical solution f_{ij} to be

$$|f|_1 = \frac{1}{N_d} \sum_{(i,j) \in E_d} |f_{ij}|$$

with N_d being the number of elements in E_d .

6.1 l^1 -stability under an assumption on the initial data

Given the initial data $f_{ij}^0, (i, j) \in E_d$. Denote the numerical solution at time T to be $f_{ij}^L, (i, j) \in E_d$. To prove the l^1 -stability, we need to show that $|f^L|_1 \leq C|f^0|_1$.

Due to the linearity of the scheme, the equation for the error between the analytical and the numerical solution is the same as (3.2), so in this section, f_{ij} will denote the error. We assume there is no error at the boundary, thus $f_{ij}^n = 0$ at the boundary. If the l^1 -norm of the error introduced at each time step in incoming boundary cells is ensured to be $o(1)$ part of $|f^n|_1$, our following analysis still applies.

Since $V_x(x) = 0$ except at $x = x_{m+1/2}$, Scheme I is given by:

1) if $\xi_j > 0, i \neq m + 1$,

$$f_{ij}^{n+1} = (1 - \xi_j \lambda_x^t) f_{ij} + \xi_j \lambda_x^t f_{i-1,j}; \quad (6.2)$$

2) if $\xi_j < 0, i \neq m$,

$$f_{ij}^{n+1} = (1 - |\xi_j| \lambda_x^t) f_{ij} + |\xi_j| \lambda_x^t f_{i+1,j}; \quad (6.3)$$

3) if $\xi_j > \sqrt{2D}$,

$$f_{m+1,j}^{n+1} = (1 - \xi_j \lambda_x^t) f_{m+1,j} + \xi_j \lambda_x^t (c_{j,k} f_{m,k} + c_{j,k+1} f_{m,k+1}); \quad (6.4)$$

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

$$f_{m+1,j}^{n+1} = (1 - \xi_j \lambda_x^t) f_{m+1,j} + \xi_j \lambda_x^t f_{m+1,k}; \quad (6.5)$$

5) if $\xi_j < 0$,

$$f_{mj}^{n+1} = (1 - |\xi_j| \lambda_x^t) f_{mj} + |\xi_j| \lambda_x^t (c_{jk} f_{m+1,k} + c_{j,k+1} f_{m+1,k+1}), \quad (6.6)$$

where $0 \leq c_{jk} \leq 1$ and $c_{jk} + c_{j,k+1} = 1$. In (6.4) k is determined by $\xi_k \leq \sqrt{\xi_j^2 - 2D} < \xi_{k+1}$, in (6.6) $\xi_k = -\xi_j$, and in (6.5) $\xi_k \leq -\sqrt{\xi_j^2 + 2D} < \xi_{k+1}$. We omit the superscript n of f_{ij} on the right hand side.

Using the triangle inequality in (6.2)-(6.6), one typically gets the following

$$|f^{n+1}|_1 \leq \frac{1}{N_d} \sum_{(i,j) \in E_d} \alpha_{ij} |f_{ij}^n|, \quad (6.7)$$

where the coefficients α_{ij} are positive. One can check that, under the hyperbolic CFL condition (3.3), $\alpha_{ij} \leq 1$ except for possibly $(i,j) \in D_m^2 \cup D_{m+1}^4$ with the definitions:

$$D_m^2 = \{(m,j) | 0 < \xi_j < \sqrt{\xi_N^2 - 2D} + \Delta\xi\},$$

$$D_{m+1}^4 = \{(m+1,j) | \xi_j < -\sqrt{\Delta\xi^2/4 + 2D} + \Delta\xi\}.$$

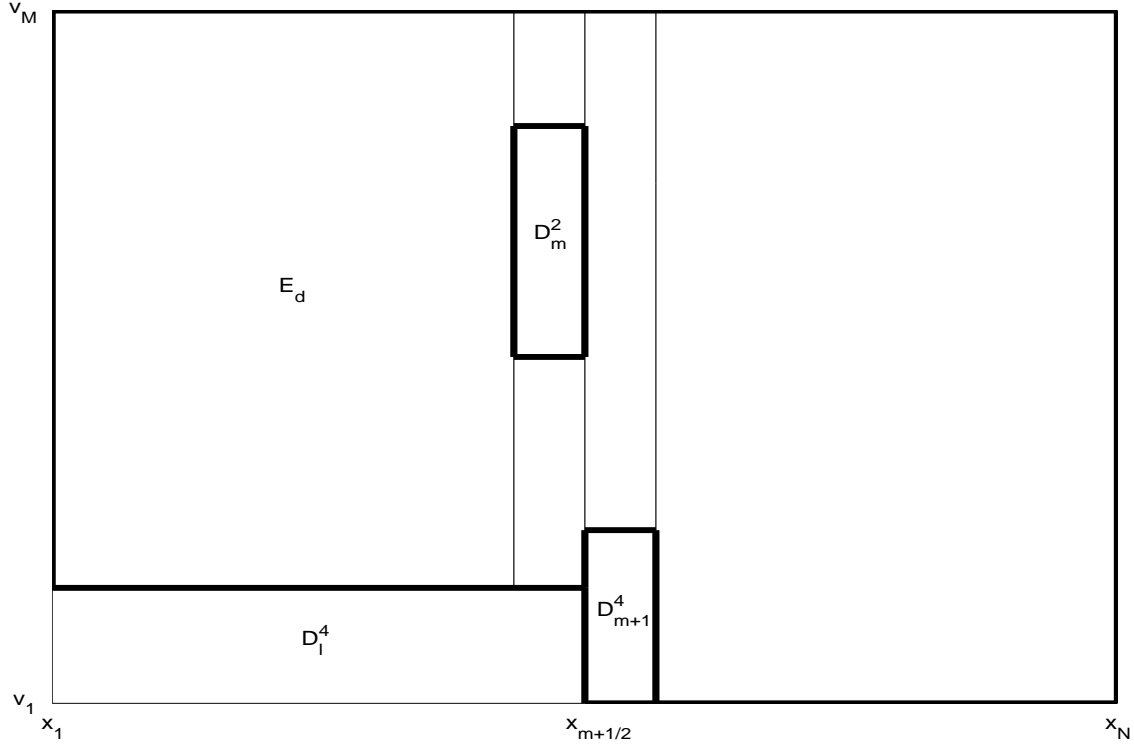


Figure 6.1 Sketch of the index sets D_m^2, D_{m+1}^4, D_l^4 .

Denote

$$M_1 = \max_{(i,j) \in D_m^2} \alpha_{ij}, \quad M_2 = \max_{(i,j) \in D_{m+1}^4} \alpha_{ij}.$$

Our next step is to prove that M_1, M_2 are bounded independent of the mesh size. Let us first examine M_1 .

Define the set

$$S_j^m = \left\{ j' \mid \xi_{j'} > \sqrt{2D}, \left| \sqrt{\xi_{j'}^2 - 2D} - \xi_j \right| < \Delta\xi \right\} \quad \text{for } (m, j) \in D_m^2.$$

Let the number of elements in S_j^m be N_j^m . One can check that $N_j^m \leq 2$ because every two elements $j'_1, j'_2 \in S_j^m$ satisfy $\left| \sqrt{\xi_{j'_1}^2 - 2D} - \sqrt{\xi_{j'_2}^2 - 2D} \right| \geq |\xi_{j'_1} - \xi_{j'_2}| \geq \Delta\xi$.

On the other hand, one can easily check from (6.4), for $(m, j) \in D_m^2$,

$$\alpha_{mj} < 1 + N_j^m \leq 3,$$

so the boundedness of M_1 is proved.

Next we study M_2 . Define the set

$$S_j^{m+1} = \left\{ j' \mid \left| -\sqrt{\xi_{j'}^2 + 2D} - \xi_j \right| < \Delta\xi \right\} \quad \text{for } (m+1, j) \in D_{m+1}^4.$$

Let $\xi_{max} = \max\{|\xi_1|, |\xi_M|\}$. Using the CFL condition, $\frac{\xi_{max}\Delta t}{\Delta x} \leq 1$. So from (6.6) one can get, for $(m+1, j) \in D_{m+1}^4$, the estimate for $\alpha_{m+1, j}$:

$$\alpha_{m+1, j} < 1 + \sum_{j' \in S_j^{m+1}} |\xi_{j'}| \lambda_x^t \leq 1 + \frac{1}{\xi_{max}} \sum_{j' \in S_j^{m+1}} |\xi_{j'}|. \quad (6.8)$$

Since $\xi_{j'}$, for $j' \in S_j^{m+1}$, are in fact an arithmetic progression with increment $\Delta\xi$. Denote the minimum and maximum element in S_j^{m+1} to be m_1, m_2 respectively. Since $\xi_{m_1}, \xi_{m_2} < 0$, one has $|\xi_{m_2}| \leq |\xi_{m_1}|$. The last summation in (6.8) turns out to be

$$\sum_{j' \in S_j^{m+1}} |\xi_{j'}| = \frac{|\xi_{m_1}| + |\xi_{m_2}|}{2} \left(\frac{|\xi_{m_1}| - |\xi_{m_2}|}{\Delta\xi} + 1 \right) \leq \frac{\xi_{m_1}^2 - \xi_{m_2}^2}{2\Delta\xi} + \xi_{max}. \quad (6.9)$$

On the other hand, because $m_1, m_2 \in S_j^{m+1}$,

$$\begin{aligned} & \sqrt{\xi_{m_1}^2 + 2D} - \sqrt{\xi_{m_2}^2 + 2D} \leq 2\Delta\xi, \\ \Rightarrow & \sqrt{\xi_{m_1}^2 + 2D} \leq \sqrt{\xi_{m_2}^2 + 2D} + 2\Delta\xi, \\ \Rightarrow & \xi_{m_1}^2 \leq \xi_{m_2}^2 + 2\sqrt{\xi_{m_2}^2 + 2D}\Delta\xi + 4\Delta\xi^2, \\ \Rightarrow & \frac{\xi_{m_1}^2 - \xi_{m_2}^2}{2\Delta\xi} \leq \sqrt{\xi_{m_2}^2 + 2D} + 2\Delta\xi \leq \xi_{max} + 2\Delta\xi. \end{aligned} \quad (6.10)$$

Combine (6.8)-(6.10), we get

$$\alpha_{m+1, j} < 1 + \frac{1}{\xi_{max}}(2\xi_{max} + 2\Delta\xi) = 3 + 2\frac{\Delta\xi}{\xi_{max}}$$

with $(m+1, j) \in D_{m+1}^4$. Therefore the boundedness of M_2 is proved.

In summary, we have

$$M_1 < 3, \quad M_2 < 3 + 2\frac{\Delta\xi}{\xi_{max}},$$

both are bounded independent of mesh size.

Denote $M'_1 = \max(0, M_1 - 1)$, $M'_2 = \max(0, M_2 - 1)$. From (6.7),

$$|f^{n+1}|_1 \leq |f^n|_1 + \frac{M'_1}{N_d} \sum_{(i, j) \in D_m^2} |f_{ij}^n| + \frac{M'_2}{N_d} \sum_{(i, j) \in D_{m+1}^4} |f_{ij}^n|. \quad (6.11)$$

We now impose an assumption:

Assumption 1

There exists a positive constant ξ_z such that

$$\forall (i, j) \in S_z = \{(i, j) \mid x_i < x_{m+\frac{1}{2}}, \quad 0 < \xi_j < \xi_z\}, \quad (6.12)$$

it holds that

$$|f_{ij}^0| \leq C_1 |f^0|_1. \quad (6.13)$$

Remark: The semiclassical limit initial data (1.4) does not satisfy this condition. Thus Scheme I, when directly applied to this problem, may have stability problems, as shown in the next subsection. However, if the decomposition idea mentioned in the Introduction is used, Scheme I is still suitable, which is what will be done in the numerical experiments of Section 9.

We now establish the following theorem:

Theorem 6.1. *Under Assumption 1, there exists an $h_0 > 0$, when $\Delta x < h_0$, the l^1 -stability property*

$$|f^L|_1 \leq C |f^0|_1$$

of the scheme (6.2)-(6.6) holds.

Proof. From (6.11),

$$|f^L|_1 \leq |f^0|_1 + \frac{M'_1}{N_d} \sum_{n=0}^{L-1} \left\{ \sum_{(i,j) \in D_m^2} |f_{ij}^n| \right\} + \frac{M'_2}{N_d} \sum_{n=0}^{L-1} \left\{ \sum_{(i,j) \in D_{m+1}^4} |f_{ij}^n| \right\}. \quad (6.14)$$

It remains to estimate

$$S_1 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j) \in D_m^2} |f_{ij}^n| \right\} \quad (6.15)$$

and

$$S_2 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j) \in D_{m+1}^4} |f_{ij}^n| \right\}. \quad (6.16)$$

We begin with estimating S_2 .

Define the set

$$S_r = \{(i, j) \mid x_i > x_{m+\frac{1}{2}}, (m+1, j) \in D_{m+1}^4\}.$$

$\forall (i, j) \in S_r$, due to the zero boundary condition and the upwind nature of the scheme, one has

$$f_{ij}^n = \sum_{(p,q) \in S_r} \beta_{pq}^{ijn_0} f_{pq}^0, \quad (i, j) \in S_r \quad (6.17)$$

with $\beta_{pq}^{ijn0} \geq 0$.

Notice $D_{m+1}^4 \subset S_r$,

$$S_2 \leq \sum_{(p,q) \in S_r} \left(\sum_{n=0}^{L-1} \sum_{(i,j) \in D_{m+1}^4} \beta_{pq}^{ijn0} \right) |f_{pq}^0| \equiv \sum_{(p,q) \in S_r} F(p,q) |f_{pq}^0|, \quad (6.18)$$

where we have defined

$$F(p,q) = \sum_{n=0}^{L-1} \sum_{(i,j) \in D_{m+1}^4} \beta_{pq}^{ijn0}, \quad (p,q) \in S_r. \quad (6.19)$$

The next step is to estimate these coefficients. Define

$$\beta_{pq}^{ij0} = \sum_{n=0}^{\infty} \beta_{pq}^{ijn0}, \quad (p,q) \in S_r,$$

then (6.19) gives

$$F(p,q) = \sum_{(i,j) \in D_{m+1}^4} \sum_{n=0}^{L-1} \beta_{pq}^{ijn0} \leq \sum_{(i,j) \in D_{m+1}^4} \beta_{pq}^{ij0}.$$

Hence it is useful to evaluate β_{pq}^{ij0} .

Notice β_{pq}^{ij0} is not zero only when $p \geq i$ and $q = j$ due to the upwind flux and constant potential. We first evaluate β_{pq}^{ij0} when $p = i$ and $q = j$. Denote $c_1^j = 1 - \frac{|\xi_j| \Delta t}{\Delta x}$, $c_2^j = \frac{|\xi_j| \Delta t}{\Delta x}$. From scheme (6.3)

$$\beta_{ij}^{ij0} = \sum_{n=0}^{\infty} \beta_{ij}^{ijn0} = \sum_{n=0}^{\infty} (c_1^j)^n = \frac{1}{1 - c_1^j} = \frac{1}{c_2^j}. \quad (6.20)$$

Since $(i,j) \in S_r$ and $c_2^j \geq \sqrt{2D} \lambda_x^t$, so

$$\frac{1}{c_2^j} \leq \frac{1}{\sqrt{2D} \lambda_x^t} \equiv \lambda_1.$$

We now evaluate β_{pj}^{ij0} when $p > i$. From scheme (6.3),

$$\beta_{pq}^{ij,n+1,0} = c_1^j \beta_{pq}^{ijn0} + c_2^j \beta_{pq}^{i+1,jn0}, \quad (6.21)$$

then a sum of n from 0 to ∞ in (6.21) gives

$$\beta_{pq}^{ij0} = \beta_{pq}^{i+1,j0}, \quad i < p. \quad (6.22)$$

We now can evaluate $F(p, q)$ for $(p, q) \in S_r$.

$$F(p, q) \leq \sum_{(i,j) \in D_{m+1}^4} \beta_{pq}^{ij0} = \beta_{pq}^{m+1,q,0} = \beta_{pq}^{m+2,q,0} = \dots = \beta_{pq}^{p,q,0} \leq \lambda_1. \quad (6.23)$$

Therefore, from (6.18) we get

$$\begin{aligned} S_2 &\leq \sum_{(p,q) \in S_r} F(p, q) |f_{pq}^0| \leq \lambda_1 \sum_{(p,q) \in S_r} |f_{pq}^0| \\ &\leq \lambda_1 \sum_{(p,q) \in E_d} |f_{pq}^0| = \lambda_1 N_d |f^0|_1. \end{aligned} \quad (6.24)$$

Our next step is to estimate S_1 . Define the set

$$S_l = \{(i, j) \mid x_i < x_{m+\frac{1}{2}}, (m, j) \in D_m^2\}.$$

Similarly when $(i, j) \in S_l$, one has

$$f_{ij}^n = \sum_{(p,q) \in S_l} \gamma_{pq}^{ijn0} f_{pq}^0, \quad (i, j) \in S_l. \quad (6.25)$$

Dividing set D_m^2 into two parts:

$$D_m^{2,1} = \{(i, j) \in D_m^2 \mid \xi_j \geq \xi_z\}, \quad D_m^{2,2} = \{(i, j) \in D_m^2 \mid \xi_j < \xi_z\},$$

and also define the corresponding two parts of S_l

$$S_l^1 = \{(i, j) \in S_l \mid \xi_j \geq \xi_z\}, \quad S_l^2 = \{(i, j) \in S_l \mid \xi_j < \xi_z\}.$$

Note that S_l^2 is a subset of S_z in (6.12).

Correspondingly, S_1 is also divided into two parts

$$S_1 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j) \in D_m^{2,1}} |f_{ij}^n| \right\} + \sum_{n=0}^{L-1} \left\{ \sum_{(i,j) \in D_m^{2,2}} |f_{ij}^n| \right\} = S_{11} + S_{12}. \quad (6.26)$$

Similar to the previous case, we can get the upper bound of the first term

$$S_{11} \leq \lambda_2 N_d |f^0|_1 \quad (6.27)$$

with $\lambda_2 \equiv \frac{1}{\xi_z \lambda_x^t}$. Substituting (6.25) into S_{12} gives

$$S_{12} \leq \sum_{(p,q) \in S_l^2} \left(\sum_{n=0}^{L-1} \sum_{(i,j) \in D_m^{2,2}} \gamma_{pq}^{ijn0} \right) |f_{pq}^0|.$$

Using Assumption 1,

$$\begin{aligned}
S_{12} &\leq C_1 |f^0|_1 \sum_{(p,q) \in S_l^2} \left(\sum_{n=0}^{L-1} \sum_{(i,j) \in D_m^{2,2}} \gamma_{pq}^{ijn0} \right) \\
&= C_1 |f^0|_1 \sum_{n=0}^{L-1} \sum_{(i,j) \in D_m^{2,2}} \left(\sum_{(p,q) \in S_l^2} \gamma_{pq}^{ijn0} \right). \tag{6.28}
\end{aligned}$$

Now we evaluate $\sum_{(p,q) \in S_l^2} \gamma_{pq}^{ijn0}$ when $(i, j) \in D_m^{2,2}$. Write (6.25) as

$$f_{ij}^n = \sum_{(p,q) \in S_l^2} \gamma_{pq}^{ijn0} f_{pq}^0, \quad (i, j) \in D_m^{2,2}. \tag{6.29}$$

When the initial values are constant 1, including the ghost cells at the boundary, the numerical solutions at the next time step still remain unchanged, while the coefficients γ_{pq}^{ijn0} in (6.29) do not include those corresponding to the ghost cells, thus

$$\sum_{(p,q) \in S_l^2} \gamma_{pq}^{ijn0} \leq 1, \quad \forall (i, j) \in D_m^{2,2}.$$

Continuing from (6.28),

$$\begin{aligned}
S_{12} &\leq C_1 |f^0|_1 \sum_{n=0}^{L-1} \sum_{(i,j) \in D_m^{2,2}} 1 \leq \frac{C_1 |f^0|_1 L N_d}{N} \\
&= \frac{C_1 T N_d}{(x_{N+\frac{1}{2}} - x_{\frac{1}{2}}) \lambda_x^t} |f^0|_1 \equiv \lambda_3 N_d |f^0|_1 \tag{6.30}
\end{aligned}$$

with $\lambda_3 = \frac{C_1 T}{(x_{N+\frac{1}{2}} - x_{\frac{1}{2}}) \lambda_x^t}$ being an $O(1)$ quantity.

Now from (6.26), (6.27) and (6.30),

$$S_1 \leq (\lambda_2 + \lambda_3) N_d |f^0|_1. \tag{6.31}$$

Combing (6.14), (6.24) and (6.31),

$$\begin{aligned}
|f^L|_1 &\leq |f^0|_1 + M'_1 \lambda_1 |f^0|_1 + M'_2 (\lambda_2 + \lambda_3) |f^0|_1 \\
&= [1 + M'_1 \lambda_1 + M'_2 (\lambda_2 + \lambda_3)] |f^0|_1 \\
&\equiv C |f^0|_1
\end{aligned}$$

where $C \equiv 1 + M'_1 \lambda_1 + M'_2 (\lambda_2 + \lambda_3)$. Thus Theorem 1 is proved. \square

6.2 An unstable example

There arises another question about whether condition (6.13) in Assumption 1 is necessary for the l^1 -stability. In this subsection we give a counter example which shows that if this condition is violated, the solution may become unbounded in l^1 norm.

Here we impose the assumption:

Assumption 2

There exists a positive constant ξ_z such that $\forall (i, j) \in S_z$ in (6.12), it holds that

$$|f_{ij}^0| \leq \frac{C_1 |f^0|_1}{\Delta x^q}, \quad q > 0 \quad (6.32)$$

with C_1 independent of the mesh size.

Remark: Assumption 2 reduces to Assumption 1 in the case $q = 0$.

We first introduce some notations.

Define the sets

$$\begin{aligned} S'_m &= \{k | \sqrt{2D} + \Delta\xi \leq \xi_k \leq \frac{1}{3}\sqrt{20D} - \Delta\xi\}, \\ S_m &= \{k | \exists j \in S'_m, \text{ s.t. } |\xi_k - \xi_j| < \frac{1}{2}\Delta\xi \text{ or } \xi_k = \xi_j + \frac{1}{2}\Delta\xi\}. \end{aligned}$$

Let N_s be the number of elements in S_m . We name the elements in S_m as $k_i, i = 1, 2, \dots, N_s$ such that $k_1 < k_2 < \dots < k_{N_s}$.

Define an one-to-one map from S_m to S'_m as

$$T_s(k) = j \text{ s.t. } j \in S'_m, \quad |\xi_k - \xi_j| \leq \frac{1}{2}\Delta\xi, \quad k \in S_m.$$

It is clear that $\xi_{T_s(k_i)} \geq \sqrt{2D} + i\Delta\xi, \quad i = 1, 2, \dots, N_s$.

Let $q' = \min(\frac{q}{2}, \frac{1}{2})$. We choose T such that $T\lambda_t^x < x_{m+\frac{1}{2}} - x_{\frac{1}{2}}$ and $T\lambda_t^x < x_{N+\frac{1}{2}} - x_{m+\frac{1}{2}}$, thus $L < m$ and $L < N - m - 1$. Let

$$L_0 = \text{int}(L^{1-q'})L, \quad (6.33)$$

where $\text{int}(x)$ is the biggest integer equal to or less than x .

Define a function $G(k)$ as

$$G(k) = \text{int}(L\xi_k\lambda_x^t), \quad k \in S_m.$$

Clearly, $G(k_1) \leq G(k_2) \leq \dots \leq G(k_{N_s})$.

Since $L < m$, so $G(k) < m$ for $k \in S_m$. Define the following set of index of cells

$$H = \{(i, j) | j \in S_m, m - G(j) < i \leq m\}.$$

Let N_h be the number of elements in H . Our next step is to check the condition under which $N_h > L_0$.

Lemma 6.1. $N_h > L_0$ under the mesh size restrictions

$$\Delta x < \frac{\sqrt{2D}}{96\sqrt{10}\lambda_x^\xi}, \quad (6.34)$$

$$\Delta x < \frac{1}{4\sqrt{10}(\sqrt{10}-3)\sqrt{2D}\lambda_x^\xi} \frac{T\lambda_x^t}{T\lambda_x^t + \lambda_\xi^t}, \quad (6.35)$$

$$\Delta x < \frac{1}{\lambda_x^t} \left(\frac{\lambda_x^t \lambda_\xi^t}{12\sqrt{10}T^{1-q'}} \right)^{\frac{1}{q'}}. \quad (6.36)$$

Proof. According to the definitions,

$$\begin{aligned} N_h &= \sum_{k \in S_m} G(k) = \sum_{k \in S_m} \text{int}(L\xi_k \lambda_x^t) > \left(L\lambda_x^t \sum_{k \in S_m} \xi_k \right) - N_s \\ &> L\lambda_x^t \sum_{k \in S'_m} \left(\sqrt{\xi_k^2 - 2D} - \Delta\xi \right) - \frac{1}{\Delta\xi} \frac{(\sqrt{10}-3)\sqrt{2D}}{3} \\ &> L\lambda_x^t \sum_{i=1}^{N_s} \left(\sqrt{(\sqrt{2D} + i\Delta\xi)^2 - 2D} \right) - \frac{1}{3}L \left(\lambda_x^t + \frac{\lambda_\xi^t}{T} \right) (\sqrt{10}-3) \sqrt{2D} \\ &> \frac{3L}{\sqrt{20D}} \lambda_x^t \sum_{i=1}^{N_s} \left[(\sqrt{2D} + i\Delta\xi) \sqrt{(\sqrt{2D} + i\Delta\xi)^2 - 2D} \right] \\ &\quad - \frac{1}{3}L \left(\lambda_x^t + \frac{\lambda_\xi^t}{T} \right) (\sqrt{10}-3) \sqrt{2D} \\ &= \frac{L\lambda_x^t}{\sqrt{20D}\Delta\xi} \sum_{i=1}^{N_s} \left[3(\sqrt{2D} + i\Delta\xi) \sqrt{(\sqrt{2D} + i\Delta\xi)^2 - 2D\Delta\xi} \right] \\ &\quad - \frac{1}{3}L \left(\lambda_x^t + \frac{\lambda_\xi^t}{T} \right) (\sqrt{10}-3) \sqrt{2D} \\ &> \frac{L\lambda_x^t}{\sqrt{20D}\Delta\xi} \int_{\sqrt{2D}}^{\frac{\sqrt{20D}}{3} - 4\Delta\xi} 3x\sqrt{x^2 - 2D} dx - \frac{1}{3}L \left(\lambda_x^t + \frac{\lambda_\xi^t}{T} \right) (\sqrt{10}-3) \sqrt{2D} \\ &> \frac{L\lambda_x^t}{\sqrt{20D}\Delta\xi} \left(\frac{1}{3}\sqrt{2D} - \sqrt{\frac{8\sqrt{20D}\Delta\xi}{3}} \right) - \frac{1}{3}L \left(\lambda_x^t + \frac{\lambda_\xi^t}{T} \right) (\sqrt{10}-3) \sqrt{2D} \end{aligned} \quad (6.37)$$

We impose the following restriction on the mesh sizes

$$\sqrt{\frac{8\sqrt{20D}\Delta\xi}{3}} < \frac{\sqrt{2D}}{6}, \quad (6.38)$$

$$\left(1 + \frac{\lambda_\xi^t}{T\lambda_x^t} \right) \frac{(\sqrt{10}-3)\sqrt{2D}}{3} \Delta\xi < \frac{1}{12\sqrt{10}}, \quad (6.39)$$

then continue from (6.37),

$$N_h > \frac{L\lambda_x^t}{12\sqrt{10}\Delta\xi} = \frac{L\lambda_x^t\lambda_\xi^t}{12\sqrt{10}\Delta t}.$$

According to (6.33), $L_0 < LL^{1-q'} = \frac{LT^{1-q'}}{(\Delta t)^{1-q'}}$. Therefore, in order that $N_h > L_0$, one needs to impose the mesh size restriction

$$\Delta t < \left(\frac{\lambda_x^t\lambda_\xi^t}{12\sqrt{10}T^{1-q'}} \right)^{\frac{1}{q'}}. \quad (6.40)$$

One can rewrite the mesh size restriction (6.38), (6.39) and (6.40) to that on Δx which are (6.34)-(6.36).

Now, under the mesh size restriction (6.34)-(6.36), it holds that $N_h > L_0$. □

We now prove the following theorem:

Theorem 6.2. $\forall q > 0$ in Assumption 2, $\forall h_0 > 0$, $\exists \Delta x < h_0$, $T > 0$, $\forall B > 0$, $\exists f_{ij}^0, (i, j) \in E_d$ satisfying Assumption 2, such that

$$|f^L|_1 > B|f^0|_1.$$

Proof. We define a function F_H in H as

$$F_H(i, j) = m - G(j) + 1 + \sum_{l=1}^{s-1} G(k_l) \quad \text{if } j = k_s, \quad (i, j) \in H.$$

F_H in fact is an one-to-one map from H to $(1, 2, \dots, N_h)$. Now define the set

$$H_L = \{(i, j) | (i, j) \in H, F_H(i, j) \leq L_0\}.$$

Since $N_h > L_0$ by Lemma 5.1, the number of elements in H_L is L_0 .

We can now introduce the initial value f_{ij}^0 satisfying the condition of Theorem 2:

$$f_{ij}^0 = c_0, \quad (i, j) \in H_L, \quad (6.41)$$

$$f_{ij}^0 = 0, \quad (i, j) \in E_d \setminus H_L, \quad (6.42)$$

where $c_0 > 0$ is a constant.

We first check that these initial values satisfy Assumption 2. Since

$$\frac{|f_{ij}^0|}{|f^0|_1} = \frac{N_d}{L_0} < \frac{2MN}{L^{2-q'}} = \frac{2(x_{N+\frac{1}{2}} - x_{\frac{1}{2}})(\xi_{M+\frac{1}{2}} - \xi_{\frac{1}{2}})\lambda_x^{t^{2-q'}}}{\lambda_x^\xi T^{2-q'} \Delta x^{q'}},$$

thus Assumption 2 is satisfied if

$$\frac{2(x_{N+\frac{1}{2}} - x_{\frac{1}{2}})(\xi_{M+\frac{1}{2}} - \xi_{\frac{1}{2}})\lambda_x^{t^{2-q'}}}{\lambda_x^\xi T^{2-q'} \Delta x^{q'}} < \frac{C_1}{\Delta x^q}. \quad (6.43)$$

Condition (6.43) is satisfied under the following mesh size restriction

$$\Delta x < \left(\frac{C_1 \lambda_x^\xi T^{2-q'}}{2(x_{N+\frac{1}{2}} - x_{\frac{1}{2}})(\xi_{M+\frac{1}{2}} - \xi_{\frac{1}{2}})\lambda_x^{t^{2-q'}}} \right)^{\frac{1}{q-q'}} \quad (6.44)$$

because we have chosen $q' < q$.

Next we analyze the relation between $|f^L|_1$ and $|f^0|_1$. Since $L < N - m - 1$, the solution at the boundary cells remains zero for all the time steps. If we define the sets

$$\begin{aligned} S_m^m &= \{(i, j) | i = m, j \in S_m\}, \\ S_m^l &= \{(i, j) | x_i < x_{m+\frac{1}{2}}, j \in S_m\}, \\ S_m^r &= \{(i, j) | x_i > x_{m+\frac{1}{2}}, j \in S_m'\}, \end{aligned}$$

then at each time step, only solutions at cells belonging to S_m^l or S_m^r are possibly nonzero. Namely

$$f_{ij}^n = 0 \quad \text{for } (i, j) \in E_d \setminus \{S_m^l \cup S_m^r\}. \quad (6.45)$$

Since our scheme is positive preserving, and the initial values (6.41) and (6.42) are nonnegative, the numerical solutions at each time step are always nonnegative. Then similar to the proof of (6.7), at each time step

$$\begin{aligned} |f^{n+1}|_1 &= \frac{1}{N_d} \sum_{(i,j) \in E_d} f_{ij}^{n+1} \\ &= \frac{1}{N_d} \sum_{(i,j) \in E_d} \alpha_{ij} f_{ij}^n \\ &= \frac{1}{N_d} \sum_{(i,j) \in S_m^l} \alpha_{ij} f_{ij}^n + \frac{1}{N_d} \sum_{(i,j) \in S_m^r} \alpha_{ij} f_{ij}^n + \frac{1}{N_d} \sum_{(i,j) \in E_d \setminus \{S_m^l \cup S_m^r\}} f_{ij}^n, \end{aligned} \quad (6.46)$$

Note the last term in (6.46) is zero by (6.45).

For scheme (6.2) one sees that among those α_{ij} with $(i, j) \in S_m^l \cup S_m^r$, $\alpha_{ij} \neq 1$ only when $(i, j) \in S_m^m$, so continuing from (6.46) gives

$$|f^{n+1}|_1 = \frac{1}{N_d} \sum_{(m,j) \in S_m^m} \alpha_{mj} f_{mj}^n + \frac{1}{N_d} \sum_{(i,j) \in E_d \setminus S_m^m} f_{ij}^n. \quad (6.47)$$

We now estimate α_{mj} for $(m, j) \in S_m^m$. From schemes (6.2) and (6.4), for $(m, j) \in S_m^m$, by setting $j' = T_s(j)$, one has

$$\alpha_{mj} = 1 - \xi_j \lambda_x^t + \xi_{j'} \lambda_x^t c_{j'j}, \quad (6.48)$$

where $c_{j'j}$ are the coefficients in (6.4).

According to the definitions of S_m and S'_m , $c_{j'j} \geq \frac{1}{2}$, $\xi_j < \frac{1}{3}\sqrt{2D}$, $\xi_{j'} > \sqrt{2D}$ in (6.48). So (6.48) gives

$$\alpha_{mj} > 1 + \frac{\sqrt{2D}}{6} \lambda_x^t. \quad (6.49)$$

Then (6.49) together with (6.47) give

$$\begin{aligned} |f^{n+1}|_1 &> \frac{\sqrt{2D}}{6} \lambda_x^t \frac{1}{N_d} \sum_{(m,j) \in S_m^m} f_{mj}^n + \frac{1}{N_d} \sum_{(i,j) \in E_d} f_{ij}^n \\ &= \frac{\sqrt{2D}}{6} \lambda_x^t \frac{1}{N_d} \sum_{(m,j) \in S_m^m} f_{mj}^n + |f^n|_1. \end{aligned} \quad (6.50)$$

Summing up (6.50) from $n = 0$ to $L - 1$, one gets

$$|f^L|_1 > |f^0|_1 + \frac{\sqrt{2D}}{6} \lambda_x^t \frac{1}{N_d} \sum_{n=0}^{L-1} \sum_{(m,j) \in S_m^m} f_{mj}^n. \quad (6.51)$$

Write

$$f_{ij}^n = \sum_{(p,q) \in S_m^l} \eta_{pq}^{ijn0} f_{pq}^0, \quad (i, j) \in S_m^l. \quad (6.52)$$

Since $S_m^m \in S_m^l$, substituting (6.52) into (6.51) gives

$$\begin{aligned} |f^L|_1 &> |f^0|_1 + \frac{1}{6} \sqrt{2D} \lambda_x^t \frac{1}{N_d} \sum_{(p,q) \in S_m^l} \left(\sum_{n=0}^{L-1} \sum_{(m,j) \in S_m^m} \eta_{pq}^{mjn0} \right) f_{pq}^0 \\ &= |f^0|_1 + \frac{1}{6} \sqrt{2D} \lambda_x^t \frac{1}{N_d} \sum_{(p,q) \in H_L} \left(\sum_{n=0}^{L-1} \sum_{(m,j) \in S_m^m} \eta_{pq}^{mjn0} \right) c_0 \end{aligned}$$

$$\begin{aligned}
&= |f^0|_1 + \frac{1}{6} \sqrt{2D} \lambda_x^t \frac{c_0}{N_d} \sum_{(m,j) \in S_m^m} \left(\sum_{(p,j) \in H_L} \sum_{n=0}^{L-1} \eta_{pj}^{mjn0} \right) \\
&\geq |f^0|_1 + \frac{1}{6} \sqrt{2D} \lambda_x^t \frac{c_0}{N_d} \sum_{l=1}^{s-1} \left(\sum_{(p,k_l) \in H} \sum_{n=0}^{L-1} \eta_{pk_l}^{mk_l n0} \right), \tag{6.53}
\end{aligned}$$

where $k_s \in S_m$ is the quantity such that $\exists i$ satisfying $m - G(k_s) < i \leq m$ and $F_H(i, k_s) = L_0$. Thus we need to estimate $\sum_{(p,j) \in H} \sum_{n=0}^{L-1} \eta_{pj}^{mjn0}$ for $(m, j) \in S_m^m$. From scheme (6.2), one has for $(k, j) \in H$,

$$\eta_{pj}^{kj,n+1,0} = (1 - \xi_j \lambda_x^t) \eta_{pj}^{kj,n0} + \xi_j \lambda_x^t \eta_{pj}^{k-1,j,n0}. \tag{6.54}$$

Adding (6.54) from $n = 0$ to $L - 1$ leads to

$$\eta_{pj}^{kjL0} + \sum_{n=0}^{L-1} \eta_{pj}^{kj,n0} = (1 - \xi_j \lambda_x^t) \sum_{n=0}^{L-1} \eta_{pj}^{kj,n0} + \xi_j \lambda_x^t \sum_{n=0}^{L-1} \eta_{pj}^{k-1,j,n0},$$

therefore,

$$\begin{aligned}
\sum_{n=0}^{L-1} \eta_{pj}^{kj,n0} &= \sum_{n=0}^{L-1} \eta_{pj}^{k-1,j,n0} - \frac{1}{\xi_j \lambda_x^t} \eta_{pj}^{kjL0} \\
&= \sum_{n=0}^{L-1} \eta_{pj}^{k-2,j,n0} - \frac{1}{\xi_j \lambda_x^t} [\eta_{pj}^{kjL0} + \eta_{pj}^{k-1,jL0}] \\
&= \dots \\
&= \sum_{n=0}^{L-1} \eta_{pj}^{pj,n0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=p+1}^k \eta_{pj}^{ljL0} \\
&= \sum_{n=0}^{L-1} \eta_{kj}^{kj,n0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=p}^{k-1} \eta_{lj}^{kjL0}. \tag{6.55}
\end{aligned}$$

Applying (6.55) when $k = m$, one gets the relation

$$\sum_{n=0}^{L-1} \eta_{pj}^{mj,n0} = \sum_{n=0}^{L-1} \eta_{mj}^{mj,n0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=p}^{m-1} \eta_{lj}^{mjL0}. \tag{6.56}$$

For a fixed $j \in S_m$, adding (6.56) for p such that $(p, j) \in H$ gives

$$\sum_{(p,j) \in H} \sum_{n=0}^{L-1} \eta_{pj}^{mj,n0} = G(j) \sum_{n=0}^{L-1} \eta_{mj}^{mj,n0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=m-G(j)+1}^{m-1} (l - m + G(j)) \eta_{lj}^{mjL0}. \tag{6.57}$$

According to the definition of S_m and S'_m , when $j \in S_m$, $\xi_j < \frac{1}{3}\sqrt{2D}$. The CFL condition (3.3) implies that $\sqrt{2D}\lambda_x^t < 1$, so $\xi_j\lambda_x^t < \frac{1}{3}$ when $j \in S_m$. Define $\mu_j = \xi_j\lambda_x^t$, one has $\eta_{lj}^{mjL0} = (1 - \mu_j)^{L+l-m}\mu_j^{m-l}C_L^{m-l}$, hence,

$$\begin{aligned} \sum_{l=m-G(j)+1}^{m-1} \eta_{lj}^{mjL0} &= \sum_{l=m-G(j)+1}^{m-1} (1 - \mu_j)^{L+l-m}\mu_j^{m-l}C_L^{m-l} \\ &= \sum_{l=1}^{G(j)-1} (1 - \mu_j)^{L-l}\mu_j^l C_L^l = \sum_{l=1}^{\text{int}(\mu_j L)-1} (1 - \mu_j)^{L-l}\mu_j^l C_L^l < \frac{1}{2}. \end{aligned}$$

The proof of the last inequality is in the Appendix A. Continuing from (6.57) gives

$$\begin{aligned} \sum_{(p,j) \in H} \sum_{n=0}^{L-1} \eta_{pj}^{mjn0} &> G(j) \sum_{n=0}^{L-1} \eta_{mj}^{mjn0} - \frac{1}{\xi_j\lambda_x^t} \frac{G(j)}{2} \\ &= G(j) \frac{1 - (1 - \xi_j\lambda_x^t)^L}{\xi_j\lambda_x^t} - \frac{1}{\xi_j\lambda_x^t} \frac{G(j)}{2}. \end{aligned} \quad (6.58)$$

By the definitions of S_m and S'_m , for $j \in S_m$,

$$\begin{aligned} \xi_j &> \sqrt{(\sqrt{2D} + \Delta\xi)^2 - 2D} - \Delta\xi \\ &> \sqrt{2\sqrt{2D}\Delta\xi} - \Delta\xi. \end{aligned} \quad (6.59)$$

In order for $\xi_j\lambda_x^t > \frac{2}{L} = \frac{2\lambda_x^t}{T}\Delta\xi$, from (6.59),

$$\begin{aligned} \sqrt{2\sqrt{2D}\Delta\xi} - \Delta\xi &> \frac{2}{T\lambda_x^t}\Delta\xi \\ \Leftrightarrow \Delta\xi &< \frac{2\sqrt{2D}}{\left(\frac{2}{T\lambda_x^t} + 1\right)^2} \\ \Leftrightarrow \Delta x &< \frac{2\sqrt{2D}}{\left(\frac{2}{T\lambda_x^t} + 1\right)^2\lambda_x^t}. \end{aligned} \quad (6.60)$$

Under mesh size restriction (6.60), $\xi_j\lambda_x^t > \frac{2}{L} > \frac{1}{L}$, thus

$$(1 - \xi_j\lambda_x^t)^L < \left(1 - \frac{1}{L}\right)^L < \frac{1}{e} < \frac{1}{2.5}.$$

By using (6.58), one gets

$$\sum_{(p,j) \in H} \sum_{n=0}^{L-1} \eta_{pj}^{mjn0} > \frac{G(j)}{10\xi_j\lambda_x^t} > \frac{L - \frac{1}{\xi_j\lambda_x^t}}{10} > \frac{L}{20}, \quad (6.61)$$

where in the last inequality we used $\xi_j \lambda_x^t > \frac{2}{L}$ under mesh size restriction (6.60).

Next one needs to estimate s appeared in (6.53) as the upper bound of the summation. From the definition of s in (6.53),

$$\sum_{l=1}^s G(k_l) \geq L_0. \quad (6.62)$$

On the other hand, for $1 \leq s' \leq N_s$,

$$\begin{aligned} \sum_{l=1}^{s'} G(k_l) &< L\lambda_x^t \sum_{l=1}^{s'} \xi_{k_l} + s' < L\lambda_x^t \sum_{l=1}^{s'} \sqrt{\xi_{k_l}^2 - 2D} + s'\lambda_x^t L\Delta\xi + s' \\ &< \frac{L\lambda_x^t}{3\sqrt{2D}} \sum_{l=1}^{s'} 3\xi_{k_l} \sqrt{\xi_{k_l}^2 - 2D} + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s' \\ &< \frac{L\lambda_x^t}{3\sqrt{2D}\Delta\xi} \int_{\sqrt{2D}}^{\sqrt{2D}+(s'+1)\Delta\xi} 3\xi \sqrt{\xi^2 - 2D} d\xi + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s' \\ &< \frac{L\lambda_x^t}{3\sqrt{2D}\Delta\xi} \left[2\sqrt{2D}(s'+1)\Delta\xi \right]^{\frac{3}{2}} + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s'. \end{aligned} \quad (6.63)$$

By choosing $s' = s_N^{1-\frac{5}{6}q'}$, (6.63) gives

$$\begin{aligned} \sum_{l=1}^{s'} G(k_l) &< \frac{8\lambda_x^t (2D)^{\frac{1}{4}} L \sqrt{\Delta\xi}}{3} s'^{\frac{3}{2}} + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s' \\ &< \frac{8\lambda_x^t (2D)^{\frac{1}{4}} L \sqrt{\Delta\xi}}{3} s_N^{\frac{3}{2}-\frac{5}{4}q'} + \frac{s_N \lambda_x^t T}{\lambda_\xi^t} + s_N \\ &< \frac{8\lambda_x^t (2D)^{\frac{1}{4}} \sqrt{T} L}{3\sqrt{\lambda_\xi^t} \sqrt{L}} \left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right)^{\frac{3}{2}-\frac{5}{4}q'} \\ &\quad + \frac{\left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right)}{\lambda_\xi^t} \lambda_x^t T + \left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right) \\ &= \frac{8\lambda_x^t (2D)^{\frac{1}{4}} \sqrt{T} \left(\frac{\lambda_\xi^t}{T} \left(\frac{\sqrt{10}}{3} - 1 \right) \sqrt{2D} \right)^{\frac{3}{2}-\frac{5}{4}q'}}{3\sqrt{\lambda_\xi^t}} L^{2-\frac{5}{4}q'} \\ &\quad + \left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right) \lambda_x^t L + \frac{\left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right) \lambda_\xi^t L}{T}. \end{aligned} \quad (6.64)$$

If one imposes the mesh size restrictions

$$\begin{aligned} \frac{8\lambda_x^t(2D)^{\frac{1}{4}}\sqrt{T}\left(\frac{\lambda_\xi^t}{T}\left(\frac{\sqrt{10}}{3}-1\right)\sqrt{2D}\right)^{\frac{3}{2}-\frac{5}{4}q'}}{3\sqrt{\lambda_\xi^t}}L^{2-\frac{5}{4}q'} &< \frac{1}{4}L^{2-q'}, \\ \left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_x^tL &< \frac{1}{4}L^{2-q'}, \\ \frac{\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^tL}{T} &< \frac{1}{4}L^{2-q'}, \end{aligned}$$

which corresponds to

$$\Delta x < \frac{T}{\lambda_x^t} \left(\frac{3\sqrt{\lambda_\xi^t}}{32\lambda_x^t(2D)^{\frac{1}{4}}\sqrt{T}\left(\frac{\lambda_\xi^t}{T}\left(\frac{\sqrt{10}}{3}-1\right)\sqrt{2D}\right)^{\frac{3}{2}-\frac{5}{4}q'}} \right)^{\frac{4}{q'}}, \quad (6.65)$$

$$\Delta x < \frac{T}{\lambda_x^t} \left(\frac{1}{4\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_x^t} \right)^{\frac{1}{1-q'}}, \quad (6.66)$$

$$\Delta t < \frac{T}{\lambda_x^t} \left(\frac{T}{4\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t} \right)^{\frac{1}{1-q'}}, \quad (6.67)$$

then under (6.65)-(6.67) one has, for $s' = s_N^{1-\frac{5}{6}q'}$,

$$\sum_{l=1}^{s'} G(k_l) < \frac{3}{4}L^{2-q'} < L_0. \quad (6.68)$$

Comparing (6.68) with (6.62) gives

$$s > s_N^{1-\frac{5}{6}q'} > \left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}{T} \right)^{1-\frac{5}{6}q'} L^{1-\frac{5}{6}q'} + 1. \quad (6.69)$$

Now combining with (6.61) and (6.69), (6.53) gives

$$\begin{aligned} |f^L|_1 &> |f^0|_1 + \frac{\sqrt{2D}}{120}\lambda_x^t\frac{c_0}{N_d} \left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}{T} \right)^{1-\frac{5}{6}q'} L^{2-\frac{5}{6}q'} \\ &\geq |f^0|_1 + \frac{\sqrt{2D}}{120}\lambda_x^t\frac{L_0c_0}{N_d} \left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}{T} \right)^{1-\frac{5}{6}q'} L^{\frac{1}{6}q'} \end{aligned} \quad (6.70)$$

$$= \left\{ 1 + \frac{\sqrt{2D}}{120} \lambda_x^t \left[\frac{\frac{1}{2} \left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right) \lambda_\xi^t}{T} \right]^{1-\frac{5}{6}q'} L^{\frac{1}{6}q'} \right\} |f^0|_1. \quad (6.71)$$

So $\forall B > 0$, one can choose mesh size such that

$$1 + \frac{\sqrt{2D}}{120} \lambda_x^t \left(\frac{\frac{1}{2} \left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right) \lambda_\xi^t}{T} \right)^{1-\frac{5}{6}q'} L^{\frac{1}{6}q'} > B$$

or

$$\Delta x < \frac{T}{\lambda_\xi^t} \left(\frac{\sqrt{2D}}{120B} \lambda_x^t \left(\frac{\frac{1}{2} \left(\frac{\sqrt{20D}}{3} - \sqrt{2D} \right) \lambda_\xi^t}{T} \right)^{1-\frac{5}{6}q'} \right)^{\frac{6}{q'}}, \quad (6.72)$$

under which it holds that

$$|f^L|_1 > B|f^0|_1.$$

□

7 Stability theory of Scheme II

In this section we study the l^1 and l^∞ stability of Scheme II. Its positivity is obvious under the hyperbolic CFL condition (3.3).

Theorem 7.1. *If the forward Euler time discretization is used, then the flux is given by Algorithm II yields the scheme (4.1) which is l^1 -contracting and l^∞ -stable.*

Proof. For simplicity, we discuss the case when the potential has only one discontinuity at grid point $x_{m+\frac{1}{2}}$ with jump $V_{m+\frac{1}{2}}^- - V_{m+\frac{1}{2}}^+ = D > 0$, and $V'(x) < 0$ at smooth points. The other cases, namely, when $V'(x) \geq 0$, or the potential having several discontinuity points with increased or decreased potential jumps, can be discussed similarly.

We consider the typical situation when $\xi_1 < -\sqrt{2D}$, $\xi_M > \sqrt{2D}$, so that all the three situations discussed in Section 2 are included. We assume the mesh is defined such that $0, \pm\sqrt{2D}$ are grid points in the ξ -direction. We define some sets of indexes

$$D_m^+ = \{(m, j) | \xi_j > 0\},$$

$$D_{m+1}^+ = \{(m+1, j) | \xi_{j-\frac{1}{2}} \geq \sqrt{2D}\},$$

$$\begin{aligned}
D_m^- &= \left\{ (m, j) \mid -\sqrt{\xi_1^2 - 2D} \leq \xi_{j-\frac{1}{2}} \leq 0 \right\}, \\
D_{m+1}^- &= \left\{ (m+1, j) \mid \xi_{j+\frac{1}{2}} \leq -\sqrt{2D} \right\}, \\
D_l^4 &= \left\{ (i, j) \mid x_i \leq x_m, \xi_{j+\frac{1}{2}} \leq -\sqrt{\xi_1^2 - 2D} \right\}.
\end{aligned}$$

These domains are shown in Figure (7.1).

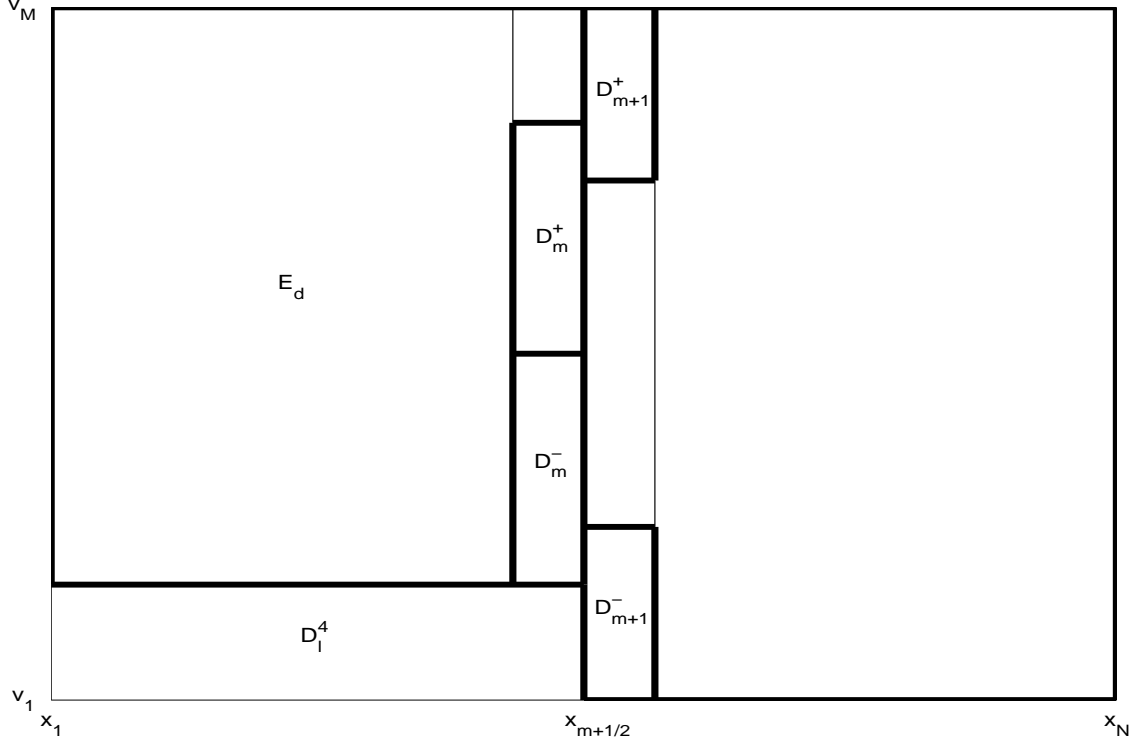


Figure 7.1 Sketch of the index sets $D_m^+, D_{m+1}^+, D_m^-, D_{m+1}^-, D_l^4$.

Again the computational domain is chosen as (6.1):

$$E_d = \{(i, j) \mid i = 1, \dots, N, j = 1, \dots, M\} \setminus D_l^4.$$

Now denote $F_i = \frac{1}{\Delta x} \left| V_{i+\frac{1}{2}}^- - V_{i-\frac{1}{2}}^+ \right|$. Our scheme (4.1) with Algorithm II can be made precisely as

1) if $\xi_j > 0, i \neq m+1$,

$$f_{ij}^{n+1} = (1 - F_i \lambda_\xi^t - \xi_j \lambda_x^t) f_{ij} + F_i \lambda_\xi^t f_{i,j-1} + \xi_j \lambda_x^t f_{i-1,j}; \quad (7.1)$$

2) if $\xi_j < 0, i \neq m$,

$$f_{ij}^{n+1} = (1 - F_i \lambda_\xi^t - |\xi_j| \lambda_x^t) f_{ij} + F_i \lambda_\xi^t f_{i,j-1} + |\xi_j| \lambda_x^t f_{i+1,j}; \quad (7.2)$$

3) if $\xi_j > 0$,

$$f_{m+1,j}^{n+1} = (1 - F_{m+1}\lambda_\xi^t - \xi_j\lambda_x^t) f_{m+1,j} + F_{m+1}\lambda_\xi^t f_{m+1,j-1} + \xi_j\lambda_x^t f_{m+\frac{1}{2},j}^+; \quad (7.3)$$

4) if $\xi_j < 0$,

$$f_{mj}^{n+1} = (1 - F_m\lambda_\xi^t - |\xi_j|\lambda_x^t) f_{mj} + F_m\lambda_\xi^t f_{m,j-1} + |\xi_j|\lambda_x^t f_{m+\frac{1}{2},j}^-, \quad (7.4)$$

where we omit the superscript n on the right hand side.

By summing up (7.1)-(7.4) for $(i,j) \in E_d$, one typically gets the following expression

$$\begin{aligned} \sum_{(i,j) \in E_d} f_{ij}^{n+1} &= \sum_{(i,j) \in E_d} \alpha_{ij} f_{ij} + \sum_{(m+1,j) \in D_{m+1}^+} \xi_j \lambda_x^t f_{m+\frac{1}{2},j}^+ + \sum_{(m,j) \in D_m^-} \xi_j \lambda_x^t f_{m+\frac{1}{2},j}^- \\ &\equiv I_1 + I_2 + I_3 \end{aligned} \quad (7.5)$$

As in the proof of stability of Scheme I, we assume that f satisfies the zero boundary condition. In this situation, the coefficients α_{ij} in (7.5) satisfy

$$\alpha_{ij} \leq 1, \quad (i,j) \in E_d \setminus \{D_m^+ \cup D_{m+1}^-\}, \quad (7.6)$$

$$\alpha_{ij} \leq 1 - |\xi_j|\lambda_x^t, \quad (i,j) \in D_m^+ \cup D_{m+1}^-. \quad (7.7)$$

We now study the relation between I_2 and $\sum_{(m,j) \in D_m^+} |\xi_j \lambda_x^t f_{mj}|$. Let

$$p_{N+1} = \sqrt{\xi_{N+\frac{1}{2}}^2 - 2D},$$

and assume

$$\xi_k < p_{N+1} \leq \xi_{k+1} \leq \xi_{N+\frac{1}{2}}.$$

Assume $\xi_{J_2-\frac{1}{2}} = 0$ for some J_2 . Since

$$I_2 \leq \sum_{j=J_2}^{k-1} |\xi_j f_{mj}| + \frac{p_{N+1} - \xi_k}{\Delta\xi} |\xi_k f_{mk}| \leq \sum_{(m,j) \in D_m^+} |\xi_j f_{mj}|,$$

thus

$$I_2 \leq \sum_{(m,j) \in D_m^+} |\xi_j \lambda_x^t f_{mj}|. \quad (7.8)$$

Similarly, one gets

$$I_3 \leq \sum_{(m+1,j) \in D_{m+1}^-} |\xi_j \lambda_x^t f_{m+1,j}|. \quad (7.9)$$

Combining (7.5), (7.6), (7.7), (7.8) and (7.9) gives

$$\sum_{(i,j) \in E_d} |f_{ij}^{n+1}| \leq \sum_{(i,j) \in E_d} |f_{ij}^n|. \quad (7.10)$$

This is the l^1 -contracting property of this scheme.

Next we prove the l^∞ -stability. In the cells where $\xi_j > 0, i \neq m+1$ or $\xi_j < 0, i \neq m$, one uses (7.1) or (7.2). Observing that the coefficients on the right hand side of (7.1) or (7.2) are positive and the sum of them is 1, so in fact these schemes are l^∞ -contracting. It remains to study the cells where $\xi_j > 0, i = m+1$ or $\xi_j < 0, i = m$, corresponding to (7.3) or (7.4).

We first consider (7.3). It can be checked that when $\xi_{j-\frac{1}{2}} < \sqrt{2D}$, $f_{m+\frac{1}{2},j}^+ = f_{m+1,k}$ with k such that $\xi_k = -\xi_j$, thus the l^∞ -contracting property still holds. When $\xi_{j-\frac{1}{2}} \geq \sqrt{2D}$, denote

$$\xi'_1 = \sqrt{\left(\xi_{j-\frac{1}{2}}\right)^2 - 2D}, \quad \xi'_2 = \sqrt{\left(\xi_{j+\frac{1}{2}}\right)^2 - 2D}. \quad (7.11)$$

Since $V_{m+\frac{1}{2}}^+ < V_{m+\frac{1}{2}}^-$, one has $\xi'_2 - \xi'_1 > \Delta\xi$. Therefore, it is impossible that $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi'_2 \leq \xi_{k+\frac{1}{2}}$ for any k . Assume $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi_{k+\frac{1}{2}} < \dots < \xi_{k+s-\frac{1}{2}} < \xi'_2 \leq \xi_{k+s+\frac{1}{2}}$ with $s \geq 1$. In this case

$$\begin{aligned} f_{m+\frac{1}{2},j}^+ &= \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k f_{mk} + \xi_{k+1} f_{m,k+1} + \dots \right. \\ &\quad \left. + \xi_{k+s-1} f_{m,k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s} f_{m,k+s} \right\}. \end{aligned} \quad (7.12)$$

Substituting (7.12) into (7.3) yields

$$\begin{aligned} f_{m+1,j}^{n+1} &= (1 - F_{m+1} \lambda_\xi^t - \xi_j \lambda_x^t) f_{m+1,j} + F_{m+1} \lambda_\xi^t f_{m+1,j-1} \\ &\quad + \lambda_x^t \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k f_{mk} + \xi_{k+1} f_{m,k+1} + \dots \right. \\ &\quad \left. + \xi_{k+s-1} f_{m,k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s} f_{m,k+s} \right\}. \end{aligned} \quad (7.13)$$

Observing that the coefficients on the right hand side of (7.13) is still positive. Thus it remains to check the sum of these coefficients given by

$$I_4 = 1 - \xi_j \lambda_x^t + \lambda_x^t \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k + \xi_{k+1} + \dots + \xi_{k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s} \right\}$$

$$= 1 + \xi_j \lambda_x^t \left\{ \frac{\frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k + \xi_{k+1} + \cdots + \xi_{k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s}}{\xi_j} - 1 \right\}. \quad (7.14)$$

Let

$$\begin{aligned} \xi'_k &= \frac{\xi_k + \xi_{k+s}}{2} = \frac{\xi_{k+\frac{1}{2}} + \xi_{k+s-\frac{1}{2}}}{2}, \\ a'_1 &= \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \in (0, 1], \\ a'_2 &= \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \in (0, 1], \end{aligned}$$

then

$$\xi_k = \xi'_k - \frac{s\Delta\xi}{2}, \quad \xi_{k+s} = \xi'_k + \frac{s\Delta\xi}{2}.$$

Also notice

$$\xi'_k - \frac{1}{2}(\xi'_1 + \xi'_2) = \frac{1}{2} \left[(\xi_{k+\frac{1}{2}} - \xi'_1) + (\xi_{k+s-\frac{1}{2}} - \xi'_2) \right] = \frac{1}{2}(a'_1 - a'_2)\Delta\xi,$$

hence one gets

$$\begin{aligned} & \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k + \xi_{k+1} + \cdots + \xi_{k+s-1} + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi_{k+s} \right\} \\ &= \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi'_k + \xi'_k + \cdots + \xi'_k + \frac{\xi'_2 - \xi_{k+s-\frac{1}{2}}}{\Delta\xi} \xi'_k \right\} + \frac{s\Delta\xi}{2\xi_j} (a'_2 - a'_1) \\ &= \frac{(\xi'_2 - \xi'_1)\xi'_k}{\xi_j \Delta\xi} + \frac{s\Delta\xi}{2\xi_j} (a'_2 - a'_1) \\ &= \frac{(\xi'_2 - \xi'_1)(\xi'_1 + \xi'_2)}{2\xi_j \Delta\xi} + \frac{s\Delta\xi}{2\xi_j} (a'_2 - a'_1) - \frac{(\xi'_2 - \xi'_1)}{2\xi_j} (a'_2 - a'_1) \\ &= \frac{(\xi'^2_2 - \xi'^2_1)}{(\xi_{j+\frac{1}{2}} - \xi_{j-\frac{1}{2}})(\xi_{j+\frac{1}{2}} + \xi_{j-\frac{1}{2}})} + \frac{(1 - a'_1 - a'_2)\Delta\xi}{2\xi_j} (a'_2 - a'_1) \\ &< 1 + \frac{\Delta\xi}{8\xi_j} < 1 + \frac{\Delta\xi}{8\sqrt{2D}}. \end{aligned} \quad (7.15)$$

Substituting (7.15) into (7.14), the sum of the coefficients in (7.13) is estimated as

$$I_4 < 1 + \xi_j \lambda_x^t \frac{\Delta\xi}{8\sqrt{2D}} < 1 + \frac{1}{8\lambda_\xi^t \sqrt{2d}} \Delta t, \quad (7.16)$$

where the last inequality is deduced by using the CFL condition.

Now we consider case (7.4). Denote

$$\xi'_1 = -\sqrt{\left(\xi_{j-\frac{1}{2}}\right)^2 + 2D}, \quad \xi'_2 = -\sqrt{\left(\xi_{j+\frac{1}{2}}\right)^2 + 2D}. \quad (7.17)$$

In this case, we know $\xi'_2 - \xi'_1 < \Delta\xi$. So there are two cases $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi'_2 \leq \xi_{k+\frac{1}{2}}$ or $\xi_{k-\frac{1}{2}} \leq \xi'_1 < \xi_{k+\frac{1}{2}} < \xi'_2 \leq \xi_{k+\frac{3}{2}}$ corresponding respectively to

$$f_{m+\frac{1}{2},j}^- = \frac{1}{\xi_j} \frac{\xi'_2 - \xi'_1}{\Delta\xi} \xi_k f_{m+1,k} \quad (7.18)$$

or

$$f_{m+\frac{1}{2},j}^- = \frac{1}{\xi_j} \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} \xi_k f_{m+1,k} + \frac{\xi'_2 - \xi_{k+\frac{1}{2}}}{\Delta\xi} \xi_{k+1} f_{m+1,k+1} \right\}. \quad (7.19)$$

Substituting (7.18) or (7.19) into (7.4) gives

$$f_{mj}^{n+1} = (1 - F_m \lambda_\xi^t - |\xi_j| \lambda_x^t) f_{mj} + F_m \lambda_\xi^t f_{m,j-1} + \lambda_x^t \frac{\xi'_2 - \xi'_1}{\Delta\xi} |\xi_k| f_{m+1,k}, \quad (7.20)$$

or

$$\begin{aligned} f_{mj}^{n+1} &= (1 - F_m \lambda_\xi^t - |\xi_j| \lambda_x^t) f_{mj} + F_m \lambda_\xi^t f_{m,j-1} \\ &+ \lambda_x^t \left\{ \frac{\xi_{k+\frac{1}{2}} - \xi'_1}{\Delta\xi} |\xi_k| f_{m+1,k} + \frac{\xi'_2 - \xi_{k+\frac{1}{2}}}{\Delta\xi} |\xi_{k+1}| f_{m+1,k+1} \right\}. \end{aligned} \quad (7.21)$$

In each case, the coefficients on the right hand side are positive. Thus it remains to check the sum of the coefficients, which is, respectively,

$$1 + |\xi_j| \lambda_x^t \left\{ \frac{(\xi'_2 - \xi'_1) |\xi_k|}{\Delta\xi |\xi_j|} - 1 \right\} \quad (7.22)$$

or

$$1 + |\xi_j| \lambda_x^t \left\{ \frac{(\xi_{k+\frac{1}{2}} - \xi'_1) |\xi_k| + (\xi'_2 - \xi_{k+\frac{1}{2}}) |\xi_{k+1}|}{\Delta\xi |\xi_j|} - 1 \right\}. \quad (7.23)$$

Let D_k be $\frac{(\xi'_2 - \xi'_1) |\xi_k|}{\Delta\xi |\xi_j|}$ or $\frac{(\xi_{k+\frac{1}{2}} - \xi'_1) |\xi_k| + (\xi'_2 - \xi_{k+\frac{1}{2}}) |\xi_{k+1}|}{\Delta\xi |\xi_j|}$. One has

$$D_k < \frac{(\xi'_2 - \xi'_1) [\frac{1}{2}(|\xi'_1| + |\xi'_2|) + \Delta\xi]}{\Delta\xi |\xi_j|} = \frac{\frac{1}{2}(|\xi'_1| + |\xi'_2|) + \Delta\xi}{\frac{1}{2}(|\xi'_1| + |\xi'_2|)} < 1 + \frac{\Delta t}{\lambda_\xi^t \sqrt{2D}},$$

thus the sums (7.22) and (7.23) are both bounded above by

$$1 + \frac{1}{\lambda_\xi^t \sqrt{2D}} \Delta t. \quad (7.24)$$

Combining (7.16) and (7.24), and letting $C_0 = \frac{1}{\lambda_\xi^t \sqrt{2D}}$ be an $O(1)$ quantity, we get

$$|f^{n+1}|_\infty < (1 + C_0 \Delta t) |f^n|_\infty,$$

thus

$$|f^L|_\infty < (1 + C_0 \Delta t)^L |f^0|_\infty < e^{C_0 T} |f^0|_\infty. \quad (7.25)$$

This is the l^∞ -stability property of this scheme. □

Similar to Scheme I, Scheme II is also positive under the CFL condition such as (3.3).

8 Discontinuous solutions and numerical accuracy

When the solution of the Liouville equation is smooth, the formally second order shock capturing finite difference scheme will produce second order numerical approximations. Consequently the physical observables obtained by evaluating the numerical δ -integral concentrated on these numerical solution, such as those in (1.8)-(1.9), should generally be of first order. However, when the potential V is discontinuous, the solution of the Liouville equation, even with smooth initial data, may produce discontinuities at downstream part of the potential discontinuity. These discontinuities influence the accuracy of the numerical δ -integral through which the desired physical observables are obtained.

8.1 Discontinuities produced in the downstream part

For the Liouville equation with a discontinuous potential, if the initial data are smooth, the level set function exhibits discontinuities in the downstream side of the potential discontinuity.

We use a 1D example to illustrate this. Let ϕ be the level set function that solves the 1d Liouville equation with the potential given by

$$V(x) = \begin{cases} A, & x < -b; \\ -\frac{Ax}{b}, & -b < x < 0; \\ 0, & x > 0, \end{cases} \quad (8.1)$$

with A, b positive. Let the initial velocity profile be a constant velocity $\xi_0 > 0$ and the initial density is denoted by $\rho_0(x)$. The initial value of the level set function is

$$\phi(x, \xi, 0) = \xi - \xi_0.$$

We consider the solution at $t = T$. In this example the potential is continuous, and the initial level set function is continuous, so this level set function should still be continuous at $t = T$. Now look at the set

$$S_1 = \{(x, \xi_0) \mid -b < x < 0\},$$

which is part of the initial zero level set. The bicharacteristic of the Liouville equation (2.1) is

$$\begin{cases} \frac{dx}{dt} = \xi, & x(0) = x_0; \\ \frac{d\xi}{dt} = -V'(x), & \xi(0) = \xi_0. \end{cases} \quad (8.2)$$

Denote the solution of (8.2) by

$$x = x(x_0, \xi_0, t), \quad \xi = \xi(x_0, \xi_0, t),$$

then define the set

$$S_2 = \{(x, \xi) \mid x = x(x_0, \xi_0, T), \xi = \xi(x_0, \xi_0, T), (x_0, \xi_0) \in S_1\},$$

which is a subset of the zero level set of $\phi(x, \xi, T)$.

Select an element $(x_1, \xi_1) \in S_2$. We now want to evaluate $\phi_\xi(x_1, \xi_1, T)$. Assume $(x_1, \xi_1) = (x(-c, \xi_0, T), \xi(-c, \xi_0, T))$. Consider the case that T is large enough so that (x_1, ξ_1) is a downstream point. Then the relation between x_1 and c is

$$x_1(c) = T\sqrt{\xi_0^2 + \frac{2Ac}{b}} - \frac{b}{A} \left(\xi_0^2 + \frac{2Ac}{b} \right).$$

The density at $x = x_1$ at time T is the inverse of the Jacobian of $x(c)$ multiplied by the initial density

$$\rho(x_1, T) = \frac{\rho_0(-c)}{\left| \frac{dx_1(c)}{dc} \right|} = \frac{b\rho_0(-c)}{\left| \frac{TA}{\sqrt{\xi_0^2 + \frac{2Ac}{b}}} - 2b \right|}.$$

On the other hand, it is known

$$\rho(x_1, T) = \rho_0(-c) \int_{\xi_1 - \epsilon}^{\xi_1 + \epsilon} \delta(\phi(x_1, \xi, T)) d\xi = \frac{\rho_0(-c)}{|\phi_\xi(x_1, \xi_1, T)|}.$$

So we have

$$|\phi_\xi(x_1, \xi_1, T)| = \left| \frac{tA}{\sqrt{\xi_0^2 + \frac{2Ac}{b}}} - 2b \right| b^{-1}.$$

If we take the limit $b \rightarrow 0$, we know $|\phi_\xi(x_1, \xi_1, T)| \rightarrow \infty$.

Moreover, the time needed for (x_1, ξ_1) to be in the downstream domain, which is the time for the point $(-c, \xi_0)$ to reach $x = 0$ along its bi-characteristic, should be $T(c) = \frac{b}{A} \sqrt{\xi_0^2 + \frac{2Ac}{b}}$. Notice $T(c) \rightarrow 0$ as $b \rightarrow 0$, we know in this example when taking limit to the discontinuous potential, the level set function should only contain discontinuities in the downstream domain.

8.2 Influence of discontinuities on the accuracy of the numerical evaluation of moments

In the previous subsection, we showed that the discontinuities inevitably emerge in the downstream part of the potential discontinuity. As is well known, the l^1 -convergence rate for finite difference schemes to compute a discontinuous solution of a linear equation is at most halfth order [14], [27]. Here we show that a halfth order error is also introduced when evaluating the moments (1.8) (1.9) based on the discontinuous part of the solution.

We use the 1D linear advection equation with the Riemann initial data to illustrate this. Consider equation

$$u_t + au_x = 0 \quad (8.3)$$

with initial data

$$u(x, 0) = \begin{cases} 1, & x < 0; \\ -1, & x > 0. \end{cases} \quad (8.4)$$

Since the finite difference solution is closer to the solution of the modified equation

$$u_t + au_x = Du_{xx} \quad (8.5)$$

than the exact solution of the original linear advection equation (8.3), we check the accuracy of the numerical moments based on the solution of the modified equation (8.5).

If the upwind scheme is used then $D = \frac{a}{2}\Delta x(1 - a\lambda_x^t)$ [15, 26]. Thus $D \sim \Delta x$.

The exact solution of the equation (8.5) with initial data (8.4) is

$$\tilde{u}(x, t) = -\frac{2}{\sqrt{\pi}} \int_0^{\frac{x-at}{\sqrt{4Dt}}} e^{-z^2} dz. \quad (8.6)$$

The exact solution of (8.3) with initial data (8.4) at t is

$$u(x, t) = \begin{cases} 1, & x < at; \\ -1, & x > at. \end{cases} \quad (8.7)$$

which has the property

$$\int \delta(u(x, t)) dx = 0.$$

When evaluating the δ -integration concentrated on (8.6), one gets

$$\int \delta(\tilde{u}(x, t)) dx = \frac{1}{|\tilde{u}'(at, t)|} = \frac{\sqrt{4\pi Dt}}{e^{-(\frac{x-at}{\sqrt{4Dt}})^2}} \Big|_{x=at} = \sqrt{4\pi Dt}.$$

Since $D \sim \Delta x$, the accuracy of numerical δ -integral based on (8.6) is only halfth order. This implies that the evaluation of δ -integration in (1.8)(1.9) based on the finite difference solution for (8.3) is also only halfth order.

9 Numerical examples

In this section we present three numerical examples to show the performance and accuracy of the proposed methods. In the numerical computations the second order TVD Runge-Kutta time discretization [24] is used.

Example 9.1. A 1D problem with an exact L^∞ -solution. Consider the 1D Liouville equation

$$f_t + \xi f_x - V_x f_\xi = 0 \quad (9.1)$$

with a discontinuous potential given by

$$V(x) = \begin{cases} 0.2, & x < 0; \\ 0, & x > 0. \end{cases}$$

The initial data is given by

$$f(x, \xi, 0) = \begin{cases} 1, & x \leq 0, \xi > 0, \sqrt{x^2 + \xi^2} < 1; \\ 1, & x \geq 0, \xi < 0, \sqrt{x^2 + \xi^2} < 1; \\ 0, & \text{otherwise;} \end{cases} \quad (9.2)$$

as shown in the upper part of Figure 9.1 which depicts the non-zero part of $f(x, \xi, 0)$.

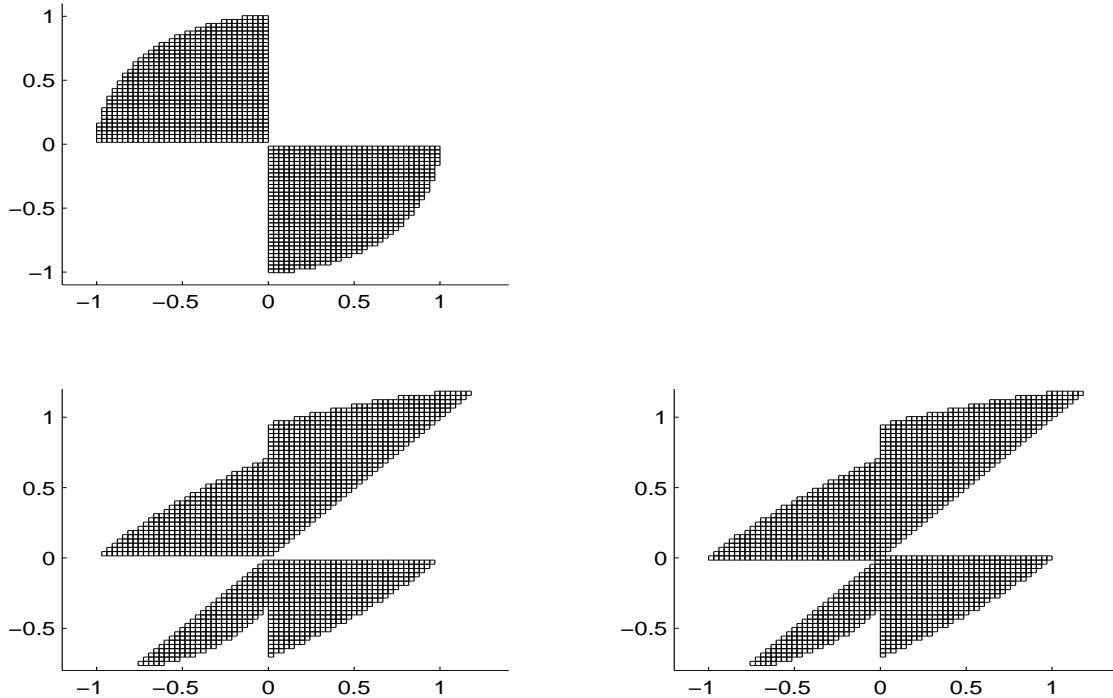


Figure 9.1 Example 9.1, solution in the phase space. Upper: non-zero part of the initial data; Lower left: non-zero part of exact solution $f(x, \xi, 1)$; Lower right: the part of numerical solution $f(x, \xi, 1) > 0.5$ computed by the 100×101 mesh. The horizontal axis is the position, the vertical axis is the velocity.

The exact solution at $t = 1$ is given by

$$f(x, \xi, 1) = \begin{cases} 1, & x \geq 0, \xi < \sqrt{0.4}, \xi > x; \\ 1, & x \geq 0, \xi < 0, x < 1, \xi > \frac{x - \sqrt{2 - x^2}}{2}; \\ 1, & x \leq 0, \xi < x, \xi > -\sqrt{0.6}, x < (1 - \frac{\sqrt{0.6 - \xi^2}}{\sqrt{\xi^2 + 0.4}})\xi; \\ 1, & x \leq 0, \xi > 0, x > -1, \xi < \frac{x + \sqrt{2 - x^2}}{2}; \\ 1, & x \geq 0, \xi > \sqrt{0.4}, \xi > x, \xi < \sqrt{1.4}, x > (1 - \frac{\sqrt{1.4 - \xi^2}}{\sqrt{\xi^2 - 0.4}})\xi; \\ 0, & \text{otherwise,} \end{cases}, \quad (9.3)$$

as shown in the lower left in Figure 9.1.

The numerical solution computed with a 100×101 mesh on the domain $[-1.5, 1.5] \times [-1.5, 1.5]$ using Scheme I is shown in the lower right in Figure 9.1. It shows a good agreement with the exact solution.

Table 9.1 compares the l^1 -error of the numerical solutions computed using 50×51 , 100×101 and 200×201 meshes respectively. From these data, the convergence rate of the numerical solution in the l^1 -norm is about 0.66 for both Scheme I and Scheme II. This agrees with our study in section 8, and the well established theory [14], [27], that the l^1 -error by a finite difference scheme for a discontinuous solution of linear equation is at most halfth order.

Table 9.1 Example 9.1, l^1 error of the numerical solutions with different meshes

mesh	50×51	100×101	200×201
Scheme I	0.245192	0.155871	0.093817
Scheme II	0.246248	0.156963	0.094275

Example 9.2. Computing the physical observables of a 1D problem with measure-valued solution. As mentioned in the Introduction, such problems arise in the computation of semiclassical limit of the Schrödinger equation. Consider the same problem as in example 9.1, with the initial data

$$f(x, \xi, 0) = \delta(\xi - w(x)), \quad (9.4)$$

where

$$w(x) = \begin{cases} 0.9, & x \leq -2; \\ 0.9 - \frac{0.9}{4}(x+2)^2, & -2 < x \leq 0; \\ -0.9 + \frac{0.9}{4}(x-2)^2; & 0 < x < 2. \\ -0.9, & x \geq 2. \end{cases} \quad (9.5)$$

Figure 9.2 plot $w(x)$ with the dashed line.

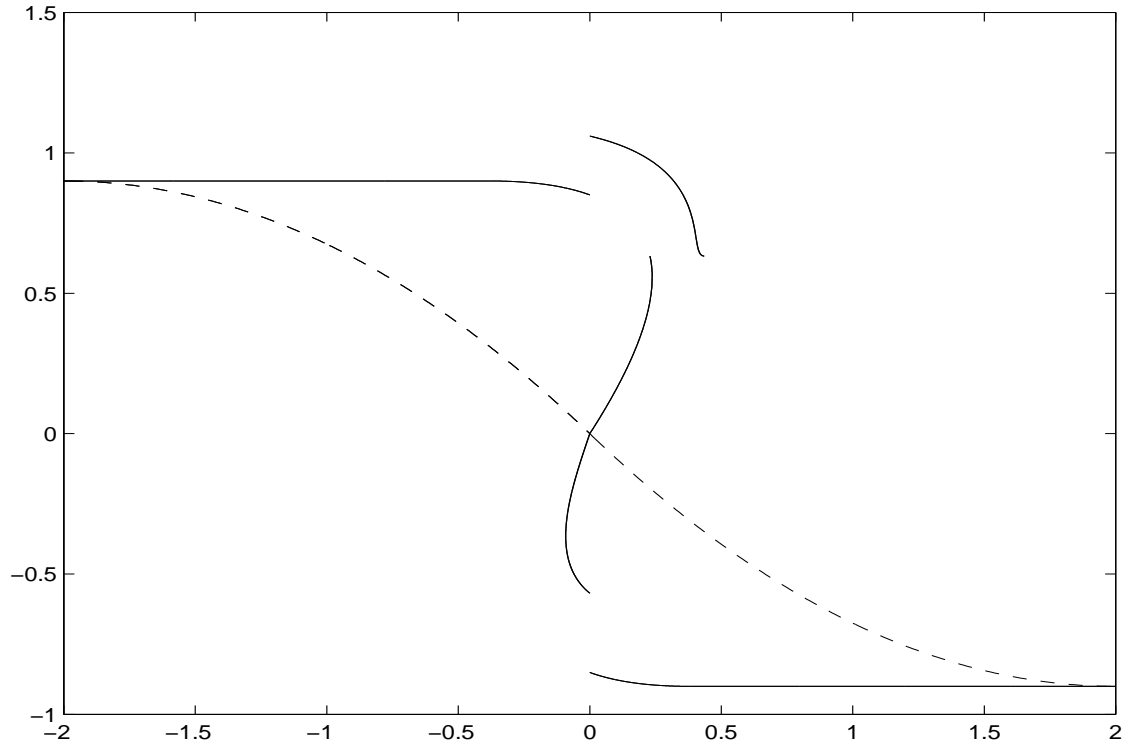


Figure 9.2 Example 9.2, velocity. Dashed line: $w(x)$; Solid line: multivalued velocity at $t = 1.8$. The horizontal axis is the position, the vertical axis is the velocity.

In this example we are interested in the approximation of the moments, such as the density

$$\rho(x, t) = \int f(x, \xi, t) d\xi$$

and the averaged velocity

$$u(x, t) = \frac{\int f(x, \xi, t) \xi d\xi}{\int f(x, \xi, t) d\xi}$$

These quantities are computed by the decomposition techniques described in the Introduction. We first solve the level set function ϕ and modified density function

ψ which satisfy the Liouville equation (9.1) with initial data $\xi - w(x)$ and 1 respectively. Then the desired physical observables ρ and u are computed from the numerical singular integrals (1.8), (1.9), which are computed by approximating the delta function in the integrand by a discrete delta function

$$\delta_\omega(x) = \begin{cases} \frac{1}{2\omega}(1 + \cos(\frac{|\pi x|}{\omega})), & |x| \leq \omega; \\ 0, & |x| > \omega, \end{cases} \quad (9.6)$$

and then evaluating the integral on a uniform mesh [28, 5]. The ω in (9.6) is half of the support size of the discrete delta function. In our computation we choose

$$w = \max(|\psi_v|, 1)h,$$

where $|\psi_v|$ denotes the Jacobian of $\Psi = (\psi_j)$ with respect to \mathbf{v} :

$$|\partial\Psi/\partial(v_1, \dots, v_d)|,$$

and is approximated by the central differencing. In example 9.2 $d = 1$ and in example 9.3 $d = 2$.

The exact velocity profile and the corresponding density at $t = 1.8$ are given in Appendix B. Figure 9.2 shows the exact multivalued velocity.

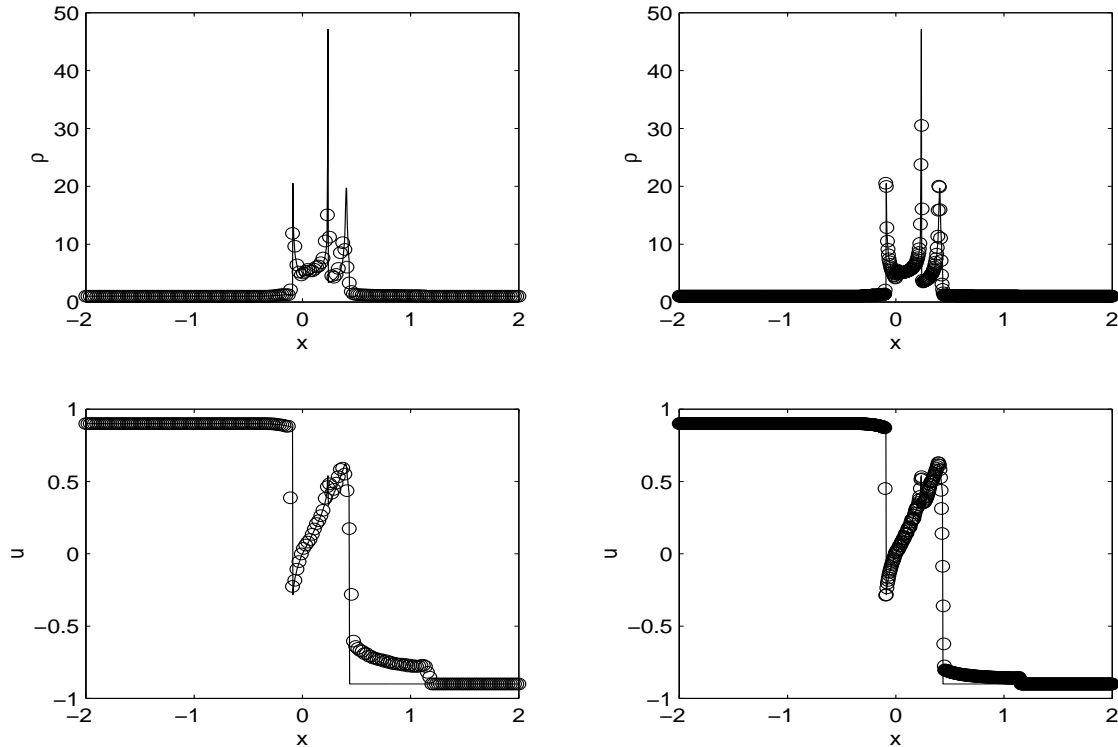


Figure 9.3 Example 9.2, density $\rho(x, t)$ and averaged velocity $u(x, t)$ at $t = 1.8$. Solid line: the exact solutions; 'o': the numerical solutions. Upper: density; Lower: the averaged velocity. Left: 200×161 mesh; Right: 800×641 mesh.

Figure 9.3 shows the calculated density $\rho(x, t)$ and averaged velocity $u(x, t)$ with different meshes using Scheme I together with the exact solutions. Note in the velocity the halfth order error produced around the discontinuity travels to the right and stops at around $x = 1.2$. There are also such errors produced in density, but they can not be observed in the figure since these errors are small compared with the maximum density value.

Table 9.2 compares the l^1 -error of the numerical densities $\rho(x, t)$ computed with 200×161 , 400×321 and 800×641 meshes on the domain $[-2, 2] \times [-1.6, 1.6]$. We notice that Scheme II has slightly larger errors than Scheme I. This is understandable because in order to maintain the l^1 -contracting property, Scheme II may use more cell values to perform the numerical interpolation in evaluating the split fluxes.

Table 9.2 l^1 error of the numerical density $\rho(x, t)$ with different meshes

mesh	200×161	400×321	800×641
Scheme I	1.691542	0.967246	0.670656
Scheme II	1.694563	0.992385	0.679215

Table 9.3 compares the l^1 -error of the numerical averaged velocities u computed with 200×161 , 400×321 and 800×641 meshes on the domain $[-2, 2] \times [-1.6, 1.6]$. It shows the halfth order convergence.

Table 9.3 l^1 error of the numerical averaged velocity ρ on different meshes

mesh	200×161	400×321	800×641
Scheme I	0.170247	0.116522	0.073458
Scheme II	0.170900	0.128646	0.081642

Example 9.3. Computing the physical observables of a 2D problem with a measure-valued solution. Consider the 2D Liouville equation

$$f_t + \xi f_x + \eta f_y - V_x f_\xi - V_y f_\eta = 0$$

with a discontinuous potential given by

$$V(x, y) = \begin{cases} 0.1, & x > 0, y > 0, \\ 0, & \text{else,} \end{cases}$$

and the delta-function initial data

$$f(x, y, \xi, \eta, 0) = \rho(x, y, 0)\delta(\xi - p(x, y))\delta(\eta - q(x, y)),$$

where

$$\rho(x, y, 0) = \begin{cases} 0, & x > -0.1, y > -0.1; \\ 1, & \text{else,} \end{cases}$$

$$p(x, y) = q(x, y) = \begin{cases} 0.4, & x > 0, y > 0, \\ 0.6, & \text{else.} \end{cases}.$$

In this example we are interested in the computation of numerical density which is the zeroth moment of this delta-type solution

$$\rho(x, y, t) = \int \int f(x, y, \xi, \eta, t) d\xi d\eta.$$

The computational domain is chosen to be $[x, y, \xi, \eta] \in [-0.2, 0.2] \times [-0.2, 0.2] \times [0.3, 0.9] \times [0.3, 0.9]$.

The exact density at $t = 0.4$ is

$$\rho(x, y, 0.4) = \begin{cases} 1, & x < 0 \text{ or } y < 0; \\ 1.5, & 0 \leq x \leq 14/150, y \geq \frac{3x}{2}; \\ 1.5, & 0 \leq y \leq 14/150, y \leq \frac{2x}{3}; \\ 0, & \text{otherwise,} \end{cases}$$

as shown in the upper left part in Figure 9.4.

The other part in Figures 9.4 show respectively the calculated density ρ with 14^4 , 26^4 and 50^4 meshes in the phase space using Scheme I in space.

Table 9.4 compares the l^1 errors on $[0, 0.2] \times [0, 0.2]$ of numerical densities computed with 14^4 , 26^4 and 50^4 meshes in phase space. Again the error of Scheme II is larger than Scheme I. The convergence order is about 1/2.

Table 9.4 l^1 error of numerical densities on $[0, 0.2] \times [0, 0.2]$ using different meshes

mesh	14^4	26^4	50^4
Scheme I	0.01851	0.01417	0.01029
Scheme II	0.01864	0.01527	0.01257

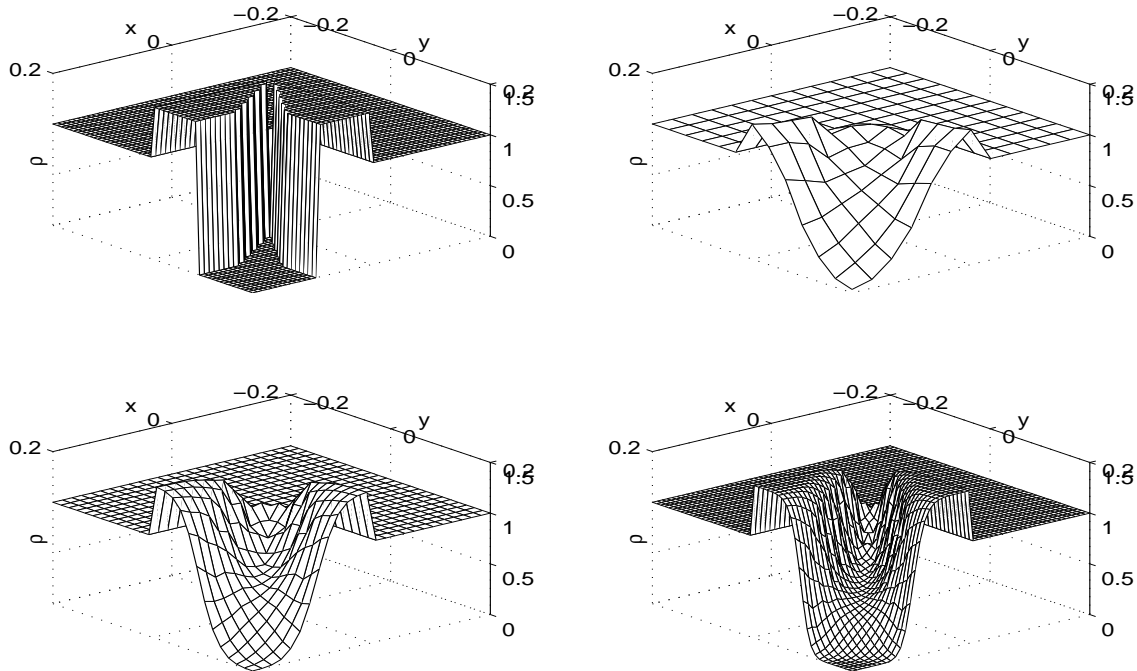


Figure 9.4 Example 9.3, density at $t = 0.4$ in space. Upper left: the exact solution; Upper right: the numerical solution using 14^4 mesh; Lower left: the numerical solution using 26^4 mesh; Lower right: the numerical solution using 50^4 mesh.

10 Conclusion

In this paper, we introduce two classes of Hamiltonian-preserving schemes for the Liouville equation with discontinuous potentials. By using the constant Hamiltonian across the potential barrier, we introduced a selection criterion for a unique, physically relevant solution to the underlying linear hyperbolic equation with singular coefficients. These schemes have a hyperbolic CFL condition, which is a significant improvement over a conventional discretization. We established positivity, and stability theory in both l^1 and l^∞ norms, of these discretizations, and conducted numerical experiments to study the numerical accuracy.

This idea has also recently been extended to the Liouville equation arising from geometrical optics limit of the linear wave equation with a discontinuous local wave speed [13]. In addition, the same idea can also be extended to problems with external fields, such as the electrical or electromagnetic fields. There Vlasov-Poisson or Vlasov-Maxwell systems arise. Currently we are exploring the Hamiltonian-preserving schemes in these more general applications, as well as the case when the interface is a curved geometry.

Appendix A

Lemma A.1. Assume $0 < \mu < \frac{1}{2}$, N is a positive integer, then

$$\sum_{l=0}^{[\mu N]-1} (1-\mu)^{N-l} \mu^l C_N^l < \frac{1}{2}, \quad (\text{A.1})$$

where $[x]$ represents the biggest integer equal to or less than x .

Proof. Notice that

$$\sum_{l=0}^N (1-\mu)^{N-l} \mu^l C_N^l = 1,$$

so proof of (A.1) is equivalent to prove

$$\begin{aligned} & \sum_{l=0}^{[\mu N]-1} (1-\mu)^{N-l} \mu^l C_N^l < \sum_{l=[\mu N]}^N (1-\mu)^{N-l} \mu^l C_N^l \\ \Leftrightarrow & \sum_{l=0}^{[\mu N]-1} \left(\frac{\mu}{1-\mu} \right)^l C_N^l < \sum_{l=[\mu N]}^N \left(\frac{\mu}{1-\mu} \right)^l C_N^l. \end{aligned} \quad (\text{A.2})$$

Denote $k = [\mu N]$, then $2k \leq 2\mu N < N \Rightarrow k < N + 1 - k$. Denote $\Upsilon_l = \left(\frac{\mu}{1-\mu} \right)^l C_N^l$, $l = 0, 1, \dots, N$, we first compare the two terms Υ_{k-1} and Υ_k :

$$\frac{\Upsilon_k}{\Upsilon_{k-1}} = \frac{N+1-k}{k} \frac{\mu}{1-\mu} = \frac{N+1-k}{k} \frac{\mu N}{N-\mu N} \geq \frac{N+1-k}{k} \frac{k}{N-k} > 1.$$

By comparing Υ_{k-2} and Υ_{k+1} , one has

$$\begin{aligned} \frac{\Upsilon_{k+1}}{\Upsilon_{k-2}} &= \frac{\Upsilon_{k+1}}{\Upsilon_k} \frac{\Upsilon_k}{\Upsilon_{k-1}} \frac{\Upsilon_{k-1}}{\Upsilon_{k-2}} > \frac{\Upsilon_{k+1}}{\Upsilon_k} \frac{\Upsilon_{k-1}}{\Upsilon_{k-2}} \\ &= \frac{N+1-(k+1)}{k+1} \frac{N+1-(k-1)}{k-1} \left(\frac{\mu}{1-\mu} \right)^2 \\ &\geq \frac{(N+1-k)^2 - 1}{k^2 - 1} \left(\frac{k}{N-k} \right)^2 > 1. \end{aligned} \quad (\text{A.3})$$

By induction, one can generally prove the following results,

$$\frac{\Upsilon_{k+l-1}}{\Upsilon_{k-l}} > 1, \quad 1 \leq l \leq k \Rightarrow \Upsilon_l < \Upsilon_{2k-1-l}, \quad 0 \leq l \leq k-1.$$

Thus the inequality (A.2) is proved. \square

Appendix B

This Appendix gives the exact velocity profile and density at $t = 1.8$ for the problem in Example 9.2.

Set $t = 1.8$, $X = -2 + \sqrt{\frac{4}{0.9}(0.9 - \sqrt{0.4})} + \sqrt{0.4t}$.

- In domain $-2 < x < -2 + 0.9t$ or $2 - 0.9t < x < 2$, the velocity is single phased given by

$$u(x) = \begin{cases} 0.9, & -2 < x < -2 + 0.9t; \\ -0.9, & 2 - 0.9t < x < 2, \end{cases}$$

the corresponding density is the constant 1.

- In domain $-2 + 0.9t < x < -0.09150169603022$, the velocity is single phased given by

$$u(x) = 0.9 - \frac{0.9}{4} \left(\frac{2}{0.9t} - \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2} \right)^2,$$

the corresponding density is given by

$$\rho(x) = \frac{2}{0.9t \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2}}.$$

- In domain $-0.09150169603022 < x < 0$, the velocity has three phases.

$$u_1(x) = 0.9 - \frac{0.9}{4} \left(\frac{2}{0.9t} - \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2} \right)^2,$$

while u_2, u_3 both satisfy the expression

$$-\frac{0.9t}{4} \left(-\left(2 - \frac{2}{0.9t}\right)^2 + \left(-\sqrt{\frac{4}{0.9} \left(0.9 - \sqrt{u_2^2 + 0.4}\right)} + 2/0.9/t \right)^2 \right) \frac{u_2}{\sqrt{u_2^2 + 0.4}} = x,$$

and $-0.36444353343385 < u_2 < 0$, $-0.56860919537261 < u_3 < -0.36444353343385$.

The first branch of the density is

$$\rho_1(x) = \frac{2}{0.9t \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2}}.$$

To determine densities ρ_2, ρ_3 , denote the derivative of $u_2(x), u_3(x)$ to be $u'_2(x), u'_3(x)$ respectively. Define the functions

$$\begin{aligned} W(w) &= -\sqrt{w^2 + 0.4}, \\ X(W) &= 2 - \sqrt{\frac{4}{0.9}(0.9 + W)}, \\ Y(X) &= \frac{0.9}{2}(X - 2), \end{aligned}$$

then

$$\begin{aligned} \rho_2(x) &= \left| \frac{u_2(x)u'_2(x)}{W(u_2(x))Y(X(W(u_2(x))))} \right|, \\ \rho_3(x) &= \left| \frac{u_3(x)u'_3(x)}{W(u_3(x))Y(X(W(u_3(x))))} \right|. \end{aligned}$$

- In domain $0 < x < X$, the velocity has three phases. u_1 is determined by

$$\frac{0.9t}{4} \left(\left(2 - \frac{2}{0.9t} \right)^2 - \left(\sqrt{\frac{4}{0.9} \left(0.9 - \sqrt{u_1^2 - 0.4} \right)} - \frac{2}{0.9t} \right)^2 \right) \frac{u_1}{\sqrt{u_1^2 - 0.4}} = x,$$

with $0.97449009909131 < u_1 < 1.05986622602208$, and

$$\begin{aligned} u_2(x) &= 0.9 - \frac{0.9}{4} \left(-\frac{2}{0.9t} - \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2} \right)^2, \\ u_3(x) &= -0.9 + \frac{0.9}{4} \left(-\frac{2}{0.9t} + \sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2} \right)^2. \end{aligned}$$

Denote the derivative of $u_1(x)$ to be $u'_1(x)$. Define the functions

$$\begin{aligned} W(w) &= \sqrt{w^2 - 0.4}, \\ X(W) &= \sqrt{\frac{4}{0.9}(0.9 - W)} - 2, \\ Y(X) &= -\frac{0.9}{2}(X + 2), \end{aligned}$$

then the densities are

$$\begin{aligned} \rho_1(x) &= \left| \frac{u_1(x)u'_1(x)}{W(u_1(x))Y(X(W(u_1(x))))} \right|, \\ \rho_2(x) &= \frac{2}{0.9t\sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2}}, \\ \rho_3(x) &= \frac{2}{0.9t\sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2}}. \end{aligned}$$

- In domain $X < x < -2 + 0.9t + \frac{1}{0.9t}$, the velocity has four phases. u_1 is determined by

$$\frac{0.9t}{4} \left(\left(2 - \frac{2}{0.9t} \right)^2 - \left(\sqrt{\frac{4}{0.9} \left(0.9 - \sqrt{u_1^2 - 0.4} \right) - \frac{2}{0.9t}} \right)^2 \right) \frac{u_1}{\sqrt{u_1^2 - 0.4}} = x,$$

with $0.96921825670040 < u_1 < 0.97449009909131$, and

$$\begin{aligned} u_2(x) &= 0.9 - \frac{0.9}{4} \left(-\frac{2}{0.9t} + \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2} \right)^2, \\ u_3(x) &= 0.9 - \frac{0.9}{4} \left(-\frac{2}{0.9t} - \sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2} \right)^2, \\ u_4(x) &= -0.9 + \frac{0.9}{4} \left(-\frac{2}{0.9t} + \sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2} \right)^2. \end{aligned}$$

Denote the derivative of $u_1(x)$ to be $u_1'(x)$. Define the functions

$$\begin{aligned} W(w) &= \sqrt{w^2 - 0.4}, \\ X(W) &= \sqrt{\frac{4}{0.9}(0.9 - W) - 2}, \\ Y(X) &= -\frac{0.9}{2}(X + 2), \end{aligned}$$

then the densities are

$$\begin{aligned} \rho_1(x) &= \left| \frac{u_1(x)u_1'(x)}{W(u_1(x))Y(X(W(u_1(x))))} \right|, \\ \rho_2(x) &= \frac{2}{0.9t\sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2}}, \\ \rho_3(x) &= \frac{2}{0.9t\sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2}}, \\ \rho_4(x) &= \frac{2}{0.9t\sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t} \right)^2}}. \end{aligned}$$

- In domain $-2 + 0.9t + \frac{1}{0.9t} < x < 0.35899646920179$, the velocity has two phases. u_1 is determined by

$$\frac{0.9t}{4} \left(\left(2 - \frac{2}{0.9t} \right)^2 - \left(\sqrt{\frac{4}{0.9} \left(0.9 - \sqrt{u_1^2 - 0.4} \right) - \frac{2}{0.9t}} \right)^2 \right) \frac{u_1}{\sqrt{u_1^2 - 0.4}} = x,$$

with $0.63245703734354 < u_1 < 0.96921825670040$, and

$$u_2(x) = -0.9 + \frac{0.9}{4} \left(-\frac{2}{0.9t} + \sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2} \right)^2.$$

Denote the derivative of $u_1(x)$ to be $u_1'(x)$. Define the functions

$$\begin{aligned} W(w) &= \sqrt{w^2 - 0.4}, \\ X(W) &= \sqrt{\frac{4}{0.9}(0.9 - W) - 2}, \\ Y(X) &= -\frac{0.9}{2}(X + 2), \end{aligned}$$

then the densities are

Density ρ_2 is given by

$$\begin{aligned} \rho_1(x) &= \left| \frac{u_1(x)u_1'(x)}{W(u_1(x))Y(X(W(u_1(x))))} \right|, \\ \rho_2(x) &= \frac{2}{0.9t\sqrt{-\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2}}. \end{aligned}$$

- In domain $0.35899646920179 < x < 2 - 0.9t$, the velocity is single phased given by

$$u(x) = -0.9 + \frac{0.9}{4} \left(-\frac{2}{0.9t} + \sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2} \right)^2,$$

the corresponding density is given by

$$\rho(x) = \frac{2}{0.9t\sqrt{\frac{4x}{0.9t} + \left(2 - \frac{2}{0.9t}\right)^2}}.$$

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