The l^1-stability of a Hamiltonian-preserving scheme for the Liouville equation with discontinuous potentials *

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Abstract

We study the l^1-stability of a Hamiltonian-preserving scheme, developed in [3], for the Liouville equation with a discontinuous potential in one space dimension. We prove that, for suitable initial data, the scheme is stable in the l^1-norm under a hyperbolic CFL condition. We also provide a counter example to show that for other initial data, in particular, the measure-valued initial data, the numerical solution may become unbounded.

1 Introduction

In [3], we constructed a class of numerical schemes for the d-dimensional Liouville equation in classical mechanics:

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

where $f(t, \mathbf{x}, \mathbf{v})$ is the density distribution of a classical particle at position $\mathbf{x}$, time t and travelling with velocity $\mathbf{v}$. $V(\mathbf{x})$ is the potential. The main interest is in the case of a discontinuous potential $V(\mathbf{x})$, corresponding to a potential barrier. When

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V is discontinuous, the Liouville equation (1.1) is a linear hyperbolic equation with a measure-valued coefficient. One needs to provide additional condition in order to select a unique, physically relevant solution across the barrier. The main idea of the Hamiltonian-preserving schemes developed in [3] was to build into the numerical flux the particle behavior at the barrier.

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

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

which is a Hamiltonian system with the Hamiltonian

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

It is known from classical mechanics that the Hamiltonian remains constant across a potential barrier. By using this mechanism in the numerical flux, the schemes developed in [3] provide a physically relevant solution to the underlying problem. It was proved that the two schemes developed in [3], under a hyperbolic CFL condition, are positive, and stable under both l^∞ and l^1 norms in one space dimension. The detailed proof of Scheme I, using a finite difference approach involving interpolations in the phase space, was left out due to the length restriction of the publishing journal, thus is provided in this article.

In Sections 2, we first present Scheme I developed in [3]. In Section 3, we prove the l^1-stability of this scheme for suitable initial data. We give a counter example in Section 4 to show that for more general initial data, in particular the measure-valued initial data, the numerical solution may become unbounded.

2 A Hamiltonian-preserving scheme

Consider the Liouville equation in one space dimension:

$$f_t + \xi f_x - V_x f_\xi = 0 \tag{2.1}$$

with a discontinuous potential $V(x)$.

Without loss of generality, we employ an uniform mesh with grid points at $x_{i+\frac{1}{2}}, i = 0, \cdots, N$, in the x-direction and $\xi_{j+\frac{1}{2}}, j = 0, \cdots, M$ in the ξ-direction. The cells are centered at $(x_i, \xi_j), i = 1, \cdots, N, j = 1, \cdots, M$ 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 $0 = t_0 < t_1 < \cdots < t_L = T$. 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

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

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

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i |DV_i|}{\Delta\xi}\right] \le 1. \tag{2.3}$$

  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 $\Delta t = O(\Delta x \Delta\xi)$.

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:*

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

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

The main ingredient in the Hamiltonian-preserving schemes developed in [3], like the early work for shallow-water equations [5], was to build into the numerical flux the particle behavior at the barrier. Since the density distribution f remains unchanged across the potential barrier, thus

$$f(t,x^+,\xi^+) = f(t,x^-,\xi^-) \tag{2.5}$$

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 [3].

We now present the first Hamiltonian-preserving scheme, called *Scheme I* in [3].

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

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

The flux-splitting, semidiscrete scheme (with time continuous) reads

$$\partial_t f_{ij} + \xi_j \frac{f^-_{i+\frac{1}{2},j} - f^+_{i-\frac{1}{2},j}}{\Delta x} - \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0, \tag{2.6}$$

where the numerical fluxes $f_{i,j+\frac{1}{2}}$ 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 the algorithm is to define the split numerical fluxes $f^-_{i+\frac{1}{2},j}, f^+_{i-\frac{1}{2},j}$ at each cell interface. (2.5) will be used to define these fluxes.

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

The algorithm

- $\xi_j > 0$

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

  ❑ if $V^-_{i+\frac{1}{2}} > V^+_{i+\frac{1}{2}}$,

  ✰ 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 $\xi_k \le \xi^- < \xi_{k+1}$ for some k

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

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 $V^-_{i+\frac{1}{2}} < V^+_{i+\frac{1}{2}}$,

☆ 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 $\xi_k \le \xi^+ < \xi_{k+1}$ for some k

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 $V^-_{i+\frac{1}{2}} > V^+_{i+\frac{1}{2}}$

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

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

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

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

In [3] we proved that, when the first order upwind scheme is used spatially, and the forward Euler method is used in time, and the potential V has a single jump, Scheme I is positive and l^∞-contracting under the CFL condition:

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|}{\Delta \xi} \right] \le 1. \tag{2.7}$$

Note that the quantity $\left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|$ represents the gradient of potential at its *smooth* point, which has a *finite* upper bound. Thus the scheme satisfies a hyperbolic CFL condition.

3 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 consider the simple case when $V(x)$ is a step function, with a jump $-D, D > 0$ at $x_{m+\frac{1}{2}}$. Namely

$$V^-_{m+\frac{1}{2}} - V^+_{m+\frac{1}{2}} = D, \quad V^\pm_{i+\frac{1}{2}} = V^-_{m+\frac{1}{2}}, i < m, \quad V^\pm_{i+\frac{1}{2}} = V^+_{m+\frac{1}{2}}, i > m.$$

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

Define an index set

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

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

$$E_d = \{(i,j) | i = 1, \cdots, N, j = 1, \cdots, M\} \setminus D_l^4. \tag{3.1}$$

Figure 3.1 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.

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 the scheme itself, 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 $\xi_j > 0, i \neq m+1$,

$$f_{ij}^{n+1} = (1 - \xi_j \lambda_x^t) f_{ij} + \xi_j \lambda_x^t f_{i-1,j}\,; \tag{3.2}$$

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

$$f_{ij}^{n+1} = (1 - |\xi_j| \lambda_x^t) f_{ij} + |\xi_j| \lambda_x^t f_{i+1,j}\,; \tag{3.3}$$

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

$$f_{m+1,j}^{n+1} = (1 - \xi_j \lambda_x^t) f_{m+1,j} + \xi_j \lambda_x^t (c_{j,k} f_{m,k} + c_{j,k+1} f_{m,k+1})\,; \tag{3.4}$$

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

$$f_{m+1,j}^{n+1} = (1 - \xi_j \lambda_x^t) f_{m+1,j} + \xi_j \lambda_x^t f_{m+1,k}\,; \tag{3.5}$$

5) if $\xi_j < 0$,

$$f_{mj}^{n+1} = (1 - |\xi_j| \lambda_x^t) f_{mj} + |\xi_j| \lambda_x^t (c_{jk} f_{m+1,k} + c_{j,k+1} f_{m+1,k+1}), \tag{3.6}$$

where $0 \leq c_{jk} \leq 1$ and $c_{jk} + c_{j,k+1} = 1$. In (3.4) k is determined by $\xi_k \leq \sqrt{\xi_j^2 - 2D} < \xi_{k+1}$, in (3.5) $\xi_k = -\xi_j$, and in (3.6) $\xi_k \leq -\sqrt{\xi_j^2 + 2D} < \xi_{k+1}$. We omit the superscript n of f_{ij} on the right hand side.

Using the triangle inequality in (3.2)-(3.6), one typically gets the following

$$|f^{n+1}|_1 \leq \frac{1}{N_d} \sum_{(i,j) \in E_d} \alpha_{ij} |f_{ij}^n|, \tag{3.7}$$

where the coefficients α_{ij} are positive. One can check that, under the hyperbolic CFL condition (2.7), $\alpha_{ij} \leq 1$ except for possibly $(i,j) \in D_m^2 \cup D_{m+1}^4$ with the definitions:

$$D_m^2 = \{(m,j) | 0 < \xi_j < \sqrt{\xi_N^2 - 2D} + \Delta\xi\},$$
$$D_{m+1}^4 = \{(m+1,j) | \xi_j < -\sqrt{\Delta\xi^2/4 + 2D} + \Delta\xi\}.$$

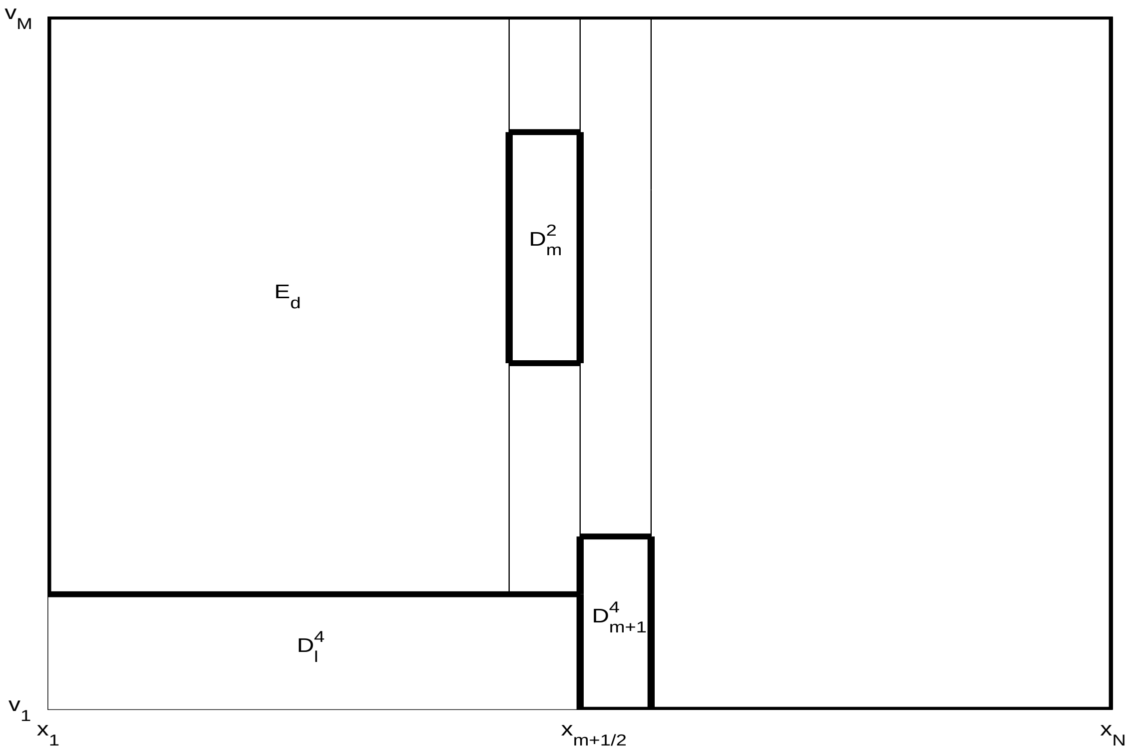

Figure 3.1 Sketch of the index sets D_m^2, D_{m+1}^4, D_l^4.

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

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

Let the number of elements in S_j^m be N_j^m. One can check that $N_j^m \le 2$ because every two elements $j_1', j_2' \in S_j^m$ satisfy $|\sqrt{\xi_{j_1'}^2 - 2D} - \sqrt{\xi_{j_2'}^2 - 2D}| \ge |\xi_{j_1'} - \xi_{j_2'}| \ge \Delta\xi$.

On the other hand, one can easily check from (3.4), for $(m,j) \in D_m^2$,

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

so the boundedness of M_1 is proved.

Next we study M_2. Define the set

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

Let $\xi_{max} = \max\{|\xi_1|, |\xi_M|\}$. Using the CFL condition, $\frac{\xi_{max}\Delta t}{\Delta x} \le 1$. So from (3.6) one can get, for $(m+1, j) \in D^4_{m+1}$, the estimate for $\alpha_{m+1,j}$:

$$\alpha_{m+1,j} < 1 + \sum_{j' \in S_j^{m+1}} |\xi_{j'}| \lambda_x^t \le 1 + \frac{1}{\xi_{max}} \sum_{j' \in S_j^{m+1}} |\xi_{j'}|. \tag{3.8}$$

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 $|\xi_{m_2}| \le |\xi_{m_1}|$. The last summation in (3.8) turns out to be

$$\sum_{j' \in S_j^{m+1}} |\xi_{j'}| = \frac{|\xi_{m_1}| + |\xi_{m_2}|}{2} \left(\frac{|\xi_{m_1}| - |\xi_{m_2}|}{\Delta\xi} + 1 \right) \le \frac{\xi_{m_1}^2 - \xi_{m_2}^2}{2\Delta\xi} + \xi_{max}. \tag{3.9}$$

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

$$\begin{aligned} & \sqrt{\xi_{m_1}^2 + 2D} - \sqrt{\xi_{m_2}^2 + 2D} \le 2\Delta\xi\,, \\ \Rightarrow\ & \sqrt{\xi_{m_1}^2 + 2D} \le \sqrt{\xi_{m_2}^2 + 2D} + 2\Delta\xi\,, \\ \Rightarrow\ & \xi_{m_1}^2 \le \xi_{m_2}^2 + 2\sqrt{\xi_{m_2}^2 + 2D}\Delta\xi + 4\Delta\xi^2\,, \\ \Rightarrow\ & \frac{\xi_{m_1}^2 - \xi_{m_2}^2}{2\Delta\xi} \le \sqrt{\xi_{m_2}^2 + 2D} + 2\Delta\xi \le \xi_{max} + 2\Delta\xi. \end{aligned} \tag{3.10}$$

Combine (3.8)-(3.10), 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 $(m+1, j) \in D^4_{m+1}$. 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 (3.7),

$$|f^{n+1}|_1 \le |f^n|_1 + \frac{M_1'}{N_d} \sum_{(i,j) \in D_m^2} |f_{ij}^n| + \frac{M_2'}{N_d} \sum_{(i,j) \in D_{m+1}^4} |f_{ij}^n|\,. \tag{3.11}$$

We now impose an assumption:

Assumption 1

There exists a positive constant ξ_z such that

$$\forall (i,j) \in S_z = \{(i,j)| \quad x_i < x_{m+\frac{1}{2}}, \quad 0 < \xi_j < \xi_z\}, \tag{3.12}$$

it holds that

$$|f^0_{ij}| \leq C_1 |f^0|_1 \,. \tag{3.13}$$

Remark: When arisen from the semiclassical limit of the linear Schrödinger equation, the Liouville equation is supplied with measure-valued initial data [1, 4], which does not satisfy this assumption. Thus Scheme I, when directly applied to this problem, may have stability problems, as shown in the next subsection. However, in [2], a decomposition of the initial data was introduced, which allows one to solve the semiclassical limit problem with only bounded initial data. Thus Scheme I is still suitable by using this decomposition, as shown in [3].

We now establish the following theorem:

Theorem 3.1. *Under Assumption 1, the scheme (3.2)-(3.6) is l^1-stable*

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

Proof. From (3.11),

$$|f^L|_1 \leq |f^0|_1 + \frac{M_1'}{N_d} \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D^2_m} |f^n_{ij}| \right\} + \frac{M_2'}{N_d} \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D^4_{m+1}} |f^n_{ij}| \right\}. \tag{3.14}$$

It remains to estimate

$$S_1 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D^2_m} |f^n_{ij}| \right\} \tag{3.15}$$

and

$$S_2 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D^4_{m+1}} |f^n_{ij}| \right\}. \tag{3.16}$$

We begin with estimating S_2.

Define the set

$$S_r = \{(i,j)| \quad x_i > x_{m+\frac{1}{2}}, (m+1,j) \in D^4_{m+1}\}.$$

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

$$f^n_{ij} = \sum_{(p,q)\in S_r} \beta^{ijn0}_{pq} f^0_{pq}, \quad (i,j) \in S_r \tag{3.17}$$

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

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

$$S_2 \leq \sum_{(p,q)\in S_r} \left(\sum_{n=0}^{L-1} \sum_{(i,j)\in D_{m+1}^4} \beta_{pq}^{ijn0} \right) |f_{pq}^0| \equiv \sum_{(p,q)\in S_r} F(p,q)|f_{pq}^0|, \tag{3.18}$$

where we have defined

$$F(p,q) \quad = \quad \sum_{n=0}^{L-1} \sum_{(i,j)\in D_{m+1}^4} \beta_{pq}^{ijn0}, \quad (p,q) \in S_r. \tag{3.19}$$

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 (3.19) 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 (3.3)

$$\beta_{ij}^{ij0} = \sum_{n=0}^{\infty} \beta_{ij}^{ijn0} = \sum_{n=0}^{\infty} (c_1^j)^n = \frac{1}{1 - c_1^j} = \frac{1}{c_2^j}. \tag{3.20}$$

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 (3.3),

$$\beta_{pq}^{ij,n+1,0} \quad = \quad c_1^j \beta_{pq}^{ijn0} + c_2^j \beta_{pq}^{i+1,jn0}, \tag{3.21}$$

then a sum of n from 0 to ∞ in (3.21) gives

$$\beta_{pq}^{ij0} \quad = \quad \beta_{pq}^{i+1,j0}, \quad i < p. \tag{3.22}$$

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

$$F(p,q) \leq \sum_{(i,j)\in D^4_{m+1}} \beta^{ij0}_{pq} = \beta^{m+1,q,0}_{pq} = \beta^{m+2,q,0}_{pq} = \cdots = \beta^{p,q,0}_{pq} \leq \lambda_1. \tag{3.23}$$

Therefore, from (3.18) we get

$$\begin{aligned} S_2 &\leq \sum_{(p,q)\in S_r} F(p,q)|f^0_{pq}| \leq \lambda_1 \sum_{(p,q)\in S_r} |f^0_{pq}| \\ &\leq \lambda_1 \sum_{(p,q)\in E_d} |f^0_{pq}| = \lambda_1 N_d |f^0|_1. \end{aligned} \tag{3.24}$$

Our next step is to estimate S_1. Define the set

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

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

$$f^n_{ij} = \sum_{(p,q)\in S_l} \gamma^{ijn0}_{pq} f^0_{pq}, \quad (i,j) \in S_l. \tag{3.25}$$

Dividing set D^2_m into two parts:

$$D^{2,1}_m = \{(i,j) \in D^2_m | \xi_j \geq \xi_z\}, \quad D^{2,2}_m = \{(i,j) \in D^2_m | \xi_j < \xi_z\},$$

and also define the corresponding two parts of S_l

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

Note that S^2_l is a subset of S_z in (3.12).

Correspondingly, S_1 is also divided into two parts

$$S_1 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D^{2,1}_m} |f^n_{ij}| \right\} + \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D^{2,2}_m} |f^n_{ij}| \right\} = S_{11} + S_{12}. \tag{3.26}$$

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

$$S_{11} \leq \lambda_2 N_d |f^0|_1 \tag{3.27}$$

with $\lambda_2 \equiv \frac{1}{\xi_z \lambda^t_x}$. Substituting (3.25) into S_{12} gives

$$S_{12} \leq \sum_{(p,q)\in S^2_l} \left(\sum_{n=0}^{L-1} \sum_{(i,j)\in D^{2,2}_m} \gamma^{ijn0}_{pq} \right) |f^0_{pq}|.$$

Using Assumption 1,

$$
\begin{aligned}
S_{12} &\leq C_1|f^0|_1 \sum_{(p,q)\in S_l^2} \left(\sum_{n=0}^{L-1} \sum_{(i,j)\in D_m^{2,2}} \gamma_{pq}^{ijn0} \right) \\
&= C_1|f^0|_1 \sum_{n=0}^{L-1} \sum_{(i,j)\in D_m^{2,2}} \left(\sum_{(p,q)\in S_l^2} \gamma_{pq}^{ijn0} \right). \qquad (3.28)
\end{aligned}
$$

Now we evaluate $\sum_{(p,q)\in S_l^2} \gamma_{pq}^{ijn0}$ when $(i,j) \in D_m^{2,2}$. Write (3.25) as

$$
f_{ij}^n = \sum_{(p,q)\in S_l^2} \gamma_{pq}^{ijn0} f_{pq}^0, \quad (i,j) \in D_m^{2,2}. \qquad (3.29)
$$

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 (3.29) 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 (3.28),

$$
\begin{aligned}
S_{12} &\leq C_1|f^0|_1 \sum_{n=0}^{L-1} \sum_{(i,j)\in D_m^{2,2}} 1 \leq \frac{C_1|f^0|_1 L N_d}{N} \\
&= \frac{C_1 T N_d}{(x_{N+\frac{1}{2}} - x_{\frac{1}{2}})\lambda_x^t} |f^0|_1 \equiv \lambda_3 N_d |f^0|_1 \qquad (3.30)
\end{aligned}
$$

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 (3.26), (3.27) and (3.30),

$$
S_1 \leq (\lambda_2 + \lambda_3) N_d |f^0|_1. \qquad (3.31)
$$

Combing (3.14), (3.24) and (3.31),

$$
\begin{aligned}
|f^L|_1 &\leq |f^0|_1 + M_1'\lambda_1|f^0|_1 + M_2'(\lambda_2 + \lambda_3)|f^0|_1 \\
&= [1 + M_1'\lambda_1 + M_2'(\lambda_2 + \lambda_3)]|f^0|_1 \\
&\equiv C|f^0|_1
\end{aligned}
$$

where $C \equiv 1 + M_1'\lambda_1 + M_2'(\lambda_2 + \lambda_3)$. Thus Theorem 3.1 is proved. □

4 A counter example for instability

There arises another question about whether condition (3.13) in Assumption 1 is necessary for the l^1-stability. In this subsection we give an 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 (3.12), it holds that

$$|f_{ij}^0| \leq \frac{C_1 |f^0|_1}{\Delta x^q}, \quad q > 0 \tag{4.1}$$

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

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

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

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

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

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

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

$$L_0 = \text{int}(L^{1-q'})L, \tag{4.2}$$

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

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 4.1. $N_h > L_0$ *under the mesh size restrictions*

$$\Delta x < \frac{\sqrt{2D}}{96\sqrt{10}\lambda_x^\xi}, \tag{4.3}$$

$$\Delta x < \frac{1}{4\sqrt{10}(\sqrt{10}-3)\sqrt{2D}\lambda_x^\xi}\frac{T\lambda_x^t}{T\lambda_x^t+\lambda_\xi^t}, \tag{4.4}$$

$$\Delta x < \frac{1}{\lambda_x^t}(\frac{\lambda_x^t\lambda_\xi^t}{12\sqrt{10}T^{1-q'}})^{\frac{1}{q'}}. \tag{4.5}$$

Proof. According to the definitions,

$$\begin{aligned}
N_h &= \sum_{k\in S_m} G(k) = \sum_{k\in S_m} \mathrm{int}\left(L\xi_k\lambda_x^t\right) > \left(L\lambda_x^t\sum_{k\in S_m}\xi_k\right) - N_s \\
&> L\lambda_x^t\sum_{k\in S_m'}\left(\sqrt{\xi_k^2-2D}-\Delta\xi\right) - \frac{1}{\Delta\xi}\frac{(\sqrt{10}-3)\sqrt{2D}}{3} \\
&> L\lambda_x^t\sum_{i=1}^{N_s}\left(\sqrt{(\sqrt{2D}+i\Delta\xi)^2-2D}\right) - \frac{1}{3}L\left(\lambda_x^t+\frac{\lambda_\xi^t}{T}\right)\left(\sqrt{10}-3\right)\sqrt{2D} \\
&> \frac{3L}{\sqrt{20D}}\lambda_x^t\sum_{i=1}^{N_s}\left[\left(\sqrt{2D}+i\Delta\xi\right)\sqrt{\left(\sqrt{2D}+i\Delta\xi\right)^2-2D}\right] \\
&\quad -\frac{1}{3}L\left(\lambda_x^t+\frac{\lambda_\xi^t}{T}\right)\left(\sqrt{10}-3\right)\sqrt{2D} \\
&= \frac{L\lambda_x^t}{\sqrt{20D}\Delta\xi}\sum_{i=1}^{N_s}\left[3\left(\sqrt{2D}+i\Delta\xi\right)\sqrt{\left(\sqrt{2D}+i\Delta\xi\right)^2-2D}\Delta\xi\right] \\
&\quad -\frac{1}{3}L\left(\lambda_x^t+\frac{\lambda_\xi^t}{T}\right)\left(\sqrt{10}-3\right)\sqrt{2D} \\
&> \frac{L\lambda_x^t}{\sqrt{20D}\Delta\xi}\int_{\sqrt{2D}}^{\frac{\sqrt{20D}}{3}-4\Delta\xi} 3x\sqrt{x^2-2D}dx - \frac{1}{3}L\left(\lambda_x^t+\frac{\lambda_\xi^t}{T}\right)\left(\sqrt{10}-3\right)\sqrt{2D} \\
&> \frac{L\lambda_x^t}{\sqrt{20D}\Delta\xi}\left(\frac{1}{3}\sqrt{2D}-\sqrt{\frac{8\sqrt{20D}\Delta\xi}{3}}\right) - \frac{1}{3}L\left(\lambda_x^t+\frac{\lambda_\xi^t}{T}\right)\left(\sqrt{10}-3\right)\sqrt{2D}
\end{aligned} \tag{4.6}$$

We impose the following restriction on the mesh sizes

$$\sqrt{\frac{8\sqrt{20D}\Delta\xi}{3}} < \frac{\sqrt{2D}}{6}, \tag{4.7}$$

$$(1+\frac{\lambda_\xi^t}{T\lambda_x^t})\frac{(\sqrt{10}-3)\sqrt{2D}}{3}\Delta\xi < \frac{1}{12\sqrt{10}}, \tag{4.8}$$

then continue from (4.6),

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

According to (4.2), $L_0 < LL^{1-q'} = \frac{LT^{1-q'}}{(\Delta t)^{1-q'}}$. Therefore, in order that $N_h > L_0$, one needs to impose the mesh size restriction

$$\Delta t < \left(\frac{\lambda_x^t\lambda_\xi^t}{12\sqrt{10}T^{1-q'}}\right)^{\frac{1}{q'}}. \tag{4.9}$$

One can rewrite the mesh size restriction (4.7), (4.8) and (4.9) to that on Δx which are (4.3)-(4.5).

Now, under the mesh size restriction (4.3)-(4.5), it holds that $N_h > L_0$.

□

We now prove the following theorem:

Theorem 4.1. *$\forall q > 0$ 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

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

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

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

Since $N_h > L_0$ by Lemma 4.1, 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 4.1:

$$f_{ij}^0 = c_0, \quad (i,j) \in H_L, \tag{4.10}$$

$$f_{ij}^0 = 0, \quad (i,j) \in E_d \setminus H_L, \tag{4.11}$$

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

$$\frac{2(x_{N+\frac{1}{2}} - x_{\frac{1}{2}})(\xi_{M+\frac{1}{2}} - \xi_{\frac{1}{2}}){\lambda_x^t}^{2-q'}}{\lambda_x^\xi T^{2-q'} \Delta x^{q'}} < \frac{C_1}{\Delta x^q}. \tag{4.12}$$

Condition (4.12) is satisfied under the following mesh size restriction

$$\Delta x < \left(\frac{C_1 \lambda_x^\xi T^{2-q'}}{2(x_{N+\frac{1}{2}} - x_{\frac{1}{2}})(\xi_{M+\frac{1}{2}} - \xi_{\frac{1}{2}}){\lambda_x^t}^{2-q'}} \right)^{\frac{1}{q-q'}} \tag{4.13}$$

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

$$f_{ij}^n = 0 \quad \text{for} \quad (i,j) \in E_d \setminus \{S_m^l \cup S_m^r\}. \tag{4.14}$$

Since our scheme is positive preserving, and the initial values (4.10) and (4.11) are nonnegative, the numerical solutions at each time step are always nonnegative. Then similar to the proof of (3.7), at each time step

$$\begin{aligned} |f^{n+1}|_1 &= \frac{1}{N_d} \sum_{(i,j)\in E_d} f_{ij}^{n+1} \\ &= \frac{1}{N_d} \sum_{(i,j)\in E_d} \alpha_{ij} f_{ij}^n \\ &= \frac{1}{N_d} \sum_{(i,j)\in S_m^l} \alpha_{ij} f_{ij}^n + \frac{1}{N_d} \sum_{(i,j)\in S_m^r} \alpha_{ij} f_{ij}^n + \frac{1}{N_d} \sum_{(i,j)\in E_d\setminus\{S_m^l \cup S_m^r\}} f_{ij}^n, \end{aligned} \tag{4.15}$$

Note the last term in (4.15) is zero by (4.14).

For scheme (3.2) 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 (4.15) gives

$$|f^{n+1}|_1 = \frac{1}{N_d} \sum_{(m,j)\in S_m^m} \alpha_{mj} f_{mj}^n + \frac{1}{N_d} \sum_{(i,j)\in E_d \setminus S_m^m} f_{ij}^n. \tag{4.16}$$

We now estimate α_{mj} for $(m,j) \in S_m^m$. From schemes (3.2) and (3.4), for $(m,j) \in S_m^m$, by setting $j' = T_s(j)$, one has

$$\alpha_{mj} = 1 - \xi_j \lambda_x^t + \xi_{j'} \lambda_x^t c_{j'j}, \tag{4.17}$$

where $c_{j'j}$ are the coefficients in (3.4).

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 (4.17). So (4.17) gives

$$\alpha_{mj} > 1 + \frac{\sqrt{2D}}{6}\lambda_x^t. \tag{4.18}$$

Then (4.18) together with (4.16) give

$$\begin{aligned} |f^{n+1}|_1 &> \frac{\sqrt{2D}}{6}\lambda_x^t \frac{1}{N_d} \sum_{(m,j)\in S_m^m} f_{mj}^n + \frac{1}{N_d} \sum_{(i,j)\in E_d} f_{ij}^n \\ &= \frac{\sqrt{2D}}{6}\lambda_x^t \frac{1}{N_d} \sum_{(m,j)\in S_m^m} f_{mj}^n + |f^n|_1. \end{aligned} \tag{4.19}$$

Summing up (4.19) from $n = 0$ to $L-1$, one gets

$$|f^L|_1 > |f^0|_1 + \frac{\sqrt{2D}}{6}\lambda_x^t \frac{1}{N_d} \sum_{n=0}^{L-1} \sum_{(m,j)\in S_m^m} f_{mj}^n. \tag{4.20}$$

Write

$$f_{ij}^n = \sum_{(p,q)\in S_m^l} \eta_{pq}^{ijn0} f_{pq}^0, \quad (i,j) \in S_m^l. \tag{4.21}$$

Since $S_m^m \in S_m^l$, substituting (4.21) into (4.20) gives

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

$$
\begin{aligned}
&= |f^0|_1 + \frac{1}{6}\sqrt{2D}\lambda_x^t \frac{c_0}{N_d} \sum_{(m,j)\in S_m^m} \left(\sum_{(p,j)\in H_L} \sum_{n=0}^{L-1} \eta_{pj}^{mjn0} \right) \\
&\geq |f^0|_1 + \frac{1}{6}\sqrt{2D}\lambda_x^t \frac{c_0}{N_d} \sum_{l=1}^{s-1} \left(\sum_{(p,k_l)\in H} \sum_{n=0}^{L-1} \eta_{pk_l}^{mk_l n0} \right), \qquad (4.22)
\end{aligned}
$$

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 (3.2), one has for $(k,j) \in H$,

$$
\eta_{pj}^{kj,n+1,0} = \left(1 - \xi_j \lambda_x^t\right) \eta_{pj}^{kjn0} + \xi_j \lambda_x^t \eta_{pj}^{k-1,jn0}. \qquad (4.23)
$$

Adding (4.23) from $n = 0$ to $L - 1$ leads to

$$
\eta_{pj}^{kjL0} + \sum_{n=0}^{L-1} \eta_{pj}^{kjn0} = \left(1 - \xi_j \lambda_x^t\right) \sum_{n=0}^{L-1} \eta_{pj}^{kjn0} + \xi_j \lambda_x^t \sum_{n=0}^{L-1} \eta_{pj}^{k-1,jn0},
$$

therefore,

$$
\begin{aligned}
\sum_{n=0}^{L-1} \eta_{pj}^{kjn0} &= \sum_{n=0}^{L-1} \eta_{pj}^{k-1,jn0} - \frac{1}{\xi_j \lambda_x^t} \eta_{pj}^{kjL0} \\
&= \sum_{n=0}^{L-1} \eta_{pj}^{k-2,jn0} - \frac{1}{\xi_j \lambda_x^t} [\eta_{pj}^{kjL0} + \eta_{pj}^{k-1,jL0}] \\
&= \cdots \\
&= \sum_{n=0}^{L-1} \eta_{pj}^{pjn0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=p+1}^{k} \eta_{pj}^{ljL0} \\
&= \sum_{n=0}^{L-1} \eta_{kj}^{kjn0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=p}^{k-1} \eta_{lj}^{kjL0}. \qquad (4.24)
\end{aligned}
$$

Applying (4.24) when $k = m$, one gets the relation

$$
\sum_{n=0}^{L-1} \eta_{pj}^{mjn0} = \sum_{n=0}^{L-1} \eta_{mj}^{mjn0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=p}^{m-1} \eta_{lj}^{mjL0}. \qquad (4.25)
$$

For a fixed $j \in S_m$, adding (4.25) for p such that $(p,j) \in H$ gives

$$
\sum_{(p,j)\in H} \sum_{n=0}^{L-1} \eta_{pj}^{mjn0} = G(j) \sum_{n=0}^{L-1} \eta_{mj}^{mjn0} - \frac{1}{\xi_j \lambda_x^t} \sum_{l=m-G(j)+1}^{m-1} (l - m + G(j)) \eta_{lj}^{mjL0}. \qquad (4.26)
$$

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 (2.7) 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,

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

The proof of the last inequality is in the Appendix. Continuing from (4.26) gives

$$\begin{aligned}\sum_{(p,j)\in H}\sum_{n=0}^{L-1}\eta_{pj}^{mjn0} &> G(j)\sum_{n=0}^{L-1}\eta_{mj}^{mjn0} - \frac{1}{\xi_j\lambda_x^t}\frac{G(j)}{2}\\ &= G(j)\frac{1-(1-\xi_j\lambda_x^t)^L}{\xi_j\lambda_x^t} - \frac{1}{\xi_j\lambda_x^t}\frac{G(j)}{2}.\end{aligned} \tag{4.27}$$

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

$$\begin{aligned}\xi_j &> \sqrt{(\sqrt{2D}+\Delta\xi)^2-2D}-\Delta\xi\\ &> \sqrt{2\sqrt{2D}\Delta\xi}-\Delta\xi.\end{aligned} \tag{4.28}$$

In order for $\xi_j\lambda_x^t > \frac{2}{L} = \frac{2\lambda_\xi^t}{T}\Delta\xi$, from (4.28),

$$\begin{aligned}&\sqrt{2\sqrt{2D}\Delta\xi}-\Delta\xi > \frac{2}{T\lambda_x^\xi}\Delta\xi\\ \Leftrightarrow\ &\Delta\xi < \frac{2\sqrt{2D}}{(\frac{2}{T\lambda_x^\xi}+1)^2}\\ \Leftrightarrow\ &\Delta x < \frac{2\sqrt{2D}}{(\frac{2}{T\lambda_x^\xi}+1)^2\lambda_x^\xi}.\end{aligned} \tag{4.29}$$

Under mesh size restriction (4.29), $\xi_j\lambda_x^t > \frac{2}{L} > \frac{1}{L}$, thus

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

By using (4.27), one gets

$$\sum_{(p,j)\in H}\sum_{n=0}^{L-1}\eta_{pj}^{mjn0} > \frac{G(j)}{10\xi_j\lambda_x^t} > \frac{L-\frac{1}{\xi_j\lambda_x^t}}{10} > \frac{L}{20}, \tag{4.30}$$

where in the last inequality we used $\xi_j \lambda_x^t > \frac{2}{L}$ under mesh size restriction (4.29).

Next one needs to estimate s appeared in (4.22) as the upper bound of the summation. From the definition of s in (4.22),

$$\sum_{l=1}^{s} G(k_l) \geq L_0\,. \tag{4.31}$$

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

$$\begin{aligned}
\sum_{l=1}^{s'} G(k_l) &< L\lambda_x^t \sum_{l=1}^{s'} \xi_{k_l} + s' < L\lambda_x^t \sum_{l=1}^{s'} \sqrt{\xi_{k'_l}^2 - 2D} + s'\lambda_x^t L \Delta\xi + s' \\
&< \frac{L\lambda_x^t}{3\sqrt{2D}} \sum_{l=1}^{s'} 3\xi_{k'_l}\sqrt{\xi_{k'_l}^2 - 2D} + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s' \\
&< \frac{L\lambda_x^t}{3\sqrt{2D}\Delta\xi} \int_{\sqrt{2D}}^{\sqrt{2D}+(s'+1)\Delta\xi} 3\xi\sqrt{\xi^2 - 2D}\, d\xi + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s' \\
&< \frac{L\lambda_x^t}{3\sqrt{2D}\Delta\xi} \left[2\sqrt{2D}\,(s'+1)\,\Delta\xi\right]^{\frac{3}{2}} + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s'.
\end{aligned} \tag{4.32}$$

By choosing $s' = {s_N}^{1-\frac{5}{6}q'}$, (4.32) gives

$$\begin{aligned}
\sum_{l=1}^{s'} G(k_l) &< \frac{8\lambda_x^t (2D)^{\frac{1}{4}} L\sqrt{\Delta\xi}}{3} s'^{\frac{3}{2}} + \frac{s'\lambda_x^t T}{\lambda_\xi^t} + s' \\
&< \frac{8\lambda_x^t (2D)^{\frac{1}{4}} L\sqrt{\Delta\xi}}{3} {s_N}^{\frac{3}{2}-\frac{5}{4}q'} + \frac{s_N\lambda_x^t T}{\lambda_\xi^t} + s_N \\
&< \frac{8\lambda_x^t (2D)^{\frac{1}{4}} \sqrt{T} L}{3\sqrt{\lambda_\xi^t}\sqrt{L}} \left(\frac{\frac{\sqrt{20D}}{3} - \sqrt{2D}}{\Delta\xi}\right)^{\frac{3}{2}-\frac{5}{4}q'} \\
&+ \frac{\left(\frac{\frac{\sqrt{20D}}{3} - \sqrt{2D}}{\Delta\xi}\right)\lambda_x^t T}{\lambda_\xi^t} + \left(\frac{\frac{\sqrt{20D}}{3} - \sqrt{2D}}{\Delta\xi}\right) \\
&= \frac{8\lambda_x^t (2D)^{\frac{1}{4}} \sqrt{T} \left(\frac{\lambda_\xi^t}{T}\left(\frac{\sqrt{10}}{3} - 1\right)\sqrt{2D}\right)^{\frac{3}{2}-\frac{5}{4}q'}}{3\sqrt{\lambda_\xi^t}} L^{2-\frac{5}{4}q'} \\
&+ \left(\frac{\sqrt{20D}}{3} - \sqrt{2D}\right)\lambda_x^t L + \frac{\left(\frac{\sqrt{20D}}{3} - \sqrt{2D}\right)\lambda_\xi^t L}{T}.
\end{aligned} \tag{4.33}$$

If one imposes the mesh size restrictions

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

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

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

which corresponds to

$$\Delta x < \frac{T}{\lambda_x^t}\left(\frac{3\sqrt{\lambda_\xi^t}}{32\lambda_x^t (2D)^{\frac{1}{4}}\sqrt{T}\left(\frac{\lambda_\xi^t}{T}\left(\frac{\sqrt{10}}{3}-1\right)\sqrt{2D}\right)^{\frac{3}{2}-\frac{5}{4}q'}}\right)^{\frac{4}{q'}}, \tag{4.34}$$

$$\Delta x < \frac{T}{\lambda_x^t}\left(\frac{1}{4\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_x^t}\right)^{\frac{1}{1-q'}}, \tag{4.35}$$

$$\Delta t < \frac{T}{\lambda_x^t}\left(\frac{T}{4\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}\right)^{\frac{1}{1-q'}}, \tag{4.36}$$

then under (4.34)-(4.36) one has, for $s' = {s_N}^{1-\frac{5}{6}q'}$,

$$\sum_{l=1}^{s'} G(k_l) < \frac{3}{4}L^{2-q'} < L_0. \tag{4.37}$$

Comparing (4.37) with (4.31) gives

$$s > {s_N}^{1-\frac{5}{6}q'} > \left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}{T}\right)^{1-\frac{5}{6}q'} L^{1-\frac{5}{6}q'} + 1. \tag{4.38}$$

Now combining with (4.30) and (4.38), (4.22) gives

$$\begin{aligned} |f^L|_1 &> |f^0|_1 + \frac{\sqrt{2D}}{120}\lambda_x^t \frac{c_0}{N_d}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}{T}\right)^{1-\frac{5}{6}q'} L^{2-\frac{5}{6}q'} \\ &\geq |f^0|_1 + \frac{\sqrt{2D}}{120}\lambda_x^t \frac{L_0 c_0}{N_d}\left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3}-\sqrt{2D}\right)\lambda_\xi^t}{T}\right)^{1-\frac{5}{6}q'} L^{\frac{1}{6}q'} \end{aligned} \tag{4.39}$$

$$= \left\{ 1 + \frac{\sqrt{2D}}{120} \lambda_x^t \left[\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3} - \sqrt{2D}\right)\lambda_\xi^t}{T} \right]^{1-\frac{5}{6}q'} L^{\frac{1}{6}q'} \right\} |f^0|_1. \quad (4.40)$$

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

$$\Delta x < \frac{T}{\lambda_\xi^t} \left(\frac{\sqrt{2D}}{120B} \lambda_x^t \left(\frac{\frac{1}{2}\left(\frac{\sqrt{20D}}{3} - \sqrt{2D}\right)\lambda_\xi^t}{T} \right)^{1-\frac{5}{6}q'} \right)^{\frac{6}{q'}}, \quad (4.41)$$

under which it holds that

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

□

Appendix

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

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

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

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

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

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

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

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

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

By induction, one can generally prove the following results,

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

Thus the inequality (A.2) is proved. □

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