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

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Abstract

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

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

1. Introduction

In [19], we constructed a class of numerical schemes for the d-dimensional Liouville equation in classical mechanics:

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

where $f(t,\mathbf{x},\mathbf{v})$ is the density distribution of a classical particle at position $\mathbf{x}$, time t and traveling with velocity $\mathbf{v}$. $V(\mathbf{x})$ is the potential. Such problem has applications in computational high frequency waves [3,6,12,13,17,23,33,42,43]. The main interest is in the case of a discontinuous potential $V(\mathbf{x})$, corresponding to a potential barrier. When V is discontinuous, the Liouville equation (1.1) is a linear hyperbolic equation with a measure-valued coefficient. Such a problem cannot be understood mathematically using the renormalized solution by DiPerna and Lions for linear advection equations with discontinuous coefficients [5] (see also [2]). Our approach in [19–21] to such problems was to provide an interface condition to couple the Liouville equation (1.1) on both sides of the barrier or interface. The interface condition accounts for particle or wave transmission and reflection. An important property of the interface condition is that the Hamiltonian is preserved on particle trajectory in case of either transmission or reflection. By using this property to determine the particle trajectory for constructing numerical fluxes,

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the so-called Hamiltonian-preserving schemes were constructed in [19–21]. See also the related work on Hamiltonian-preserving schemes [10, 11, 14–16, 18, 22–25, 40]. Schemes so constructed provide solutions that are physically relevant for particle or wave reflection and transmission through the barriers or interfaces.

The Liouville equation is the phase space representation of Newton's second law:

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

which is a Hamiltonian system with the Hamiltonian

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

It is known from classical mechanics that the Hamiltonian remains constant across a potential barrier. This is one of the main ingredients in the Hamiltonian-preserving schemes developed in [19–21]. The two schemes developed in [19]–one based on a finite difference formulation (called Scheme I) and the other on a finite volume formulation (called Scheme II) were proved, in one space dimension with a piecewise constant potential, to be positive, and l^1 and l^∞-stable for suitable initial value problems and under a hyperbolic CFL condition except the l^1-stability of Scheme I.

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

The error estimates for Scheme I in [45] was established under the condition that the initial data is exactly given. In practical computation, however it is common that the initial data is given with errors. Therefore an interesting issue is to further investigate error estimates for Scheme I when the initial data is given with perturbation errors. In this paper we will study this issue. Due to the linearity of Scheme I, these error estimates can be obtained by applying the error estimates for Scheme I with exact initial data established in [45] and the l^1-norm estimates for the perturbation solutions. Therefore in this paper we will investigate the latter estimates. If the perturbation solution is l^1-stable, then the l^1-norm of the perturbation solution can be estimated directly from that of the initial perturbation values. However we will see that the initial perturbation values do not necessarily satisfy the condition required for the l^1-stability of Scheme I given in [46]. Therefore the perturbation solution yielded by Scheme I can be l^1-unstable. In this paper we extend the analysis in [46] to show that even if the solution of Scheme I can be l^1-unstable, the l^1-norm of the solution can still be estimated from the L^∞ and L^1-upper bounds of the initial data. Consequently we prove that Scheme I is L^1-convergent when the initial data is given with a wide class of perturbation errors and give the L^1-error bound with *explicit* coefficient. The L^1-convergence rate given in this paper is less than the order of the initial perturbation error, matching with the fact that the perturbation solution can be l^1-unstable.

This paper is organized as follows. In Section 2 we review the Hamiltonian-preserving scheme called Scheme I proposed in [19] for the Liouville equation with a discontinuous potential in one space dimension. In Section 3 we review the L^1-error estimates for Scheme I with exact initial data established in [45] for the Liouville equation with a step function potential. In Section 4 we present the main Theorems in this paper related to the L^1-error estimates for Scheme I with perturbed initial data which are proved in Section 5 by extending the analysis in [46]. We conclude the paper in Section 6. In this paper we denote $[x]^-, [x]^+$ to be the largest integer no more than x and the smallest integer no less than x respectively.

2. A Hamiltonian-Preserving Scheme

In this section we review the Hamiltonian-preserving scheme proposed in [19] to the Liouville equation in one space dimension

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

with a discontinuous potential $V(x)$.

Consider a uniform mesh with grid points at $x_{i+\frac{1}{2}}, i \in \mathbb{Z}$ in the x-direction and $\xi_{j+\frac{1}{2}}, j \in \mathbb{Z}$ in the ξ-direction. The cells are centered at $(x_i, \xi_j), (i,j) \in \mathbb{Z}^2$ 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 are 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 times are given by $t_n = n\Delta t, n \in \mathbb{N} \cup \{0\}$. We assume that the computation is performed in a bounded rectangular domain

$$\Big\{(x,y) \;\Big|\; x_{\frac{1}{2}} \le x \le x_{N+\frac{1}{2}},\ \xi_{\frac{1}{2}} \le \xi \le \xi_{M+\frac{1}{2}}\Big\}. \tag{2.2}$$

Let the cell averages of f be

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

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

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

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

In classical mechanics, a particle will either cross a potential barrier with a changing momentum, or be reflected, depending on its momentum and the strength of the potential barrier.

The Hamiltonian $H = \frac{1}{2}\xi^2 + V$ *is preserved across the potential barrier:*

$$\frac{1}{2}(\xi^+)^2 + V^+ = \frac{1}{2}(\xi^-)^2 + V^-, \tag{2.3}$$

where the superscripts $\pm$ indicate the right and left limits of the quantity at the potential barrier. This property was used in [19] to provide the interface condition for (2.1) at the barrier:

$$f(t, x^+, \xi^+) = f(t, x^-, \xi^-) \qquad \text{for transmission}, \tag{2.4}$$

$$f(t, x^\pm, \xi^\pm) = f(t, x^\pm, -\xi^\pm) \quad \text{for reflection}, \tag{2.5}$$

where ξ^+ and ξ^- are related by the constant Hamiltonian condition (2.3) in the case of transmission. With such an interface condition, we established the well-posedness of the initial value problem to the Liouville equation with a piecewise constant wave speed in [21].

The main ingredient in the Hamiltonian-preserving schemes developed in [19], like the earlier work for shallow-water equations [35], was to build into the numerical flux the interface conditions (2.4) and (2.5) at the barrier.

We now present the first Hamiltonian-preserving scheme, called *Scheme I* in [19].

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

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

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 barrier, 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, and (2.4)$-$(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 the upwind scheme, $f^-_{i+\frac{1}{2},j} = f_{ij}$. However,

$$f^+_{i+1/2,j} \equiv f(x^+_{i+1/2}, \xi^+) = f(x^-_{i+1/2}, \xi^-),$$

in the case of particle transmission, where ξ^- is obtained from $\xi^+ = \xi_j$ from (2.3). 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 particle reflection and $\xi_j < 0$ is treated in the same principle. The algorithm to generate the numerical flux is given in [19]. Here we present the simplified algorithm for the case

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

being discussed in this paper.

Algorithm I

- $\xi_j > 0$

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

  ❏ 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

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

  ❏ end

- $\xi_j < 0$

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

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

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

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

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

In [19] 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:

$$\Delta t \left(\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \left(V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}\right)/\Delta x \right|}{\Delta\xi} \right) < 1. \tag{2.6}$$

In [45, 46] we further proved that when the potential is a step function, the same scheme is l^1-stable and L^1-convergent under the CFL condition (2.6) and suitable conditions on the initial data.

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

3. The L^1-error Estimates for Scheme I

In this Section we review the L^1-error estimates for Scheme I with exact initial data established in [45]. We consider a step function potential $V(x)$ with a jump $-D, D > 0$ at $x = 0$.

Namely

$$V(0^-) - V(0^+) = D.$$

Let the computational domain be confined in the rectangular domain (2.2). We employ the uniform mesh introduced in Section 2. Define mesh ratios $\lambda_x^t = \frac{\Delta t}{\Delta x}, \lambda_x^\xi = \frac{\Delta \xi}{\Delta x}$, assumed to be fixed. Let the potential barrier $x = 0$ be at a grid point $x_{m+\frac{1}{2}}$. Then the point-wise values of V satisfy

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

where the superscripts $-, +$ represent the left and right limits at $x = 0$.

We consider the typical situation that $\xi_1 < -\sqrt{2D}, \xi_M > \sqrt{2D}$, so that all possible particle behaviors, including both transmission and reflection, are included. We choose the mesh such that 0 and $\pm\sqrt{2D}$ are grid points in the ξ-direction.

Define the index I_b satisfying

$$\xi_{I_b-\frac{3}{2}} < -\sqrt{\left(\xi_{\frac{1}{2}}\right)^2 - 2D} \le \xi_{I_b-\frac{1}{2}},$$

and the domain

$$D_b = \left\{(x, \xi) \;\middle|\; x < 0, \xi < \xi_{I_b-\frac{1}{2}}\right\}.$$

The computational domain is chosen to be

$$D_C = \left\{(x, \xi) \;\middle|\; x_{\frac{1}{2}} \le x \le x_{N+\frac{1}{2}},\ \xi_{\frac{1}{2}} \le \xi \le \xi_{M+\frac{1}{2}}\right\} \setminus D_b,$$

since D_b represents the area where particles come from outside of the domain $[x_{\frac{1}{2}}, x_{N+\frac{1}{2}}] \times [\xi_{\frac{1}{2}}, \xi_{M+\frac{1}{2}}]$ and thus is excluded from the computational domain, as discussed in [19,45]. Fig. 5.1 depicts the sets D_C and D_b.

We consider the Dirichlet boundary conditions at the incoming boundaries and assume that the initial data satisfy these boundary conditions:

$$f(x_{\frac{1}{2}}, \xi, t) = f(x_{\frac{1}{2}}, \xi, 0), \qquad 0 < \xi < \xi_{M+\frac{1}{2}}, \tag{3.1}$$

$$f(x_{N+\frac{1}{2}}, \xi, t) = f(x_{N+\frac{1}{2}}, \xi, 0), \quad \xi_{\frac{1}{2}} < \xi < 0. \tag{3.2}$$

The expression of the exact solution $f(x, \xi, t), (x, \xi) \in D_C, t > 0$ can be obtained from the initial data $f(x, \xi, 0)$ and boundary conditions (3.1), (3.2) by the method of characteristics. One can refer to [45] for the concrete expression of $f(x, \xi, t)$. Let

$$\mu_j = \lambda_x^t \left|\xi_j\right|, \qquad 1 \le j \le M, \tag{3.3}$$

which are less than 1 under the CFL condition (2.6).

With the first order numerical flux, the forward Euler method in time and the boundary conditions (3.1), (3.2), Scheme I on D_C is given by:

1) if $0 < \xi_j < \xi_{M+\frac{1}{2}}, i \ne m+1$, then

$$g_{ij}^{n+1} = (1 - \mu_j) g_{ij}^n + \mu_j g_{i-1,j}^n\,; \tag{3.4}$$

2) if $\xi_{I_b-\frac{1}{2}} < \xi_j < 0, i < m$ or $\xi_{\frac{1}{2}} < \xi_j < 0, i > m$, then

$$g_{ij}^{n+1} = (1 - \mu_j) g_{ij}^n + \mu_j g_{i+1,j}^n\,; \tag{3.5}$$

3) if $\sqrt{2D} < \xi_j < \xi_{M+\frac{1}{2}}$, then

$$g^{n+1}_{m+1,j} = (1-\mu_j) g^n_{m+1,j} + \mu_j \left(c_{j,1} g^n_{m,d_j} + c_{j,2} g^n_{m,d_j+1} \right); \tag{3.6}$$

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

$$g^{n+1}_{m+1,j} = (1-\mu_j) g^n_{m+1,j} + \mu_j g^n_{m+1,d_j}; \tag{3.7}$$

5) if $\xi_{I_b-\frac{1}{2}} < \xi_j < 0$, then

$$g^{n+1}_{mj} = (1-\mu_j) g^n_{mj} + \mu_j \left(c_{j,1} g^n_{m+1,d_j} + c_{j,2} g^n_{m+1,d_j+1} \right), \tag{3.8}$$

where $0 \le c_{j,1}, c_{j,2} \le 1$ and $c_{j,1} + c_{j,2} = 1$. d_j's in (3.6)-(3.8) are determined according to Algorithm I by

$$\xi_{d_j} \le \sqrt{(\xi_j)^2 - 2D} < \xi_{d_j+1}, \qquad \text{for } d_j \text{ in (3.6)}, \tag{3.9}$$

$$\xi_{d_j} = -\xi_j, \qquad \text{for } d_j \text{ in (3.7)}, \tag{3.10}$$

$$\xi_{d_j} \le -\sqrt{(\xi_j)^2 + 2D} < \xi_{d_j+1}, \qquad \text{for } d_j \text{ in (3.8)}. \tag{3.11}$$

The initial and incoming boundary values of the numerical solution are given by

$$g^0_{ij} = \frac{1}{\Delta x \Delta \xi} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x,\xi,0) d\xi dx, \quad (x_i, \xi_j) \in D_C, \tag{3.12}$$

$$g^n_{0,j} = \frac{1}{\Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{\frac{1}{2}}, \xi, 0) d\xi, \qquad 0 < \xi_j < \xi_{M+\frac{1}{2}}, \tag{3.13}$$

$$g^n_{N+1,j} = \frac{1}{\Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{N+\frac{1}{2}}, \xi, 0) d\xi, \qquad \xi_{\frac{1}{2}} < \xi_j < 0. \tag{3.14}$$

We introduce

$$g(x,\xi,t) = g^n_{ij}, \qquad \text{for } (x,\xi,t) \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}) \times [\xi_{j-\frac{1}{2}}, \xi_{j+\frac{1}{2}}) \times [t_n, t_{n+1}), \quad (x_i, \xi_j) \in D_C.$$

In [45] we have established the L^1-error estimates for Scheme I under the following initial data assumption:

Assumption 3.1. *The initial data $f(x,\xi,0)$ have bounded variation in the x-direction and is Lipschitz continuous in the ξ-direction. Namely*

$$\|f(.,\xi,0)\|_{BV([x_{\frac{1}{2}}, x_{N+\frac{1}{2}}])} \le A, \qquad \forall \xi \in [\xi_{\frac{1}{2}}, \xi_{M+\frac{1}{2}}], \tag{3.15}$$

$$|f(x,\xi',0) - f(x,\xi'',0)| \le B|\xi' - \xi''|, \quad \forall x \in \left[x_{\frac{1}{2}}, x_{N+\frac{1}{2}}\right],\ \xi', \xi'' \in \left[\xi_{\frac{1}{2}}, \xi_{M+\frac{1}{2}}\right]. \tag{3.16}$$

These initial data conditions can be satisfied by applying the decomposition technique proposed in [12] for solving the Liouville equation with measure-valued initial data arisen in the semiclassical limit of the linear Schrödinger equation.

Let $T = t_L = L\Delta t$. The main theorem given in [45] is as follows:

Theorem 3.1. *Under Assumption* 3.1 *on the initial data, the CFL condition* (2.6) *and the following mesh size restriction*

$$\Delta\xi \leq \frac{3-2\sqrt{2}}{2}\sqrt{2D}, \tag{3.17}$$

Scheme I (3.4)-(3.14) *has the following L^1-error bound compared to the exact solution:*

$$\|g(\cdot,\cdot,T)-f(\cdot,\cdot,T)\|_{L^1(D_C)} \leq C_1\sqrt{\Delta x}+C_2\ln\left(\frac{1}{\Delta x}\right)\Delta x+\mathcal{O}(\Delta x), \tag{3.18}$$

where

$$\begin{aligned} C_1 = &\left(4A+2\sqrt{2D}B\right)\sqrt{\frac{T+\Delta t}{2e}}\left(\frac{\xi_{M+\frac{1}{2}}}{(2D)^{\frac{1}{4}}}\sqrt{\frac{\xi_{M+\frac{1}{2}}-\sqrt{2D}}{\lambda_x^t}}+2\left|\xi_{\frac{1}{2}}\right|\left[\left(\xi_{\frac{1}{2}}\right)^2-2D\right]^{\frac{1}{4}}\right) \\ &+\left[\left(\xi_{M+\frac{1}{2}}+\left|\xi_{\frac{1}{2}}\right|+\sqrt{2D}\right)A+4DB\right]\sqrt{\frac{T+\Delta t}{2e\lambda_x^t}}, \end{aligned} \tag{3.19}$$

$$C_2 = \left(2A+\sqrt{2D}B\right)\left[2\left(\xi_{M+\frac{1}{2}}\right)^2 T\lambda_x^{\xi}/\sqrt{D}+\left|\xi_{\frac{1}{2}}\right|\right]. \tag{3.20}$$

4. The L^1-error Estimates for Scheme I with Perturbed Initial Data

In this section we present the main Theorems in this paper for the L^1-error estimates for Scheme I with perturbed initial data. We consider the same problem setup as in the previous section except we assume the initial data have some perturbation error. Assume the exact initial data $f(x,\xi,0)$ satisfies Assumption 3.1 and denote $\widehat{f}(x,\xi,0)$ to be its perturbed values. Since $f(x,\xi,0)$ is bounded in L^∞-norm, the same should be true for $\widehat{f}(x,\xi,0)$. Thus we consider the initial perturbation error satisfying

$$\left|f(x,\xi,0)-\widehat{f}(x,\xi,0)\right| < \widehat{D}, \qquad \forall (x,\xi)\in D_C, \tag{4.1}$$

$$\left\|f(\cdot,\cdot,0)-\widehat{f}(\cdot,\cdot,0)\right\|_{L^1(D_C)} < \widehat{C}(\Delta x)^r, \qquad r>0. \tag{4.2}$$

Let $\widehat{g}_{ij}^n$ be the numerical solutions computed by Scheme I with the initial data $\widehat{f}(x,\xi,0)$ and the exact Dirichlet boundary condition, namely

$$\widehat{g}_{ij}^0 = \frac{1}{\Delta x\Delta\xi}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}}\widehat{f}(x,\xi,0)d\xi dx, \quad (x_i,\xi_j)\in D_C, \tag{4.3}$$

$$\widehat{g}_{0,j}^n = \frac{1}{\Delta\xi}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{\frac{1}{2}},\xi,0)d\xi, \qquad 0<\xi_j<\xi_{M+\frac{1}{2}}, \tag{4.4}$$

$$\widehat{g}_{N+1,j}^n = \frac{1}{\Delta\xi}\int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} f(x_{N+\frac{1}{2}},\xi,0)d\xi, \qquad \xi_{\frac{1}{2}}<\xi_j<0. \tag{4.5}$$

The errors for the numerical solutions with inexact boundary conditions can be estimated by comparing the numerical solutions with exact and inexact boundary conditions and will not be discussed in this paper. Introduce

$$\widehat{g}(x,\xi,t)=\widehat{g}_{ij}^n, \qquad \text{for } (x,\xi,t)\in[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}})\times[\xi_{j-\frac{1}{2}},\xi_{j+\frac{1}{2}})\times[t_n,t_{n+1}), \quad (x_i,\xi_j)\in D_C.$$

Recall $T=L\Delta t$. We have the following main theorem for the error estimates for the numerical solutions $\widehat{g}_{ij}^L$ with the perturbed initial data:

Theorem 4.1. *Assume the initial data $f(x,\xi,0)$ satisfies Assumption 3.1, and its perturbation $\widehat{f}(x,\xi,0)$ satisfies conditions (4.1), (4.2). Then the numerical solutions $\widehat{g}_{ij}^L$ computed by Scheme I with the perturbed initial data $\widehat{f}(x,\xi,0)$ and the exact Dirichlet boundary condition are L^1-convergent to $f(x,\xi,T)$ under the CFL condition (2.6). Furthermore under the mesh size restrictions (3.17) and*

$$\Delta\xi < \frac{1}{6\lambda_x^t}, \qquad \Delta\xi < \min\left(\xi_M, \sqrt{(6\lambda_x^t)^{-2} + 2D}\right) - \sqrt{2D}, \tag{4.6}$$

$$\Delta x \le \frac{1}{16}\max\left(\frac{T}{\lambda_x^t}, x_{m+\frac12} - x_{\frac12}, \frac{4}{\lambda_x^\xi (\lambda_x^t)^2\sqrt{2D}}\right), \tag{4.7}$$

the error estimates for $\widehat{g}_{ij}^L$ are given by

$$\begin{aligned}&\|\widehat{g}(\cdot,\cdot,T) - f(\cdot,\cdot,T)\|_{L^1(D_C)}\\ \le& C_1\sqrt{\Delta x} + C_2\ln\left(\frac{1}{\Delta x}\right)\Delta x + C_3(\Delta x)^{\frac23 r} + \mathcal{O}(\Delta x),\end{aligned} \tag{4.8}$$

where C_1, C_2 are given in (3.19), (3.20), C_3 is a bounded coefficient being given by

$$C_3 = C_{30}(\Delta x)^{\frac13 r} + \max\left(C_{31}(\Delta x)^{\frac13 r}, C_{32}\right), \tag{4.9}$$

$$C_{30} = \left(4 + \frac{(1+\lambda_x^t\Delta\xi)}{2\lambda_x^t\left(\sqrt{2D} - \Delta\xi\right)}\right)\widehat{C}, \tag{4.10}$$

$$C_{31} = \frac{45\widehat{C}\sqrt{1/3\lambda_x^t + 2\Delta\xi}}{28\left(\lambda_x^t\right)^2\sqrt{D}\left(\xi_C - \frac12\Delta\xi\right)^{\frac32}}, \tag{4.11}$$

$$\xi_C = \min\left(\xi_M, \sqrt{\left(1/3\lambda_x^t - \Delta\xi\right)^2 + 2D}\right) - \sqrt{2D}, \tag{4.12}$$

$$C_{32} = \frac{\widehat{C}^{\frac23}\widehat{D}^{\frac13}\max\left(T, \left(x_{m+\frac12} - x_{\frac12}\right)\lambda_x^t, \frac{4\lambda_\xi^t}{(\lambda_x^t)^2\sqrt{2D}} + \Delta t\right)}{\left(\frac{5\sqrt{2D}}{63}\right)^{\frac13}\left(\lambda_x^t\right)^{\frac53}\left(x_{m+\frac12} - x_{\frac12}\right)^{\frac23}}. \tag{4.13}$$

Remark 4.1. The error estimate (4.8) can also be used in the case that the initial perturbation error does not converge to zero in L^1-norm with mesh refinement, for example a fixed initial perturbation error. In this case we do not have the convergence of the numerical solution $\widehat{g}(x,\xi,T)$ to the exact solution $f(x,\xi,T)$, but we can get the error bound between $\widehat{g}$ and f by setting $r = 0$ and $\widehat{C}$ to be the bound of the L^1-norm of the initial perturbation error in (4.8).

Define the discrete l^1-norm of numerical solutions g_{ij}^n to be

$$|g^n|_1 = \Delta x\Delta\xi\sum_{(x_i,\xi_j)\in D_C}\left|g_{ij}^n\right|. \tag{4.14}$$

Theorem 4.1 can be proved with Theorem 3.1 and the following theorem.

Theorem 4.2. *Assume the numerical approximations of the initial values satisfy*

$$\left|g_{ij}^0\right| < \widehat{D}, \qquad (x_i,\xi_j)\in D_C, \tag{4.15}$$

$$\left|g^0\right|_1 < \widehat{C}(\Delta x)^r, \qquad r > 0. \tag{4.16}$$

Then under the CFL condition (2.6) *and the mesh size restrictions* (4.6), (4.7) *and*

$$\Delta\xi < \sqrt{2D}/4, \tag{4.17}$$

the discrete l^1-norm of the numerical solutions computed by Scheme I with these initial values and the zero Dirichlet boundary condition are estimated by

$$\left|g^L\right|_1 < C_3(\Delta x)^{\frac{2}{3}r} + \mathcal{O}(\Delta x), \tag{4.18}$$

where C_3 is given in (4.9).

Remark 4.2. In the case that Scheme I is l^1-stable, the discrete l^1-norm of the computed solutions can be directly estimated from that of the numerical solutions initial values. In [46] we have established the l^1-stability of Scheme I under the initial data assumption

Assumption 4.1. *There exists a positive constant ξ_z such that*

$$\forall (i,j) \in S_z = \Big\{(i,j) \;\Big|\; x_i < x_{m+\frac{1}{2}},\ 0 < \xi_j < \xi_z\Big\}, \tag{4.19}$$

it holds that

$$\left|g_{ij}^0\right| \le C_1 \left|g^0\right|_1 . \tag{4.20}$$

However we also show in [46] that Scheme I can be l^1-unstable if the Assumption 4.1 is violated by the initial data. It can be seen that the initial data satisfying conditions (4.15), (4.16) do not necessarily satisfy the Assumption 4.1. Therefore the discrete l^1-norm estimates in Theorem 4.2 can not be obtained by applying the l^1-stability result of Scheme I established in [46]. In fact, the order of the mesh size in the upper bound (4.18) of the computed solutions being less than that in the upper bound (4.16) of the initial data indicates that the numerical solutions computed by Scheme I from the initial data satisfying conditions (4.15), (4.16) can be l^1-unstable. The proof for Theorem 4.2 is extended from the analysis in [46] and composes the main part of this paper.

5. Proof for the Main Theorems

In this Section we present the proof for Theorems 4.1, 4.2 in this paper. The proof for Theorem 4.1 is relatively straightforward by applying Theorems 3.1 and 4.2. Therefore the key part in this section is to prove Theorem 4.2.

5.1. Proof for Theorem 4.2

Introduce some notations

$$S_m^2 = \left\{k \middle| \xi_k > 0,\, \exists\, \xi_j > \sqrt{2D},\ \text{ s.t. } \left|\xi_k - \sqrt{{\xi_j}^2 - 2D}\right| < \Delta\xi\right\}, \tag{5.1a}$$

$$D_m^2 = \{(m,j) | j \in S_m^2\}, \qquad D_{m+1}^4 = \{(m+1,j)|\xi_j < -\sqrt{2D} + \Delta\xi\}, \tag{5.1b}$$

$$S_m^{2,1} = \left\{j \in S_m^2 \middle| \xi_j \ge \widehat{\xi}_z \equiv \frac{1}{3\lambda_x^t}\right\}, \qquad S_m^{2,2} = \left\{j \in S_m^2 \middle| \xi_j < \widehat{\xi}_z \equiv \frac{1}{3\lambda_x^t}\right\}, \tag{5.1c}$$

$$D_m^{2,1} = \{(i,j) \in D_m^2 | j \in S_m^{2,1}\}, \qquad D_m^{2,2} = \{(i,j) \in D_m^2 | j \in S_m^{2,2}\}, \tag{5.1d}$$

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

$$S_2 = \sum_{n=0}^{L-1} \left\{ \sum_{(i,j)\in D_{m+1}^4} |f_{ij}^n| \right\}, \tag{5.1e}$$

$$S_r = \{(i,j) | \;\; x_i > x_{m+\frac{1}{2}}, (m+1,j) \in D_{m+1}^4\}, \tag{5.1f}$$

$$S_l = \left\{ (i,j) \middle| \;\; x_i < x_{m+\frac{1}{2}}, (m,j) \in D_m^2 \right\}, \tag{5.1g}$$

$$S_l^2 = \{(i,j) \in S_l | j \in S_m^{2,2}\}. \tag{5.1h}$$

Fig. 5.1 depicts a sketch of the sets D_m^2 and D_{m+1}^4. Let N_s be the number of elements in $S_m^{2,2}$. We name the elements in $S_m^{2,2}$ as $k_i, i = 1,2,\cdots,N_s$ such that $k_1 < k_2 < \cdots < k_{N_s}$. Consequently $\mu_{k_1} < \mu_{k_2} < \cdots < \mu_{k_{N_s}}$, where $\mu_j, 1 \le j \le M$ are defined in (3.3).

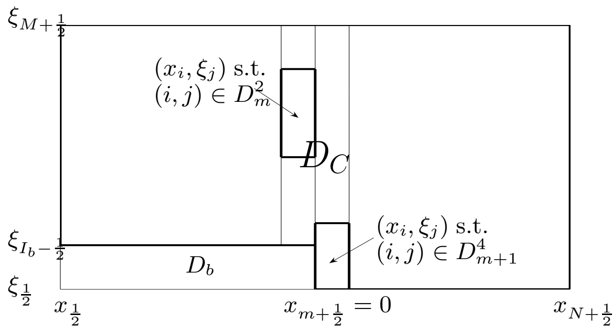

Fig. 5.1. Sketch of the sets $D_C, D_b, D_m^2, D_{m+1}^4$.

With the zero incoming boundary condition, repeatedly using the scheme (3.4) yields

$$g_{ij}^n = \sum_{(p,q)\in S_l} \gamma_{pq}^{ijn0} g_{pq}^0, \quad (i,j) \in S_l. \tag{5.2}$$

Under the hyperbolic CFL condition (2.6), $\gamma_{pq}^{ijn0} \ge 0$. $\gamma_{pq}^{ijn0} \ne 0$ only when $p \le i$ and $q = j$ due to the upwind flux and the constant potential. Define

$$T_{pq} = \sum_{n=0}^{L-1} \gamma_{pq}^{mqn0}, \quad (p,q) \in S_l. \tag{5.3}$$

The following Lemma is part of Lemma 3.2 in [46]:

Lemma 5.1. *Under the hyperbolic CFL condition* (2.6)*,* T_{pq} *defined in* (5.3) *satisfy*

$$T_{p+1,q} \ge T_{p,q}, \qquad \text{for } p < m, \tag{5.4a}$$

$$T_{p,q} < \frac{1}{\mu_q}, \qquad \text{for } (p,q) \in S_l. \tag{5.4b}$$

The following two Lemmas can be proved similarly to Lemmas 3.1, 3.3 in [46]:

Lemma 5.2. *Under the hyperbolic CFL condition* (2.6)*, the mesh size restriction*

$$\Delta\xi < \sqrt{2D}/2 \tag{5.5}$$

and the zero incoming boundary condition, Scheme I given by (3.4)-(3.8) *satisfies*

$$\left|g^L\right|_1 \le \left|g^0\right|_1 + \Delta x\Delta\xi\left(S_{11}+S_{12}\right) + \left(\frac{1}{2}+\frac{1}{2}\lambda_x^t\Delta\xi\right)\Delta x\Delta\xi S_2. \tag{5.6}$$

Lemma 5.3. *Under the hyperbolic CFL condition* (2.6)*, the mesh size restriction* (5.5) *and the zero incoming boundary condition, S_{11} and S_2 defined in* (5.1e) *satisfy*

$$S_{11} < \frac{\left|g^0\right|_1}{\lambda_x^t\widehat{\xi}_z\Delta x\Delta\xi} \equiv \frac{3\left|g^0\right|_1}{\Delta x\Delta\xi}, \quad S_2 < \frac{\left|g^0\right|_1}{\lambda_x^t\left(\sqrt{2D}-\Delta\xi\right)\Delta x\Delta\xi}. \tag{5.7}$$

We also prove the following lemma:

Lemma 5.4. *Let $N_m \le N_s$. Then under the mesh size restriction* (4.17) *one has*

$$\Delta\xi\sum_{i=1}^{N_m}\frac{1}{\xi_{k_i}} < \frac{3}{(2D)^{\frac{1}{4}}}\sqrt{(N_m+1)\Delta\xi}. \tag{5.8}$$

Proof. Denote $N_{m,2} = \left[\frac{N_m}{2}\right]^+$. Define the set

$$S_R^m = \left\{k \;\middle|\; \sqrt{2D} < \xi_k < \sqrt{2D} + N_{m,2}\Delta\xi\right\}. \tag{5.9}$$

Then the number of elements in S_R^m is $N_{m,2}$. We name the elements in S_R^m as k_i^m satisfying $\xi_{k_i^m} = \sqrt{2D} + (i-\frac{1}{2})\Delta\xi, i = 1, 2, \cdots, N_{m,2}$.

Under the mesh size restriction (4.17), $\Delta\xi < \frac{1}{2}\sqrt{\left(\xi_{k_1^m}\right)^2 - 2D}$. One has

$$\begin{aligned}
\Delta\xi\sum_{i=1}^{N_m}\frac{1}{\xi_{k_i}} <& \Delta\xi\sum_{i=1}^{N_{m,2}}\frac{1}{\sqrt{\left(\xi_{k_i^m}\right)^2-2D}} + \Delta\xi\sum_{i=1}^{N_{m,2}}\frac{1}{\sqrt{\left(\xi_{k_i^m}\right)^2-2D}-\Delta\xi} \\
<& 3\Delta\xi\sum_{i=1}^{N_{m,2}}\frac{1}{\sqrt{\left(\xi_{k_i^m}\right)^2-2D}} \\
<& \frac{3}{(8D)^{\frac{1}{4}}}\sum_{i=1}^{N_{m,2}}\frac{\Delta\xi}{\sqrt{(i-\frac{1}{2})\Delta\xi}} < \frac{3}{(8D)^{\frac{1}{4}}}\int_0^{N_{m,2}\Delta\xi}\frac{1}{\sqrt{y}}\,dy \\
=& \frac{6}{(8D)^{\frac{1}{4}}}\sqrt{N_{m,2}\Delta\xi} \le \frac{3}{(2D)^{\frac{1}{4}}}\sqrt{(N_m+1)\Delta\xi}.
\end{aligned} \tag{5.10}$$

With the above preparation, we now give the proof for Theorem 4.2

Proof of Theorem 4.2: Applying Lemmas 5.2 and 5.3, under the hyperbolic CFL condition (2.6), the mesh size restriction (5.5) and the zero incoming boundary condition one has

$$|g^L|_1 \le \left(4 + \frac{(1+\lambda_x^t\Delta\xi)}{2\lambda_x^t\left(\sqrt{2D}-\Delta\xi\right)}\right)|g^0|_1 + \Delta x\Delta\xi S_{12}. \tag{5.11}$$

Thus the following task is to estimate S_{12}. Substituting (5.2) into the expression of S_{12} in (5.1e) gives

$$S_{12} \le \sum_{(p,q)\in S_l^2} \left(\sum_{n=0}^{L-1} \sum_{(i,j)\in D_m^{2,2}} \gamma_{pq}^{ijn0} \right) |g_{pq}^0| = \sum_{(p,q)\in S_l^2} T_{pq} |g_{pq}^0|, \tag{5.12}$$

where S_l^2 and T_{pq} are defined in (5.1h) and (5.3).

Now introduce some notations. Define

$$L_2 = \left[\frac{4}{(\lambda_x^t)^2 \sqrt{2D}\Delta\xi} \right]^+, \qquad L_m = \max(L, m, L_2), \tag{5.13a}$$

$$\widetilde{k}_q = \min\left(\left[\frac{7}{5}\mu_q L_m \right]^+, m \right), \quad \widetilde{p}_q = m - \widetilde{k}_q, \qquad \text{for } q \in S_m^{2,2}. \tag{5.13b}$$

Define the set

$$J = \left\{ (p,q) \in S_l^2 \,\middle|\, \widetilde{p}_q + 1 \le p \le m \right\}. \tag{5.14}$$

Let N_J be the number of elements in J, and define

$$N_B = \left[\frac{\widehat{C}(\Delta x)^{r-1}}{\widehat{D}\Delta\xi} \right]^+. \tag{5.15}$$

We will prove the following two estimates.

1) $\Delta x \Delta\xi S_{12} < C_{31}(\Delta x)^r, \qquad \text{if } N_B > N_J,$ (5.16a)

under the mesh size restrictions (4.17), (4.6), where C_{31} is given in (4.11).

2) $\Delta x \Delta\xi S_{12} < C_{32}(\Delta x)^{\frac{2}{3}r} + O(\Delta x), \qquad \text{if } N_B \le N_J,$ (5.16b)

under the mesh size restrictions (4.17), (4.7), where C_{32} is given in (4.13).

We begin with the estimate (5.16a). Combining (5.12), (5.4b) and (4.15), and applying Lemma 5.4 give

$$\begin{aligned} S_{12} &\le \sum_{(p,q)\in S_l^2} T_{pq}|g_{pq}^0| < \sum_{q\in S_m^{2,2}} \sum_{p=1}^m \frac{1}{\mu_q}\widehat{D} < \widehat{D}m \sum_{i=1}^{N_s} \frac{1}{\mu_{k_i}} \\ &< \frac{\widehat{D}m}{\lambda_x^t \Delta\xi} \frac{3}{(2D)^{\frac{1}{4}}} \sqrt{(N_s+1)\Delta\xi}. \end{aligned} \tag{5.17}$$

From the definition of $S_m^{2,2}$ one has

$$(N_s - 1)\Delta\xi < \widehat{\xi}_z. \tag{5.18}$$

Combining (5.17) and (5.18) gives

$$S_{12} < \frac{\widehat{D}m}{\lambda_x^t \Delta\xi} \frac{3}{(2D)^{\frac{1}{4}}} \sqrt{\frac{1}{3\lambda_x^t} + 2\Delta\xi}. \tag{5.19}$$

We now estimate the number N_J. By definition

$$N_J = \sum_{q\in S_m^{2,2}} \widetilde{k}_q \ge \sum_{q\in S_m^{2,2}} \frac{7}{5}\mu_q m. \tag{5.20}$$

Define the set

$$S_R = \left\{ k \;\middle|\; \sqrt{2D} < \xi_k \le \min\left(\xi_M, \sqrt{\left(\widehat{\xi}_z - \Delta\xi\right)^2 + 2D}\right)\right\}. \tag{5.21}$$

Let N_R be the number of elements in S_R. Then

$$(N_R + \frac{1}{2})\Delta\xi + \sqrt{2D} > \min\left(\xi_M, \sqrt{\left(\widehat{\xi}_z - \Delta\xi\right)^2 + 2D}\right), \tag{5.22}$$

which gives

$$N_R\Delta\xi > \xi_C - \frac{1}{2}\Delta\xi \tag{5.23}$$

with ξ_C defined in (4.12). Under the mesh size restrictions (4.6) one has $\xi_C - \frac{1}{2}\Delta\xi > \frac{1}{2}\xi_C$.

We name the elements in S_R as k_i' satisfying $\xi_{k_i'} = \sqrt{2D} + (i - \frac{1}{2})\Delta\xi, i = 1, \cdots, N_R$. Define the map

$$\widetilde{T}(k) = j \quad \text{s.t.} \quad 0 \le \xi_j - \sqrt{(\xi_k)^2 - 2D} < \Delta\xi, \qquad \text{for } k \in S_R.$$

Then $\widetilde{T}(k) \in S_m^{2,2}$, $\forall k \in S_R$. Denote

$$T_i' = \widetilde{T}(k_i'), \quad i = 1, 2, \cdots, N_R.$$

From (5.20) one has

$$\begin{aligned} N_J \ge& \frac{7}{5}m \sum_{q \in S_m^{2,2}} \mu_q \ge \frac{7}{5}m\lambda_x^t \sum_{i=1}^{N_R} \xi_{T_i'} \ge \frac{7}{5}m\lambda_x^t \sum_{i=1}^{N_R} \sqrt{\left(\xi_{k_i'}\right)^2 - 2D} \\ >& \frac{7}{5}m\lambda_x^t(8D)^{\frac{1}{4}} \sum_{i=1}^{N_R} \sqrt{\left(i - \frac{1}{2}\right)\Delta\xi} > \frac{7}{5}m\lambda_x^t(8D)^{\frac{1}{4}} \frac{1}{\Delta\xi}\int_0^{N_R\Delta\xi} \sqrt{y}\, dy \\ =& \frac{14}{15}(8D)^{\frac{1}{4}} \frac{m\lambda_x^t}{\Delta\xi}(N_R\Delta\xi)^{\frac{3}{2}}. \end{aligned} \tag{5.24}$$

Combining (5.24) and (5.23) gives

$$N_J > \frac{14}{15}(8D)^{\frac{1}{4}} \frac{m\lambda_x^t}{\Delta\xi}\left(\xi_C - \frac{1}{2}\Delta\xi\right)^{\frac{3}{2}}. \tag{5.25}$$

Now if

$$N_B > N_J \Rightarrow \frac{\widehat{C}(\Delta x)^{r-1}}{\widehat{D}\Delta\xi} > N_J. \tag{5.26}$$

From (5.19) and (5.16) one has

$$\begin{aligned} S_{12} <& \frac{\widehat{D}m}{\lambda_x^t\Delta\xi}\frac{3}{(2D)^{\frac{1}{4}}}\sqrt{\frac{1}{3\lambda_x^t} + 2\Delta\xi} < \frac{\widehat{D}m}{\lambda_x^t\Delta\xi}\frac{3}{(2D)^{\frac{1}{4}}}\sqrt{\frac{1}{3\lambda_x^t} + 2\Delta\xi}\frac{15}{14(8D)^{\frac{1}{4}}\left(\xi_C - \frac{1}{2}\Delta\xi\right)^{\frac{3}{2}}}\frac{\Delta\xi}{m\lambda_x^t}N_J \\ <& \frac{\widehat{D}}{(\lambda_x^t)^2}\frac{45\sqrt{\frac{1}{3\lambda_x^t} + 2\Delta\xi}}{28\sqrt{D}\left(\xi_C - \frac{1}{2}\Delta\xi\right)^{\frac{3}{2}}}\frac{\widehat{C}(\Delta x)^{r-1}}{\widehat{D}\Delta\xi}, \end{aligned} \tag{5.27}$$

which gives the estimate (5.16a).

We then prove the estimate (5.16b). By definition of $S_m^{2,2}$ one has $\mu_q < \frac{1}{3}$ for $q \in S_m^{2,2}$. Since $\sqrt{2D}$ is located at mesh interface in ξ-direction one has for $\forall q \in S_m^{2,2}$

$$
\begin{aligned}
\mu_q \geq& \mu_{k_1} = \lambda_x^t \xi_{k_1} > \lambda_x^t \left[\sqrt{\left(\sqrt{2D} + \frac{1}{2}\Delta\xi\right)^2 - 2D} - \Delta\xi \right] \\
>& \lambda_x^t \left[(2D)^{\frac{1}{4}} - \sqrt{\Delta\xi} \right] \sqrt{\Delta\xi} \\
=& \lambda_x^t \left[(2D)^{\frac{1}{4}} - \sqrt{\Delta\xi} \right] \frac{1}{\sqrt{\lambda_\xi^t}} \frac{\sqrt{T}}{\sqrt{L}} = \lambda_x^t \left[(2D)^{\frac{1}{4}} - \sqrt{\Delta\xi} \right] \sqrt{\lambda_x^\xi} \frac{\sqrt{x_{m+\frac{1}{2}} - x_{\frac{1}{2}}}}{\sqrt{m}} \\
=& \lambda_x^t \left[(2D)^{\frac{1}{4}} - \sqrt{\Delta\xi} \right] \frac{\max\left(\frac{\sqrt{T}}{\sqrt{\lambda_\xi^t}}, \sqrt{\lambda_x^\xi}\sqrt{x_{m+\frac{1}{2}} - x_{\frac{1}{2}}}, \sqrt{L_2}\sqrt{\Delta\xi} \right)}{\sqrt{L_m}} \equiv \frac{\widehat{C}_1}{\sqrt{L_m}},
\end{aligned}
\tag{5.28}
$$

where

$$
\widehat{C}_1 = \lambda_x^t \left[(2D)^{\frac{1}{4}} - \sqrt{\Delta\xi} \right] \max\left(\sqrt{T/\lambda_\xi^t}, \sqrt{\lambda_x^\xi}\sqrt{x_{m+\frac{1}{2}} - x_{\frac{1}{2}}}, \sqrt{L_2}\sqrt{\Delta\xi} \right).
$$

Under the mesh size condition (4.17), $\widehat{C}_1$ satisfies

$$
\widehat{C}_1 > \lambda_x^t \frac{(2D)^{\frac{1}{4}}}{2} \sqrt{L_2 \Delta\xi} \geq \lambda_x^t \frac{(2D)^{\frac{1}{4}}}{2} \sqrt{\frac{4}{(\lambda_x^t)^2 \sqrt{2D}}} = 1.
$$

Thus one has

$$
\frac{1}{\sqrt{L_m}} < \mu_q < \frac{1}{3}, \quad \forall q \in S_m^{2,2}.
$$

It follows from the definition of $\widetilde{k}_q, \widetilde{p}_q$ in (5.13b), for $\widetilde{p}_q \geq 1$, that $\widetilde{k}_q = \left[\frac{7}{5}\mu_q L_m\right]^+$. By Lemma A.1 in Appendix one has for $\widetilde{p}_q \geq 1$

$$
\gamma_{\widetilde{p}_q,q}^{mq,L_m,0} = C_{L_m}^{\widetilde{k}_q} (1-\mu_q)^{L_m - \widetilde{k}_q} {\mu_q}^{\widetilde{k}_q} < \frac{6}{5}\mu_q,
\tag{5.29}
$$

under the conditions

$$
L_m \geq 16, \tag{5.30a}
$$

$$
1.1 \frac{1}{\sqrt{2\pi}} \sqrt{\frac{10}{7}} \frac{5}{6} \frac{{L_m}^{\frac{1}{4}}}{e^{0.036\sqrt{L_m}}} < 1, \tag{5.30b}
$$

where the notation C with both subscript and superscript denotes the binomial coefficient. Condition (5.30b) is satisfied for $\forall L_m \in \mathbb{N}$. Condition (5.30a) is satisfied under the mesh size restriction (4.7).

For $\widetilde{k}_q + 1 \leq n \leq L_m$ one has

$$
\begin{aligned}
\frac{\gamma_{\widetilde{p}_q,q}^{mqn0}}{\gamma_{\widetilde{p}_q,q}^{mq,n-1,0}} =& \frac{n}{n - \widetilde{k}_q}(1-\mu_q) \geq \frac{L_m}{L_m - \widetilde{k}_q}(1-\mu_q) \\
\geq& \frac{L_m}{L_m - \frac{7}{5}\mu_q L_m}(1-\mu_q) = \frac{1-\mu_q}{1-\frac{7}{5}\mu_q}.
\end{aligned}
\tag{5.31}
$$

Notice that $\gamma^{mqn0}_{\widetilde{p}_q,q}=0$ when $n<\widetilde{k}_q$. From (5.29) and (5.31) one has

$$T_{\widetilde{p}_q,q}=\sum_{n=0}^{L-1}\gamma^{mqn0}_{\widetilde{p}_q,q}=\sum_{n=\widetilde{k}_q}^{L-1}\gamma^{mqn0}_{\widetilde{p}_q,q}<\sum_{n=\widetilde{k}_q}^{L_m}\gamma^{mqn0}_{\widetilde{p}_q,q}<\frac{6}{5}\mu_q\left(\sum_{i=0}^{L_m-\widetilde{k}_q}\left(\frac{1-\frac{7}{5}\mu_q}{1-\mu_q}\right)^i\right)$$
$$<\frac{\frac{6}{5}\mu_q}{1-\left(\frac{1-\frac{7}{5}\mu_q}{1-\mu_q}\right)}<3,\qquad q\in S^{2,2}_m,\ \text{ if } \widetilde{p}_q\geq 1.$$

Due to the relation (5.4a), one has

$$T_{pq}<3,\quad q\in S^{2,2}_m,\quad 1\leq p\leq \widetilde{p}_q,\quad \text{if } \widetilde{p}_q\geq 1. \tag{5.32}$$

Define

$$T^m_{pq}=\begin{cases}3, & (p,q)\in S^2_l\backslash J,\\ \frac{1}{\mu_q}, & (p,q)\in J.\end{cases} \tag{5.33}$$

According to the definition of J, if $(p,q)\in S^2_l\backslash J$, then $1\leq p\leq \widetilde{p}_q$. Thus from (5.32) and (5.4b) one has

$$T_{pq}<T^m_{pq},\qquad \forall (p,q)\in S^2_l. \tag{5.34}$$

Denote

$$\varsigma_0=0,\qquad \varsigma_j=\sum_{i=1}^{j}\widetilde{k}_{k_i},\qquad\qquad j=1,\cdots,N_s, \tag{5.35a}$$

$$\tau_0=\varsigma_{N_s},\quad \tau_j=\varsigma_{N_s}+\sum_{i=1}^{j}\left(m-\widetilde{k}_{k_i}\right),\quad j=1,\cdots,N_s. \tag{5.35b}$$

One has $\varsigma_{N_s}=N_J$, $\tau_{N_s}=N_s^2\equiv mN_s$. For $1\leq j\leq N_s^2$, define

$$\widehat{T}^m_j=\begin{cases}T^m_{m-j+\varsigma_{l-1}+1,k_l}, & \varsigma_{l-1}+1\leq j\leq \varsigma_l,\ l=1,\cdots,N_s,\\ T^m_{\tau_l-j+1,k_l}, & \tau_{l-1}+1\leq j\leq\tau_l,\ l=1,\cdots,N_s.\end{cases} \tag{5.36}$$

From the definition of T^m_{pq} in (5.33), $\widehat{T}^m_j, 1\leq j\leq N_s^2$ is a permutation of $T^m_{pq},(p,q)\in S^2_l$ which is in descendent order, namely $\widehat{T}^m_j\geq \widehat{T}^m_{j+1}$, $1\leq j\leq N_s^2-1$. Define

$$\widetilde{g}^0_j=g^0_{pq},\quad \text{if } \widehat{T}^m_j \text{ is assigned as } T^m_{pq} \text{ in (5.36)},\quad 1\leq j\leq N_s^2. \tag{5.37}$$

Now if $N_B\leq N_J$, then $N_B\leq N_s^2$. Using (5.12), (5.34), (5.36), (5.37), (4.15) and (4.16), S_{12} can be estimated by

$$S_{12}\leq\sum_{(p,q)\in S^2_l}T_{pq}|g^0_{pq}|<\sum_{(p,q)\in S^2_l}T^m_{pq}|g^0_{pq}|=\sum_{j=1}^{N_s^2}\widehat{T}^m_j|\widetilde{g}^0_j|$$
$$=\sum_{j=1}^{N_B}\widehat{T}^m_j|\widetilde{g}^0_j|+\sum_{j=N_B+1}^{N_s^2}\widehat{T}^m_j|\widetilde{g}^0_j|=\sum_{j=1}^{N_B}\widehat{T}^m_j\widehat{D}-\sum_{j=1}^{N_B}\widehat{T}^m_j\left(\widehat{D}-|\widetilde{g}^0_j|\right)+\sum_{j=N_B+1}^{N_s^2}\widehat{T}^m_j|\widetilde{g}^0_j|$$
$$\leq\sum_{j=1}^{N_B}\widehat{T}^m_j\widehat{D}-\widehat{T}^m_{N_B}\sum_{j=1}^{N_B}\left(\widehat{D}-|\widetilde{g}^0_j|\right)+\widehat{T}^m_{N_B}\sum_{j=N_B+1}^{N_s^2}|\widetilde{g}^0_j|$$

$$
\begin{aligned}
&=\sum_{j=1}^{N_B}\widehat{T}_j^m\widehat{D}+\widehat{T}_{N_B}^m\left\{\sum_{j=1}^{N_s^2}|\widetilde{g}_j^0|-N_B\widehat{D}\right\}\\
&<\sum_{j=1}^{N_B}\widehat{T}_j^m\widehat{D}+\widehat{T}_{N_B}^m\left\{\frac{\widehat{C}(\Delta x)^r}{\Delta x\Delta\xi}-\frac{\widehat{C}(\Delta x)^{r-1}}{\widehat{D}\Delta\xi}\widehat{D}\right\}=\sum_{j=1}^{N_B}\widehat{T}_j^m\widehat{D}. \qquad (5.38)
\end{aligned}
$$

Since $N_B\le N_J$, denote $l_B\in\{1,2,\cdots,N_s\}$ s.t. $\varsigma_{l_B-1}<N_B\le\varsigma_{l_B}$. From definition of $\widehat{T}_j^m$ in (5.36), the expression (5.38) can be written as

$$
\begin{aligned}
\sum_{j=1}^{N_B}\widehat{T}_j^m\widehat{D}=&\widehat{D}\left\{\sum_{l=1}^{l_B-1}\frac{1}{\mu_{k_l}}\widetilde{k}_{k_l}+\frac{1}{\mu_{k_{l_B}}}\left(N_B-\varsigma_{l_B-1}\right)\right\}\le\widehat{D}\sum_{l=1}^{l_B}\frac{1}{\mu_{k_l}}\widetilde{k}_{k_l}\\
<&\widehat{D}\sum_{l=1}^{l_B}\frac{1}{\mu_{k_l}}\left(\frac{7}{5}\mu_{k_l}L_m+1\right)=\widehat{D}\left(\frac{7}{5}L_ml_B+\sum_{l=1}^{l_B}\frac{1}{\mu_{k_l}}\right). \qquad (5.39)
\end{aligned}
$$

Applying Lemma 5.4 one has

$$
\Delta\xi\sum_{l=1}^{l_B}\frac{1}{\xi_{k_l}}<\frac{3}{(2D)^{\frac14}}\sqrt{(l_B+1)\,\Delta\xi}. \qquad (5.40)
$$

In the next we estimate the number l_B. From the definition of l_B one has

$$
N_B>\varsigma_{l_B-1}=\sum_{i=1}^{l_B-1}\widetilde{k}_{k_i}\ge\sum_{i=1}^{l_B-1}\frac{7}{5}\mu_{k_i}m\ge\frac{7}{5}m\lambda_x^t\sum_{i=1}^{\left[\frac{l_B-1}{2}\right]^-}\xi_{T_i'}. \qquad (5.41)
$$

Similar to the deduction of (5.24), one gets from (5.41) that

$$
\begin{aligned}
N_B>&\frac{14}{15}(8D)^{\frac14}\frac{m\lambda_x^t}{\Delta\xi}\left(\left[\frac{l_B-1}{2}\right]^-\Delta\xi\right)^{\frac32}\\
\ge&\frac{14}{15}(8D)^{\frac14}\frac{\left(x_{m+\frac12}-x_{\frac12}\right)\lambda_x^t}{\Delta x\Delta\xi}\left[\left(\frac{l_B}{2}-1\right)\Delta\xi\right]^{\frac32}. \qquad (5.42)
\end{aligned}
$$

By definition of N_B, one has

$$
N_B<\frac{\widehat{C}(\Delta x)^{r-1}}{\widehat{D}\Delta\xi}+1. \qquad (5.43)
$$

Combining (5.42) and (5.43) gives

$$
\begin{aligned}
&\left[\left(\frac{l_B}{2}-1\right)\Delta\xi\right]^{\frac32}<\frac{15\Delta x\Delta\xi}{14(8D)^{\frac14}\left(x_{m+\frac12}-x_{\frac12}\right)\lambda_x^t}\left[\frac{\widehat{C}(\Delta x)^{r-1}}{\widehat{D}\Delta\xi}+1\right]\\
\Rightarrow\quad &l_B\Delta\xi<A_3(\Delta x)^{\frac23 r}+\mathcal{O}(\Delta x), \qquad (5.44)
\end{aligned}
$$

where

$$
A_3=2\left[\frac{15\widehat{C}}{14(8D)^{\frac14}\left(x_{m+\frac12}-x_{\frac12}\right)\lambda_x^t\widehat{D}}\right]^{\frac23}. \qquad (5.45)
$$

Combining (5.38)−(5.40) and (5.44) one has

$$\begin{aligned}\Delta x\Delta\xi S_{12} <&\widehat{D}\left(\frac{7}{5}L_m\Delta x l_B\Delta\xi+\frac{\frac{3}{(2D)^{\frac14}}\sqrt{(l_B+1)\Delta\xi}}{\lambda_x^t}\Delta x\right)\\ <&\widehat{D}\left(\frac{7}{5}L_m\Delta x A_3(\Delta x)^{\frac23 r}\right)+\mathcal{O}(\Delta x)\le C_{32}(\Delta x)^{\frac23 r}+\mathcal{O}(\Delta x),\end{aligned}$$

where C_{32} is given in (4.13). Thus we derive the estimate (5.16b).

Now combining (5.11), (4.16), (5.16a) and (5.16b) gives the estimate (4.18). □

5.2. Proof for Theorem 4.1

With Theorems 3.1 and 4.2 we now can give proof for Theorem 4.1.

Proof. Let g_{ij}^n be the numerical solutions computed with the exact initial data $f(x,\xi,0)$. Denote $z_{ij}^n=g_{ij}^n-\widehat{g}_{ij}^n$. Due to the linearity of Scheme I, z_{ij}^n is the numerical solutions computed by Scheme I with zero incoming boundary condition. Under the conditions (4.1), (4.2), the initial values z_{ij}^0 satisfy

$$\begin{aligned}\left|z_{ij}^0\right|=\left|g_{ij}^0-\widehat{g}_{ij}^0\right|=&\frac{1}{\Delta x\Delta\xi}\left|\int_{x_{i-\frac12}}^{x_{i+\frac12}}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\Big(f(x,\xi,0)-\widehat{f}(x,\xi,0)\Big)\,d\xi dx\right|\\ \le&\frac{1}{\Delta x\Delta\xi}\int_{x_{i-\frac12}}^{x_{i+\frac12}}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\Big|f(x,\xi,0)-\widehat{f}(x,\xi,0)\Big|\,d\xi dx<\widehat{D},\quad (x_i,\xi_j)\in D_C,\end{aligned}\tag{5.46}$$

$$\begin{aligned}\left|z^0\right|_1=&\Delta x\Delta\xi\sum_{(x_i,\xi_j)\in D_C}\left|g_{ij}^0-\widehat{g}_{ij}^0\right|\\ =&\sum_{(x_i,\xi_j)\in D_C}\left|\int_{x_{i-\frac12}}^{x_{i+\frac12}}\int_{\xi_{j-\frac12}}^{\xi_{j+\frac12}}\Big(f(x,\xi,0)-\widehat{f}(x,\xi,0)\Big)\,d\xi dx\right|\\ \le&\left\|f(\cdot,\cdot,0)-\widehat{f}(\cdot,\cdot,0)\right\|_{L^1(D_C)}<\widehat{C}(\Delta x)^r.\end{aligned}\tag{5.47}$$

Thus applying Theorem 4.2 gives under the CFL condition (2.6) and the mesh size restrictions (4.6), (4.7), (4.17)

$$\|g(\cdot,\cdot,T)-\widehat{g}(\cdot,\cdot,T)\|_{L^1(D_C)}=\left|z^L\right|_1<C_3(\Delta x)^{\frac23 r}+\mathcal{O}(\Delta x),\tag{5.48}$$

where C_3 is given in (4.9).

Applying Theorem 3.1 and (5.48) completes the proof for Theorem 4.1. □

6. Conclusion

In this paper we derived the L^1-error estimates for a Hamiltonian-preserving scheme called Scheme I, developed in [19], for the Liouville equation with a piecewise constant potential in one space dimension when the initial data is given with perturbation errors. The Hamiltonian-preserving scheme is designed by incorporating into the numerical fluxes the particle behavior– transmission and reflection– at the potential barrier. We proved that, with the Dirichlet incoming boundary conditions and for a class of bounded initial data, the numerical solution with a wide class of initial perturbation errors by Scheme I converges in L^1-norm to the solution of the Liouville equation defined by the particle transmission and reflection interface condition. We derived the L^1-error bounds with explicit coefficients.

Due to the linearity of Scheme I, the error estimates in this paper were obtained by applying the error estimates for the same scheme with exact initial data established in [45] and the l^1-norm estimates for the perturbation solutions. The latter estimates composes the main part of this paper. Since the initial perturbation errors may violate the condition required for the l^1-stability of Scheme I given in [46], the perturbation solution can be l^1-unstable. Therefore the l^1-norm estimates for the perturbation solutions can not be obtained by applying the l^1-stability result of Scheme I presented in [46]. In this paper we extended the analysis in [46] to show that even when the solution of Scheme I can be l^1-unstable, the l^1-norm of the solution can still be estimated from the L^∞ and L^1-upper bounds of the initial data. Based on this result we proved that Scheme I is L^1-convergent given with a wide class of initial perturbation errors. The L^1-convergence rate we derived in this paper is less than the order of the initial perturbation error, which is in consistent with the fact that the perturbation solution can be l^1-unstable.

Appendix

Lemma A.1. *Let $N \in \mathbb{N}$, $\frac{C}{\sqrt{N}} < \mu < \frac{1}{3}$, $k = [\frac{7}{5}\mu N]^+$. Then*

$$C_N^k (1-\mu)^{N-k} \mu^k < \widehat{C}\mu, \tag{A.1}$$

where C_N^k denotes the binomial coefficient, if N satisfies the conditions

$$N \geq 16 \max\left(\frac{1}{C^2}, 1\right), \tag{A.2}$$

$$1.1 \frac{1}{\sqrt{2\pi}} \sqrt{\frac{10}{7}} \frac{1}{C^{\frac{3}{2}}\widehat{C}} \frac{N^{\frac{1}{4}}}{e^{0.036C\sqrt{N}}} < 1. \tag{A.3}$$

Proof. For $N \geq 2$ one can check $k - \mu N > 0, N - k > 0, k > 0$. According to Stirling formula,

$$1 < \frac{n!}{n^n e^{-n}\sqrt{2\pi n}} < 1.1, \quad \forall n \in \mathbb{N}.$$

Thus one has

$$\begin{aligned}
C_N^k (1-\mu)^{N-k}\mu^k =& \frac{N!}{(N-k)!k!}(1-\mu)^{N-k}\mu^k \\
<& 1.1(1-\mu)^{N-k}\mu^k \frac{N^N e^N \sqrt{2\pi N}}{(N-k)^{N-k}e^{N-k}\sqrt{2\pi(N-k)}k^k e^k \sqrt{2\pi k}} \\
=& 1.1 \frac{1}{\sqrt{2\pi}} \frac{\sqrt{N}}{\sqrt{(N-k)k}} \frac{(N-\mu N)^{N-k}(\mu N)^k}{(N-k)^{N-k}k^k} \\
=& 1.1 \frac{1}{\sqrt{2\pi}} \frac{\sqrt{N}}{\sqrt{(N-k)k}} \left(1 + \frac{k-\mu N}{N-k}\right)^{N-k} \left(1 - \frac{k-\mu N}{k}\right)^k \\
=& 1.1 \frac{1}{\sqrt{2\pi}} \frac{\sqrt{N}}{\sqrt{(N-k)k}} \left[(1+A)^{\frac{1}{A}}(1-B)^{\frac{1}{B}}\right]^{k-\mu N},
\end{aligned} \tag{A.4}$$

where
$$A = \frac{k-\mu N}{N-k}, \quad B = \frac{k-\mu N}{k}.$$
By Taylor expansion one has
$$(1+A)^{\frac{1}{A}} < e^{1-\frac{A}{2}+\frac{A^2}{3}}, \quad (1-B)^{\frac{1}{B}} < e^{-1-\frac{B}{2}}, \quad \text{for } A, B > 0. \tag{A.5}$$
Combining (A.4) and (A.5) one has
$$\begin{aligned} C_N^k(1-\mu)^{N-k}\mu^k &< 1.1\frac{1}{\sqrt{2\pi}}\frac{\sqrt{N}}{\sqrt{(N-k)k}}\left[e^{-\frac{B}{2}+\frac{A^2}{3}}\right]^{k-\mu N} \\ &= 1.1\frac{1}{\sqrt{2\pi}}\frac{\sqrt{N}}{\sqrt{(N-k)k}}e^{-I_1}, \end{aligned} \tag{A.6}$$
where
$$I_1 = \frac{(k-\mu N)^2}{2k} - \frac{(k-\mu N)^3}{3(N-k)^2}. \tag{A.7}$$
We then estimate the term I_1. Define function
$$F_1(x) = \frac{x^2}{2k} - \frac{x^3}{3(N-k)^2}.$$
Then $I_1 = F_1(k-\mu N)$. Now we check the sign of $F_1'(x)$ when $x \in [\frac{2}{5}\mu N, k-\mu N]$.
$$\begin{aligned} F_1'(x) &= \frac{x}{k} - \frac{x^2}{(N-k)^2} = \frac{x}{k(N-k)^2}((N-k)^2 - kx) \\ \geq &\frac{x}{k(N-k)^2}\Big((N-k)^2 - k(k-\mu N)\Big) = \frac{x}{k(N-k)^2}(N^2 - 2kN + k\mu N) \\ > &\frac{2xN}{k(N-k)^2}\left(\frac{N}{2} - [\frac{7}{5}\mu N]^+\right) \geq \frac{2xN}{k(N-k)^2}\left(\frac{N}{2} - \left[\frac{7}{15}N\right]^+\right) \geq 0, \qquad \text{for } N \geq 14. \end{aligned}$$

Thus one has $F_1(k-\mu N) \geq F_1(\frac{2}{5}\mu N)$, namely
$$I_1 \geq \frac{(\frac{2}{5}\mu N)^2}{2k} - \frac{(\frac{2}{5}\mu N)^3}{3(N-k)^2}. \tag{A.8}$$

The right hand side of (A.8) decreases when k increases, so
$$I_1 > \frac{(\frac{2}{5}\mu N)^2}{2\left(\frac{7}{5}\mu N + 1\right)} - \frac{\left(\frac{2}{5}\mu N\right)^3}{3\left(N - \frac{7}{5}\mu N - 1\right)^2} = \mu N\left[\frac{(\frac{2}{5})^2}{2\left(\frac{7}{5}+\frac{1}{\mu N}\right)} - \frac{\left(\frac{2}{5}\right)^3}{3\left(\frac{N-1}{\mu N} - \frac{7}{5}\right)^2}\right]. \tag{A.9}$$

If one imposes the condition (A.2), then $\mu N \geq 4$, $\frac{N-1}{\mu N} > 3 \times \frac{15}{16}$, which gives $I_1 > 0.036\mu N > 0.036C\sqrt{N}$. Under this condition, from (A.6) one has
$$\begin{aligned} C_N^k(1-\mu)^{N-k}\mu^k &< 1.1\frac{1}{\sqrt{2\pi}}\frac{\sqrt{N}}{\sqrt{(N-k)k}}e^{-I_1} < 1.1\frac{1}{\sqrt{2\pi}}\frac{\sqrt{N}}{\sqrt{(N-k)k}}e^{-0.036C\sqrt{N}} \\ < 1.1&\frac{1}{\sqrt{2\pi}}\frac{\sqrt{N}}{\sqrt{(N-\frac{1}{2}N)(\frac{7}{5}\mu N)}}e^{-0.036C\sqrt{N}} < 1.1\frac{1}{\sqrt{2\pi}}\sqrt{\frac{10}{7}}\frac{1}{\sqrt{C}N^{\frac{1}{4}}}e^{-0.036C\sqrt{N}}. \end{aligned} \tag{A.10}$$

Thus if one further imposes the condition

$$1.1\frac{1}{\sqrt{2\pi}}\sqrt{\frac{10}{7}}\frac{1}{\sqrt{C}N^{\frac{1}{4}}}e^{-0.036C\sqrt{N}} < \frac{\widehat{C}C}{\sqrt{N}}, \tag{A.11}$$

which is equivalent to condition (A.3), then (A.1) is satisfied. □

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