

CONVERGENCE ESTIMATES OF A SEMI-LAGRANGIAN SCHEME FOR THE ELLIPSOIDAL BGK MODEL FOR POLYATOMIC MOLECULES

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Abstract. In this paper, we propose a new semi-Lagrangian scheme for the polyatomic ellipsoidal BGK model. In order to avoid time step restrictions coming from convection term and small Knudsen number, we combine a semi-Lagrangian approach for the convection term with an implicit treatment for the relaxation term. We show how to explicitly solve the implicit step, thus obtaining an efficient and stable scheme for any Knudsen number. We also derive an explicit error estimate on the convergence of the proposed scheme for every fixed value of the Knudsen number.

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1. INTRODUCTION

1.1. Polyatomic ES-BGK model

The BGK model [5] has been popularly employed for various flow problems of rarefied gas dynamics in place of the Boltzmann equation since it reproduces the dynamics of the Boltzmann equation in a reliable manner at much lower computational cost. The importance of developing polyatomic versions of the BGK model has been recognized soon after the inception of the model – which is very natural since most of the gas molecules consists of several atoms – and the several attempts to derive polyatomic version of the BGK model have been proposed in the literature. The polyatomic generalization of the BGK model can be realized in various manners such as the introduction of new variables describing the internal energy due to the inner configuration of the molecules [2, 4], vibrational excitation [3], and reformulation into the gas mixture framework [27, 36]. In this paper, we are interested in the polyatomic BGK model obtained from the so called ellipsoidal BGK model [2, 9, 24] (Polyatomic ES-BGK model):

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{A_{\nu, \theta}}{\kappa} (\mathcal{M}_{\nu, \theta, \delta}(f) - f),$$

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$$f(x, v, 0, I) = f_0(x, v, I). \tag{1.1}$$

The velocity-energy distribution function $f(x, v, t, I)$ represents the number density of particles in the phase space. For simplicity, we assumed periodic boundary condition in d -dimensional space. Without loss of generality, the length of the domain is assumed to be one. The parameter $I \in \mathbb{R}_+$ is related to internal energy ε due to rotation and vibration $\varepsilon(I) = I^{\frac{2}{\delta}}$, where $\delta > 0$ represents the number of degrees of freedom for the internal motion of the molecules such as the rotation and vibration. Our independent variables x and v belong to phase space $(x, v) \in \mathbb{T}^d \times \mathbb{R}^3$, with $\mathbb{T}^d \equiv \mathbb{R}^d/\mathbb{Z}^d$, and $t \geq 0$ denotes the time. The Knudsen number $\kappa > 0$ is the ratio between the mean free path of the gas molecules and the macroscopic length scale of the problem. We consider a collision frequency $A_{\nu,\theta} := 1/(1 - \nu + \nu\theta)$, for $0 < \theta \leq 1$ and $-\frac{1}{2} < \nu < 1$. The two parameters can be chosen to fit Prandtl number and transport coefficients computed by Chapman-Enskog expansion of the Boltzmann equation. The polyatomic Gaussian $\mathcal{M}_{\nu,\theta,\delta}(f)$ is given by

$$\mathcal{M}_{\nu,\theta,\delta}(f) := \frac{\rho\Lambda_\delta}{\sqrt{\det(2\pi\mathcal{T}_{\nu,\theta})(T_\theta)^{\frac{\delta}{2}}}} \exp\left(-\frac{(v - U(x, t))^\top \mathcal{T}_{\nu,\theta}^{-1}(v - U(x, t))}{2} - \frac{I^{\frac{2}{\delta}}}{T_\theta}\right), \tag{1.2}$$

where Λ_δ is a normalizing constant defined by

$$\Lambda_\delta^{-1} := \int_{\mathbb{R}_+} e^{-I^{\frac{2}{\delta}}} dI. \tag{1.3}$$

The macroscopic local density $\rho(x, t)$, bulk velocity $U(x, t)$, stress tensor $\Theta(x, t)$ and internal energy $E_\delta(x, t)$ are defined as follows:

$$\begin{aligned} \rho(x, t) &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} f(x, v, t, I) dv dI, \\ \rho(x, t)U(x, t) &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} vf(x, v, t, I) dv dI, \\ \rho(x, t)\Theta(x, t) &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} (v - U(x, t)) \otimes (v - U(x, t))f(x, v, t, I) dv dI, \\ E_\delta(x, t) &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{1}{2}|v - U(x, t)|^2 + I^{\frac{2}{\delta}}\right)f(x, v, t, I) dv dI. \end{aligned}$$

The internal energy E_δ consists of the translational energy E_{tr} and the non-translational energy $E_{I,\delta}$:

$$\begin{aligned} E_{\text{tr}} &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{1}{2}|v - U(x, t)|^2 f(x, v, t, I) dv dI, \\ E_{I,\delta} &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} I^{\frac{2}{\delta}} f(x, v, t, I) dv dI. \end{aligned}$$

The corresponding temperatures T_δ , T_{tr} and $T_{I,\delta}$ are defined by

$$E_\delta =: \frac{3 + \delta}{2}\rho T_\delta, \quad E_{\text{tr}} =: \frac{3}{2}\rho T_{\text{tr}}, \quad E_{I,\delta} =: \frac{\delta}{2}\rho T_{I,\delta}.$$

Note that T_δ is the convex combination of T_{tr} and $T_{I,\delta}$:

$$T_\delta = \frac{3}{3 + \delta}T_{\text{tr}} + \frac{\delta}{3 + \delta}T_{I,\delta}.$$

We also define the relaxation temperature T_θ and the temperature tensor $\mathcal{T}_{\nu,\theta}$ as follows:

$$T_\theta = \theta T_\delta + (1 - \theta)T_{I,\delta},$$

$$\mathcal{T}_{\nu,\theta} = \theta T_\delta Id + (1 - \theta)\{(1 - \nu)T_{tr}Id + \nu\Theta\}.$$

where Id is a 3×3 identity matrix. The polyatomic relaxation operator has five-dimensional collision invariants:

$$\int_{\mathbb{R}^3 \times \mathbb{R}_+} (\mathcal{M}_{\nu,\theta,\delta}(f) - f)\phi(v, I) \, dv \, dI = 0, \quad \phi(v, I) = \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 + I^{\frac{2}{3}} \end{pmatrix},$$

so that the conservation laws hold for mass, momentum and energy:

$$\frac{d}{dt} \int_{\mathbb{T}^d \times \mathbb{R}^3 \times \mathbb{R}_+} f\phi(v, I) \, dx \, dv \, dI = 0.$$

The celebrated H-theorem was first verified in [2] (see also [8, 9, 33, 46])

$$\frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}_+} f \ln f \, dv \, dI = \int_{\mathbb{R}^3 \times \mathbb{R}_+} (\mathcal{M}_{\nu,\theta,\delta}(f) - f) \ln f \, dv \, dI \leq 0.$$

We note that this model reduces to the monatomic ES-BGK model [24] when $\theta = 0$. On the other hand, if we take $\nu = \theta = 0$ and integrate both sides of (1.1) against I , the original BGK model is recovered [5]. It is also interesting that there is a dichotomy in the time asymptotic state of f depending on θ (see [33]). For $0 < \theta \leq 1$, f converges to $\mathcal{M}_{0,1,\delta}(f)$:

$$\mathcal{M}_{0,1,\delta}(f) := \frac{\rho\Lambda_\delta}{(2\pi T_\delta)^{\frac{3}{2}}(T_\delta)^{\frac{\delta}{2}}} \exp\left(-\frac{|v - U(x, t)|^2}{2T_\delta} - \frac{I^{\frac{2}{3}}}{T_\delta}\right),$$

while if $\theta = 0$, its time asymptotic limit is the isothermal equilibrium $\mathcal{M}_{0,0,\delta}(f)$:

$$\mathcal{M}_{0,0,\delta}(f) := \frac{\rho\Lambda_\delta}{(2\pi T_{tr})^{\frac{3}{2}}(T_{I,\delta})^{\frac{\delta}{2}}} \exp\left(-\frac{|v - U(x, t)|^2}{2T_{tr}} - \frac{I^{\frac{2}{3}}}{T_{I,\delta}}\right).$$

As regards analytical results on the polyatomic ES-BGK model, we refer to papers regarding the entropy production property [33], existence of classical solutions [32, 47] and mild solutions [34]. We also refer to [9] where authors studied how to determine the form of polyatomic Gaussian $\mathcal{M}_{\nu,\theta,\delta}(f)$. The result shows that $\mathcal{M}_{\nu,\theta,\delta}(f)$ in (1.2) is derived from an entropy minimization problem.

1.2. Implicit semi-Lagrangian scheme

Several methods have been adopted for numerical solutions of (1.1). In [28, 30], the authors employed iterative schemes to find the steady state solutions. When dealing with time-dependent problems, explicit schemes can be adopted if the Knudsen number is not too small [1, 29]. On the other hand, if one is interested in small value of κ , then an implicit treatment of collision term is necessary in order to avoid excessive restrictions on the time step. Splitting schemes can be used in which an explicit convection step is followed by an implicit relaxation step [11]. Because during the relaxation step mass momentum and energy are constant, the solution of the implicit step is relatively easy to compute. However, splitting schemes have the drawback that for small Knudsen number they are restricted to the first order accuracy in time [10, 26]. Accuracy can be improved for small Knudsen number using implicit explicit Runge–Kutta schemes [4]. In this paper, the authors use an Eulerian framework in which convection terms are treated explicitly and collision term is treated implicitly. The drawback of Eulerian schemes is the CFL-type time step restriction $|v \frac{\Delta t}{\Delta x}| < 1$ imposed by the convection term. To overcome these difficulties, we propose a semi-Lagrangian (SL) method with an implicit treatment of the relaxation term of the following form:

$$\frac{f_{i,j,k}^{n+1} - \tilde{f}_{i,j,k}^n}{\Delta t} = \frac{A_{\nu,\theta}}{\kappa} \left(\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,j,k}^{n+1} \right) - f_{i,j,k}^{n+1} \right), \tag{1.4}$$

where $f_{i,j,k}^{n+1}$ is the discrete solution of the scheme, $\tilde{f}_{i,j,k}^n$ is the approximation of the discrete solution on the foot of characteristic, and $\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k}$ denotes the numerical polyatomic ellipsoidal Gaussian (see Sect. 2 for precise definitions). However, this implicit scheme requires to solve non-linear systems.

To overcome this difficulty, we observe that the polyatomic ellipsoidal Gaussian constructed from $f_{i,j,k}^{n+1}$ in (1.4) can be replaced by the polyatomic ellipsoidal Gaussian constructed from $\tilde{f}_{i,j,k}^n$ up to small error, which makes the equation solvable as

$$f_{i,j,k}^{n+1} = \frac{\kappa \tilde{f}_{i,j,k}^n + A_{\nu,\theta} \Delta t \mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k}}{\kappa + A_{\nu,\theta} \Delta t}.$$

Note that the proposed scheme for the polyatomic ES-BGK model reduces to the SL scheme for monatomic BGK model in [22, 40, 43] and SL scheme for monatomic ES-BGK model [42] by taking appropriate values of ν and θ and integrating it over I variable.

The main result of this paper is the derivation of the error estimate based on L_q^∞ -norm (see notation in Sect. 1.3), which is stated in Theorem 3.2 as follows:

$$\|f^{Nt} - f(T^f)\|_{L_q^\infty} \leq C \left(\frac{(\Delta x)^2}{\Delta t} + (\Delta x)^2 + \Delta v + \Delta I + \Delta t \right),$$

where C is a constant depending on $T^f, q, \delta, \kappa, \theta, \nu, \Delta t$, but can be uniformly bounded regardless of $\Delta t > 0$. The main ingredient of the convergence proof is the establishment of the following uniform stability estimate of the discrete solution (see Sect. 4):

$$C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f} e^{-C_0^2 (|v_j|^a + I_k^b)} \leq \tilde{f}_{i,j,k}^n \leq e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f} \|f_0\|_{L_q^\infty} (1 + |v_j|^2)^{-q/2}.$$

We note that, unlike most of numerical stability estimates, the uniform lower bound is important since it is crucially used to prove that the polyatomic temperature never vanishes (see Lem. 4.14):

$$\left(\tilde{T}_\delta \right)_i^n \geq \left(\frac{1}{2} \frac{\bar{C}_{a,b} C_0^1}{C_\delta \|f_0\|_{L_q^\infty}} e^{-\left(\frac{1}{\kappa} + \frac{(C_{\mathcal{M}} - 1)}{\kappa + A_{\nu,\theta} \Delta t} \right) T^f} \right)^{\frac{2}{3+2\delta}},$$

so that the discrete polyatomic ellipsoidal Gaussian never degenerates into Dirac delta.

We close this subsection with a brief review on implicit SL schemes for BGK models. In [43], high order SL methods were constructed using diagonally implicit Runge–Kutta schemes [31] and high order non-oscillatory spatial reconstruction [18]. Owing to the L-stability property of time discretization, the resulting schemes enable one to use a large time step even in the fluid regime. In [22], multi-step time discretization such as the backward difference formula (BDF) were adopted in the semi-Lagrangian framework. The performance of such methods was verified through boundary value problems in [21, 39]. In [7], such SL schemes were employed as a predictor scheme corrected it by a conservative procedure to obtain an exactly conservative scheme at the discrete level. Recently, in [14] we proposed a class of high order conservative SL schemes with a high order non-oscillatory conservative reconstruction [13], and numerically show that the proposed scheme is able to capture the exact shock position of compressible Euler system. We also refer to [6, 12, 23] for SL methods applied to gas mixtures and reactive flows.

The convergence estimate for the original monatomic BGK model was investigated in [41]. The argument has been simplified and applied to the more complicate case of the ES-BGK model [42], which is the main

motivation of the current work. These two results seem to be the only available convergence estimates for fully discrete schemes for spatially inhomogeneous collisional kinetic equations.

The semi-Lagrangian methods have been widely used also for the numerical solutions of Vlasov-type equations [16, 19, 37, 38, 44, 45]. We refer to [17] for a nice survey on numerical schemes for kinetic equations.

1.3. Notation

Throughout this paper, we use the following notations:

- C denotes a constant which can be explicitly computable.
- $C_{a,b,\dots}, \bar{C}_{a,b,\dots}$ denote constants that depend on a, b, \dots .
- We use lower indices i, j, k for space, velocity, internal energy variables and an upper index n for time variable, respectively.
- We write the velocity vector v as $v \equiv (v^1, v^2, v^3)$.
- T^f denotes the final time of the numerical experiment.
- The relation $A \leq B$ for 3×3 matrices A and B means that $B - A$ is positive definite, *i.e.*, $k^\top (B - A)k \geq 0$ for all $k \equiv (k^1, k^2, k^3)^\top \in \mathbb{R}^3$.
- For $N, q \in \mathbb{N}$, the weighted L^∞ -Sobolev norm for continuous solution is defined by

$$\|f(t)\|_{L_q^\infty} := \sup_{x,v,I} \left| f(x, v, t, I) \left(1 + |v|^2 + I^{\frac{2}{3}}\right)^{\frac{q}{2}} \right|,$$

$$\|f(t)\|_{L_{N,q}^\infty} := \sum_{|\alpha|+|\beta|+\gamma \leq N} \sup_{x,v,I} \left| \partial(\alpha, \beta, \gamma) f(x, v, t, I) \left(1 + |v|^2 + I^{\frac{2}{3}}\right)^{\frac{q}{2}} \right|,$$

where $\alpha, \beta, \gamma \in \mathbb{Z}_+ \times \mathbb{Z}_+^3 \times \mathbb{Z}_+$, and the differential operator $\partial(\alpha, \beta, \gamma)$ stands for $\partial_x^\alpha \partial_v^\beta \partial_I^\gamma$. Indeed, $\|f(t)\|_{L_q^\infty} = \|f(t)\|_{L_{0,q}^\infty}$.

- The weighted L_q^∞ -Sobolev norm for discrete solution is defined by

$$\|f^n\|_{L_q^\infty} := \sup_{i,j,k} \left| f_{i,j,k}^n \left(1 + |v_j|^2 + I_k^{\frac{2}{3}}\right)^{\frac{q}{2}} \right|,$$

where $f_{i,j,k}^n$ is a numerical solution of $f(x_i, v_j, t^n, I_k)$.

- To measure the distance between discrete and continuous solutions, we use the following supremum on grid points:

$$\|f^n - f(t^n)\|_{L_q^\infty} = \sup_{i,j,k} \left| f_{i,j,k}^n - f(x_i, v_j, t^n, I_k) \right| \left(1 + |v_j|^2 + I_k^{\frac{2}{3}}\right)^{\frac{q}{2}}.$$

This paper is organized as follows: In Section 2, we derive a first order semi-Lagrangian scheme for the polyatomic ES-BGK model. Section 3 is devoted to the statement of the main result of this paper. In the following Section 4, we present several technical estimates on the discrete solution and its macroscopic variables. In Section 5, we rewrite the polyatomic ES-BGK model (1.1) for the easy comparison of continuous and discrete solution. Then, in Section 6, the difference between the continuous and discrete Gaussians is estimated. Finally, in Section 7, we prove our main theorem.

2. DESCRIPTION OF THE NUMERICAL SCHEME

2.1. Discretization

For velocity variables, we take same mesh spacing Δv in all directions, while, for the internal energy variable, we use a uniform mesh of size ΔI . For space, one-dimensional periodic unit interval is considered with a uniform mesh Δx . We assume a fixed time step Δt . Then,

$$t^n = n\Delta t, \quad n = 0, 1, \dots, N_t,$$

$$x_i = i\Delta x, \quad i = 0, \pm 1, \dots, \pm N_x, \pm(N_x + 1), \dots$$

where $N_t\Delta t = T^f$, $N_x\Delta x = 1$. Note that we consider space discretization on the whole spatial domain and then impose periodicity for technical simplicity in the convergence proof.

For velocity and internal energy variables, we use

$$\begin{aligned} v_j &\equiv (v_j^1, v_j^2, v_j^3) \equiv (j_1\Delta v, j_2\Delta v, j_3\Delta v), \quad (j_1, j_2, j_3) \in \mathbb{Z}^3, \\ I_k &= k\Delta I, \quad k = 0, 1, 2, \dots \end{aligned}$$

For later use, we denote the index sets of j and k by $\mathcal{J} := \mathbb{Z}^3$ and $\mathcal{K} := \{0, 1, 2, \dots\}$, respectively.

To be more concise, we introduce the following notations:

Definition 2.1. (1) Let $x(i, j) := x_i - v_j^1\Delta t$ and $s \equiv s(i, j)$ be the index such that

$$x(i, j) \in [x_s, x_{s+1}).$$

(2) Let $\tilde{f}_{i,j,k}^n$ be the linear interpolation of $f_{s,j,k}^n$ and $f_{s+1,j,k}^n$ on $x(i, j)$ at time t^n :

$$\tilde{f}_{i,j,k}^n := a_j f_{s,j,k}^n + (1 - a_j) f_{s+1,j,k}^n,$$

where $a_j := (x_{s+1} - x(i, j))/\Delta x$. Note that there is only j dependence on a_j due to the use of uniform grid in space variable.

2.2. Implicit semi-Lagrangian scheme

Our scheme reads

$$f_{i,j,k}^{n+1} = \frac{\kappa \tilde{f}_{i,j,k}^n + A_{\nu,\theta}\Delta t \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k}}{\kappa + A_{\nu,\theta}\Delta t}, \quad (2.1)$$

where $A_{\nu,\theta} := 1/(1 - \nu + \nu\theta)$ for $0 < \theta \leq 1$ and $-\frac{1}{2} < \nu < 1$, and

$$\tilde{f}_{i,j,k}^n := a_j f_{s,j,k}^n + (1 - a_j) f_{s+1,j,k}^n.$$

Note that a_j and s are defined in Definition 2.1. The discrete ellipsoidal Gaussian based on $\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n := \{\tilde{f}_{i,j,k}^n\}_{j \in \mathcal{J}, k \in \mathcal{K}}$ is given by

$$\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k} := \frac{\tilde{\rho}_i^n \Lambda_\delta}{\sqrt{\det(2\pi(\tilde{\mathcal{T}}_{\nu,\theta})_i^n)((\tilde{T}_\theta)_i^n)^{\frac{\delta}{2}}}} \exp\left(-\frac{(v_j - \tilde{U}_i^n)^\top ((\tilde{\mathcal{T}}_{\nu,\theta})_i^n)^{-1} (v_j - \tilde{U}_i^n)}{2} - \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n}\right), \quad (2.2)$$

with Λ_δ defined as (1.3). The macroscopic variables computed from $\{\tilde{f}_{i,j,k}^n\}$ are defined as follows:

– Mass:

$$\tilde{\rho}_i^n := \sum_{j,k} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I.$$

– Momentum:

$$\tilde{\rho}_i^n \tilde{U}_i^n := \sum_{j,k} \tilde{f}_{i,j,k}^n v_j (\Delta v)^3 \Delta I.$$

– Stress tensor:

$$\tilde{\rho}_i^n \tilde{\Theta}_i^n = \sum_{j,k} \tilde{f}_{i,j,k}^n (v_j - \tilde{U}_i^n) \otimes (v_j - \tilde{U}_i^n) (\Delta v)^3 \Delta I.$$

– Polyatomic temperature:

$$\left(\tilde{T}_\delta \right)_i^n = \frac{3}{3 + \delta} \left(\tilde{T}_{\text{tr}} \right)_i^n + \frac{\delta}{3 + \delta} \left(\tilde{T}_{I,\delta} \right)_i^n,$$

where

$$\left(\tilde{T}_{\text{tr}} \right)_i^n := \frac{2}{3} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{|v_j - \tilde{U}_i^n|^2}{2} (\Delta v)^3 \Delta I,$$

$$\left(\tilde{T}_{I,\delta} \right)_i^n := \frac{2}{\delta} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n I_k^{\frac{2}{\delta}} (\Delta v)^3 \Delta I.$$

– Relaxation temperature:

$$\left(\tilde{T}_\theta \right)_i^n := \theta \left(\tilde{T}_\delta \right)_i^n + (1 - \theta) \left(\tilde{T}_{I,\delta} \right)_i^n.$$

– Polyatomic temperature tensor:

$$\left(\tilde{T}_{\nu,\theta} \right)_i^n := \lambda \theta \left(\tilde{T}_\delta \right)_i^n Id + \lambda (1 - \theta) (1 - \nu) \left(\tilde{T}_{\text{tr}} \right)_i^n Id + (1 - \theta) \bar{\nu} \tilde{\Theta}_i^n. \quad (2.3)$$

For notational simplicity, we also introduce

$$\lambda \equiv \lambda(\nu, \theta, \kappa, \Delta t) := \frac{\kappa + A_{\nu,\theta} \Delta t}{\Delta t + \kappa}, \quad \bar{\nu} \equiv \bar{\nu}(\nu, \kappa, \Delta t) := \frac{\kappa \nu}{\Delta t + \kappa}.$$

Since the initial step can be taken to be arbitrarily correct, we assume for technical simplicity that the initial step is approximated as follows to guarantee that no error arises in the initial approximation of the initial data:

– Initial distribution:

$$f_{i,j,k}^0 = f_0(x_i, v_j, I_k), \quad \tilde{f}_{i,j,k}^0 = f_0(x_i - v_j^1 \Delta t, v_j, I_k).$$

– Mass:

$$\tilde{\rho}_i^0 = \int_{\mathbb{R}^3 \times \mathbb{R}_+} f_0(x_i - v^1 \Delta t, v, I) dv dI.$$

– Momentum:

$$\tilde{\rho}_i^0 \tilde{U}_i^0 = \int_{\mathbb{R}^3 \times \mathbb{R}_+} v f_0(x_i - v^1 \Delta t, v, I) dv dI.$$

– Stress tensor:

$$\tilde{\rho}_i^0 \tilde{\Theta}_i^0 = \int_{\mathbb{R}^3 \times \mathbb{R}_+} (v - \tilde{U}_i^0) \otimes (v - \tilde{U}_i^0) f_0(x_i - v^1 \Delta t, v, I) dv dI.$$

– Polyatomic temperature:

$$\left(\tilde{T}_\delta \right)_i^0 = \frac{3}{3 + \delta} \left(\tilde{T}_{\text{tr}} \right)_i^0 + \frac{\delta}{3 + \delta} \left(\tilde{T}_{I,\delta} \right)_i^0,$$

where

$$\begin{aligned} (\tilde{T}_{\text{tr}})_i^0 &:= \frac{2}{3} \frac{1}{\tilde{\rho}_i^0} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{|v - \tilde{U}_i^0|^2}{2} f_0(x_i - v^1 \Delta t, v, I) \, dv \, dI, \\ (\tilde{T}_{I,\delta})_i^0 &:= \frac{2}{\delta} \frac{1}{\tilde{\rho}_i^n} \int_{\mathbb{R}^3 \times \mathbb{R}_+} I^{\frac{2}{3}} f_0(x_i - v^1 \Delta t, v, I) \, dv \, dI. \end{aligned}$$

– Relaxation temperature:

$$(\tilde{T}_\theta)_i^0 := \theta (\tilde{T}_\delta)_i^0 + (1 - \theta) (\tilde{T}_{I,\delta})_i^0.$$

– Polyatomic temperature tensor:

$$(\tilde{T}_{\nu,\theta})_i^0 := \lambda \theta (\tilde{T}_\delta)_i^0 Id + \lambda (1 - \theta) (1 - \nu) (\tilde{T}_{\text{tr}})_i^0 Id + (1 - \theta) \nu \tilde{\Theta}_i^0.$$

where

$$\lambda \equiv \lambda(\nu, \theta, \kappa, \Delta t) := \frac{\kappa + A_{\nu,\theta} \Delta t}{\Delta t + \kappa}, \quad \bar{\nu} \equiv \bar{\nu}(\nu, \kappa, \Delta t) := \frac{\kappa \nu}{\Delta t + \kappa}. \quad (2.4)$$

2.3. Derivation of the first order scheme

Now we consider how the scheme (2.1) is derived. Throughout this paper, we focus on one-dimensional spatial domain ($d = 1$). We start from the backward characteristic of (1.1):

$$\begin{aligned} \frac{df}{ds} &= \frac{A_{\nu,\theta}}{\kappa} (\mathcal{M}_{\nu,\theta,\delta}(f) - f), \\ \frac{dx}{ds} &= v_j^1, \\ \frac{dv}{ds} &= \frac{dI}{ds} = 0, \end{aligned} \quad (2.5)$$

Here, one can easily have

$$x(s) \equiv x_i - v_j^1 (t^{n+1} - s), \quad v(s) \equiv v_j, \quad I(s) \equiv I_k.$$

To solve (2.5), considering the stiffness coming from κ , we apply the implicit Euler method:

$$\frac{f_{i,j,k}^{n+1} - \tilde{f}_{i,j,k}^n}{\Delta t} = \frac{A_{\nu,\theta}}{\kappa} \left(\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k} - f_{i,j,k}^{n+1} \right), \quad (2.6)$$

where the discrete ellipsoidal Gaussian is given by

$$\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k} = \frac{\rho_i^n \Lambda_\delta}{\sqrt{\det(2\pi (\mathcal{T}_{\nu,\theta})_i^n) ((T_\theta)_i^n)^{\frac{\delta}{2}}}} \exp \left(- \frac{(v_j - U_i^n)^\top ((\mathcal{T}_{\nu,\theta})_i^n)^{-1} (v_j - U_i^n)}{2} - \frac{I_k^{\frac{2}{3}}}{(T_\theta)_i^n} \right)$$

with the discrete normalizing factor:

$$\Lambda_\delta^{-1} = \sum_k e^{-I_k^{\frac{2}{3}}} \Delta I,$$

and the macroscopic fields defined similarly by replacing $\tilde{f}_{i,j,k}^n$ with $f_{i,j,k}^n$ in (2.3). However, the polyatomic temperature tensor $(\mathcal{T}_{\nu,\theta})_i^n$ is defined in a different way:

$$(\mathcal{T}_{\nu,\theta})_i^n := \theta (T_\delta)_i^n Id + (1 - \theta) (1 - \nu) (T_{\text{tr}})_i^n Id + (1 - \theta) \nu \Theta_i^n.$$

We note that (2.6) involves high computational cost since it is implicit form. To transform this implicit scheme into an explicitly computable scheme with beneficial stability properties preserved, we adopt the argument developed in [7, 22, 35, 42, 43] to our polyatomic setting.

We start with conservative quantities. We multiply both sides of (2.6) by collision invariants:

$$\phi_{j,k} := \left(1, v_j, \frac{1}{2}|v_j|^2 + I_k^{\frac{2}{\delta}} \right)$$

and take a summation over j, k to derive

$$\sum_{j,k} \left(f_{i,j,k}^{n+1} - \tilde{f}_{i,j,k}^n \right) \phi_{j,k} (\Delta v)^3 \Delta I = \sum_{j,k} \frac{A_{\nu,\theta} \Delta t}{\kappa} \left(\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k} - f_{i,j,k}^{n+1} \right) \phi_{j,k} (\Delta v)^3 \Delta I.$$

Since the right hand side vanishes for enough v and I nodes, we have

$$\begin{aligned} \rho_i^{n+1} &= \tilde{\rho}_i^n := \sum_{j,k} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I, \\ U_i^{n+1} &= \tilde{U}_i^n := \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n v_j (\Delta v)^3 \Delta I, \\ (E_\delta)_i^{n+1} &= (\tilde{E}_\delta)_i^n := \sum_{j,k} \tilde{f}_{i,j,k}^n \left(\frac{|v_j - \tilde{U}_i^n|^2}{2} + I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I. \end{aligned} \quad (2.7)$$

Using this, we approximate $(T_\delta)_i^{n+1}$, $(T_{\text{tr}})_i^{n+1}$ and $(T_{I,\delta})_i^{n+1}$ as follows:

$$\begin{aligned} (T_\delta)_i^{n+1} &= (\tilde{T}_\delta)_i^n := \frac{2}{3+\delta} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \left(\frac{|v_j - \tilde{U}_i^n|^2}{2} + I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I \\ (T_{\text{tr}})_i^{n+1} &= \frac{2}{3} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} f_{i,j,k}^{n+1} \frac{|v_j - \tilde{U}_i^n|^2}{2} (\Delta v)^3 \Delta I \\ &\approx \frac{2}{3} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{|v_j - \tilde{U}_i^n|^2}{2} (\Delta v)^3 \Delta I \\ &=: (\tilde{T}_{\text{tr}})_i^n, \\ (T_{I,\delta})_i^{n+1} &= \frac{2}{\delta} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} f_{i,j,k}^{n+1} I_k^{\frac{2}{\delta}} (\Delta v)^3 \Delta I \\ &\approx \frac{2}{\delta} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n I_k^{\frac{2}{\delta}} (\Delta v)^3 \Delta I \\ &=: (\tilde{T}_{I,\delta})_i^n. \end{aligned} \quad (2.8)$$

Note that the approximations for $(T_{\text{tr}})_i^{n+1}$ and $(T_{I,\delta})_i^{n+1}$ can be justified because we are considering a first order scheme. Now, we turn to the approximation of the stress tensor Θ_i^{n+1} . Although it is a non-conservative quantity, we can approximate it in a legitimate way as in [42]. For this, we introduce

$$\xi_{ij}^{n+1} := (v_j - U_i^{n+1}) \otimes (v_j - U_i^{n+1})$$

and multiply this to (2.6) to derive

$$\sum_{j,k} \left(f_{i,j,k}^{n+1} - \tilde{f}_{i,j,k}^n \right) \xi_{ij}^{n+1} (\Delta v)^3 \Delta I = \sum_{j,k} \frac{A_{\nu,\theta} \Delta t}{\kappa} \left(\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k} - f_{i,j,k}^{n+1} \right) \xi_{ij}^{n+1} (\Delta v)^3 \Delta I. \tag{2.9}$$

Recalling the relation $U_i^{n+1} = \tilde{U}_i^n$, we obtain

$$\xi_{ij}^{n+1} = (v_j - U_i^{n+1}) \otimes (v_j - U_i^{n+1}) = (v_j - \tilde{U}_i^n) \otimes (v_j - \tilde{U}_i^n) =: \tilde{\xi}_{ij}^n.$$

This implies that the second term on the left in (2.9) becomes

$$\sum_{j,k} \tilde{f}_{i,j,k}^n \xi_{ij}^{n+1} (\Delta v)^3 \Delta I = \sum_{j,k} \tilde{f}_{i,j,k}^n \tilde{\xi}_{ij}^n (\Delta v)^3 \Delta I = \tilde{\rho}_i^n \tilde{\Theta}_i^n, \tag{2.10}$$

where $\tilde{\Theta}_i^n$ is defined by

$$\tilde{\rho}_i^n \tilde{\Theta}_i^n = \sum_{j,k} \tilde{f}_{i,j,k}^n (v_j - \tilde{U}_i^n) \otimes (v_j - \tilde{U}_i^n) (\Delta v)^3 \Delta I.$$

On the other hand, the right hand side in (2.9) can be rewritten by

$$\begin{aligned} & \sum_{j,k} \frac{A_{\nu,\theta} \Delta t}{\kappa} \left(\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k} - f_{i,j,k}^{n+1} \right) \xi_{ij}^{n+1} (\Delta v)^3 \Delta I \\ &= \frac{A_{\nu,\theta} \Delta t}{\kappa} \left(\rho_i^{n+1} (\mathcal{T}_{\nu,\theta})_i^{n+1} - \rho_i^{n+1} \Theta_i^{n+1} \right) \\ &= \frac{A_{\nu,\theta} \Delta t}{\kappa} \left(\rho_i^{n+1} \left[\theta (T_\delta)_i^{n+1} Id + (1 - \theta) \left\{ (1 - \nu) (T_{tr})_i^{n+1} Id + \nu \Theta_i^{n+1} \right\} \right] - \rho_i^{n+1} \Theta_i^{n+1} \right) \\ &= \frac{A_{\nu,\theta} \Delta t}{\kappa} \left(\rho_i^{n+1} \left[\theta (T_\delta)_i^{n+1} + (1 - \nu) (1 - \theta) (T_{tr})_i^{n+1} \right] Id - \{ 1 - \nu + \nu \theta \} \rho_i^{n+1} \Theta_i^{n+1} \right) \\ &= \frac{\Delta t}{\kappa} \rho_i^{n+1} \left[A_{\nu,\theta} \theta (T_\delta)_i^{n+1} + (1 - A_{\nu,\theta} \theta) (T_{tr})_i^{n+1} \right] Id - \frac{\Delta t}{\kappa} \rho_i^{n+1} \Theta_i^{n+1}. \end{aligned} \tag{2.11}$$

In the last line, we use

$$A_{\nu,\theta} (1 - \theta) (1 - \nu) = \frac{(1 - \theta) (1 - \nu)}{1 - \nu + \nu \theta} = 1 - \frac{\theta}{1 - \nu + \nu \theta} = 1 - A_{\nu,\theta} \theta.$$

Then, we insert (2.10) and (2.11) into (2.9) to compute Θ_i^{n+1} as follows:

$$\Theta_i^{n+1} = \frac{\Delta t \left[A_{\nu,\theta} \theta \left(\tilde{T}_\delta \right)_i^n + (1 - A_{\nu,\theta} \theta) \left(\tilde{T}_{tr} \right)_i^n \right] Id + \kappa \tilde{\Theta}_i^n}{\Delta t + \kappa}.$$

Now, we use this and (2.8) to approximate the polyatomic stress tensor:

$$\begin{aligned} (\mathcal{T}_{\nu,\theta})_i^{n+1} &= \theta (T_\delta)_i^{n+1} Id + (1 - \theta) \left\{ (1 - \nu) (T_{tr})_i^{n+1} Id + \nu \Theta_i^{n+1} \right\} \\ &\approx \theta \left(\tilde{T}_\delta \right)_i^n Id + (1 - \theta) (1 - \nu) \left(\tilde{T}_{tr} \right)_i^n Id \\ &\quad + (1 - \theta) \nu \left[\frac{\Delta t \left[A_{\nu,\theta} \theta \left(\tilde{T}_\delta \right)_i^n + (1 - A_{\nu,\theta} \theta) \left(\tilde{T}_{tr} \right)_i^n \right] Id + \kappa \tilde{\Theta}_i^n}{\Delta t + \kappa} \right] \end{aligned}$$

$$\begin{aligned}
 &= \left(\theta + \frac{(1-\theta)\nu\Delta t A_{\nu,\theta}}{\Delta t + \kappa} \right) \left(\tilde{T}_\delta \right)_i^n Id \\
 &\quad + \left((1-\theta)(1-\nu) + \frac{(1-\theta)\nu\Delta t(1-A_{\nu,\theta})}{\Delta t + \kappa} \right) \left(\tilde{T}_{tr} \right)_i^n Id + (1-\theta)\nu \frac{\kappa \tilde{\Theta}_i^n}{\Delta t + \kappa}.
 \end{aligned}$$

We write it in a more compact manner

$$\left(\mathcal{T}_{\nu,\theta} \right)_i^{n+1} \approx \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n := \lambda \theta \left(\tilde{T}_\delta \right)_i^n Id + \lambda(1-\theta)(1-\nu) \left(\tilde{T}_{tr} \right)_i^n Id + (1-\theta)\bar{\nu} \tilde{\Theta}_i^n, \tag{2.12}$$

using

$$\lambda \equiv \lambda(\nu, \theta, \kappa, \Delta t) := \frac{\kappa + A_{\nu,\theta}\Delta t}{\Delta t + \kappa}, \quad \bar{\nu} \equiv \bar{\nu}(\nu, \kappa, \Delta t) := \frac{\kappa\nu}{\Delta t + \kappa}.$$

Similarly, we approximate $(T_\theta)_i^{n+1}$ as follows:

$$(T_\theta)_i^{n+1} \approx \left(\tilde{T}_\theta \right)_i^n := \theta \left(\tilde{T}_\delta \right)_i^n + (1-\theta) \left(\tilde{T}_{I,\delta} \right)_i^n. \tag{2.13}$$

In view of (2.7), (2.8), (2.12), (2.13), we find that $\mathcal{M}_{\nu,\theta,\delta} \left(f_{i,\mathcal{J},\mathcal{K}}^{n+1} \right)_{j,k}$ is legitimately replaced by $\mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k}$:

$$\mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k} := \frac{\tilde{\rho}_i^n \Lambda_\delta}{\sqrt{\det \left(2\pi \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n \right) \left(\left(\tilde{T}_\theta \right)_i^n \right)^{\frac{\delta}{2}}}} \exp \left(- \frac{\left(v_j - \tilde{U}_i^n \right)^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n \right)^{-1} \left(v_j - \tilde{U}_i^n \right)}{2} - \frac{I_k^{\frac{2}{\delta}}}{\left(\tilde{T}_\theta \right)_i^n} \right).$$

Finally, we substitute this into (2.6), and solve for $f_{i,j,k}^{n+1}$ to get our scheme:

$$f_{i,j,k}^{n+1} = \frac{\kappa \tilde{f}_{i,j,k}^n + A_{\nu,\theta}\Delta t \mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k}}{\kappa + A_{\nu,\theta}\Delta t}. \tag{2.14}$$

2.4. Reduction to monatomic semi-Lagrangian schemes

Before closing this section, we briefly review how our scheme can be reduced into corresponding monatomic schemes in [41, 42]. For $\theta = 0$, we get

$$\left(\tilde{\mathcal{T}}_{\nu,0} \right)_i^n = (1-\bar{\nu}) \left(\tilde{T}_{tr} \right)_i^n Id + \bar{\nu} \tilde{\Theta}_i^n.$$

After taking summation over k in (2.14), we obtain

$$g_{i,j}^{n+1} = \frac{\kappa \tilde{g}_{i,j}^n + A_{\nu,0}\Delta t \mathcal{M}_\nu \left(\tilde{g}_{i,\mathcal{J}}^n \right)}{\kappa + A_{\nu,0}\Delta t}, \tag{2.15}$$

where $g := \int_{\mathbb{R}^+} f dI$, $\tilde{g} := \int_{\mathbb{R}^+} \tilde{f} dI$, and $g_{i,j}^{n+1}$ and $\tilde{g}_{i,j}^n$ are discrete approximation of $g(x_i, v_j, t^{n+1})$ and $g(x_i - v^1\Delta t, v_j, t^n)$, respectively. Here the ellipsoidal Gaussian \mathcal{M}_ν is

$$\mathcal{M}_\nu \left(\tilde{g}_{i,\mathcal{J}}^n \right)_j := \frac{\tilde{\rho}_i^n}{\sqrt{\det \left(2\pi \left(\tilde{\mathcal{T}}_{\nu,0} \right)_i^n \right)}} \exp \left(- \frac{\left(v_j - \tilde{U}_i^n \right)^\top \left(\left(\tilde{\mathcal{T}}_{\nu,0} \right)_i^n \right)^{-1} \left(v_j - \tilde{U}_i^n \right)}{2} \right).$$

This scheme was proposed in [42] as a first order SL scheme for the monatomic ES-BGK model:

$$\begin{aligned} \frac{\partial g}{\partial t} + v \cdot \nabla_x g &= \frac{A_\nu}{\kappa} (\mathcal{M}_\nu(g) - g) \\ \mathcal{M}_\nu(g) &= \frac{\rho}{\sqrt{\det(2\pi\mathcal{T}_{\nu,0})}} \exp\left(-\frac{(v-U)^\top \mathcal{T}_{\nu,0}^{-1} (v-U)}{2}\right) \end{aligned}$$

where $A_\nu = \frac{1}{1-\nu}$. For $\theta = \nu = 0$, we have

$$\left(\tilde{\mathcal{T}}_{0,0}\right)_i^n = \left(\tilde{\mathcal{T}}_{\text{tr}}\right)_i^n Id.$$

Then, the ellipsoidal Gaussian \mathcal{M}_0 further reduces to the local Maxwellian \mathcal{M} :

$$\mathcal{M}(\tilde{g}_{i,\mathcal{J}}^n)_j := \frac{\tilde{\rho}_i^n}{\sqrt{\left(2\pi\left(\tilde{\mathcal{T}}_{\text{tr}}\right)_i^n\right)^3}} \exp\left(-\frac{|v_j - \tilde{U}_i^n|^2}{2\left(\tilde{\mathcal{T}}_{\text{tr}}\right)_i^n}\right),$$

and the resulting scheme becomes the first order SL scheme for the BGK model in [22, 40, 43]:

$$g_{i,j}^{n+1} = \frac{\kappa \tilde{g}_{i,j}^n + \Delta t \mathcal{M}(\tilde{g}_{i,\mathcal{J}}^n)_j}{\kappa + \Delta t}, \tag{2.16}$$

Although we do not explore the behavior of these SL schemes in the limit $\kappa \rightarrow 0$, it is also interesting to check if a kinetic scheme to BGK-type model becomes a consistent discretization to Euler-type system in the limit $\kappa \rightarrow 0$ at the discrete level. As related papers, we refer to [15, 20, 25].

3. MAIN RESULT

In this section, we present the explicit error estimate of our scheme measured in weighted $\|\cdot\|_{L_q^\infty}$ -norm. We state a theorem for the existence of classical solutions in [32], which is necessary for error estimates in following sections. In the following theorem, we take a final time $T^f > 0$.

Theorem 3.1 ([32]). *Let $-1/2 < \nu < 1$, $0 < \theta \leq 1$, $\delta > 0$, $q > 5 + \delta$. Suppose that the initial function f_0 satisfies the following two conditions:*

$$\begin{aligned} (1) \quad & \|f_0\|_{L_{2,q}^\infty} < \infty, \\ (2) \quad & f_0(x - vt, v, I) > C_0^1 e^{-C_0^2(|v|^a + I^b)}, \quad \text{for all } t \geq 0, \end{aligned} \tag{3.1}$$

for some constants $a, b, C_0^1, C_0^2 > 0$. Then, there exists a unique solution for (1.1) that satisfies

– (A1): f is uniformly bounded:

$$\|f(t)\|_{L_{2,q}^\infty} \leq C_{2,1} e^{C_{2,2}t} \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\}$$

for some positive constants $C_{2,1}$ and $C_{2,2}$.

– (A2): There exist positive constants C_{T^f, f_0} , $C_{T^f, f_0, \delta}$ and $C_{T^f, f_0, \delta, q}$ such that

$$\begin{aligned} \rho(x, t) &\geq C_{T^f, f_0}, \\ T_\delta(x, t) &\geq C_{T^f, f_0, \delta}, \\ \rho(x, t) + |U(x, t)| + T_\delta(x, t) &\leq C_{T^f, f_0, \delta, q}. \end{aligned}$$

Now, we state our main theorem.

Theorem 3.2. *Let $-1/2 < \nu < 1$, $0 < \theta \leq 1$, $0 < \delta \leq 2$ and $q > 5 + \delta$. Let f be the unique smooth solution of (1.1) corresponding to the initial data f_0 satisfying two initial conditions in Theorem 3.1 and $\|f_0\|_{L_{1,q+1}^\infty} < \infty$. For a positive $r_{\Delta v, \Delta I} > 0$ given in Theorem 4.5, assume that Δv and ΔI satisfy*

$$\Delta v, \Delta I < r_{\Delta v, \Delta I}.$$

Then, the discrete solution $f_{i,j,k}^n$ constructed from (2.1) satisfies the following explicit error estimate:

$$\|f^{N_t} - f(T^f)\|_{L_q^\infty} \leq C \left(\frac{(\Delta x)^2}{\Delta t} + (\Delta x)^2 + \Delta v + \Delta I + \Delta t \right)$$

where C is a constant depending on $T^f, q, \delta, \kappa, \theta, \nu, \Delta t$, but can be uniformly bounded regardless of $\Delta t > 0$.

Remark 3.3. (1) The value of $r_{\Delta v, \Delta I}$ is given in Theorem 4.5. (2) The constant C in the error bound blows up as $\kappa \rightarrow 0$.

There are three important estimates using L_q^∞ -norm, which play the key role in the proof of Theorem 3.2. (1) The first estimate is for the remainder terms R_1, R_2 defined as (5.2) (Lem. 5.6), which appears when we subtract the continuous solutions (5.1) from the discrete ones (2.14). (2) The second estimate is for the discrepancy between the continuous and the discrete distribution functions located on the characteristic feet (Lem. 6.1). (3) The third one is the discrepancy between continuous and discrete ellipsoidal Gaussian in Proposition 6.4. These results will enable us to derive a recurrence form of error estimate in the proof. We also note that stability estimates in Theorem 4.5 are the starting point of all these results.

4. STABILITY OF THE DISCRETE DISTRIBUTION FUNCTION

The goal of this section is to show that the numerical solutions and its corresponding macroscopic quantities are uniformly bounded. In Definition 4.1, we first define three constants which will be used throughout this section. Then, in Definitions 4.2 and 4.4, we state main stability estimates E^n and necessary quantities for Theorem 4.5. In order to prove Theorem 4.5, we will use an induction argument. For this, in Lemmas 4.6–4.9, we establish several technical estimates which discrete macroscopic quantities satisfy. Then, from Lemmas 4.6 to 4.9, we show that the main estimate E^0 holds for initial data (Lem. 4.11). Finally, in Lemmas 4.12–4.15, we show that E^{n-1} implies E^n , which proves Theorem 4.5.

We begin with the definition of three constants.

Definition 4.1. We define constants $\bar{C}_{a,b}, \bar{C}_{a,b,q,\delta}$ and $\bar{C}_{\delta,q-m}$ by

$$\begin{aligned} \bar{C}_{a,b} &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} e^{-C_0^2(|v|^a + I^b)} \, dv \, dI, \\ \bar{C}_{a,b,q,\delta} &:= \sup_{v,I} e^{-C_0^2(|v|^a + I^b)} \left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}, \\ \bar{C}_{\delta,q-m} &:= \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{1}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q-m}{2}}} \, dv \, dI, \quad q - m > \max(2, \delta) \end{aligned}$$

where a, b, m, q are constants and C_0^2 is defined in (3.1).

In the following, we introduce the main stability estimates of this section as E^n .

Definition 4.2. For $n \geq 1$, we say that

(1) $f_{i,j,k}^n$ satisfies E_1^n , if A^n and B^n hold:

$$\begin{aligned} (A^n) \quad & \left\| \tilde{f}_{i,j,k}^n \right\|_{L_q^\infty} \leq \left(\frac{\kappa + A_{\nu,\theta} \Delta t C_{\mathcal{M}}}{\kappa + A_{\nu,\theta} \Delta t} \right)^n \|f_0\|_{L_q^\infty} \leq e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f} \|f_0\|_{L_q^\infty}, \\ (B^n) \quad & \tilde{f}_{i,j,k}^n \geq \left(\frac{\kappa}{\kappa + A_{\nu,\theta} \Delta t} \right)^n C_0^1 e^{-C_0^2 (|v_j|^a + I_k^b)} \geq e^{-\frac{A_{\nu,\theta}}{\kappa} T^f} C_0^1 e^{-C_0^2 (|v_j|^a + I_k^b)}. \end{aligned}$$

(2) $f_{i,j,k}^n$ satisfies E_2^n , if C^n and D^n hold:

$$\begin{aligned} (C^n) \quad & \tilde{\rho}_i^n \geq \frac{1}{2} \bar{C}_{a,b} C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f} =: \tilde{\rho}_{\text{lower}}, \\ & \left(\tilde{T}_\delta \right)_i^n \geq \left(\frac{1}{2} \frac{\bar{C}_{a,b} C_0^1}{C_\delta \|f_0\|_{L_q^\infty}} e^{-\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa + A_{\nu,\theta} \Delta t}\right) A_{\nu,\theta} T^f} \right)^{\frac{2}{3+\delta}} =: \left(\tilde{T}_\delta \right)_{\text{lower}}. \\ (D^n) \quad & \|\tilde{\rho}^n\|_{L_x^\infty} \leq 2 \bar{C}_{\delta,q} e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f} \|f_0\|_{L_q^\infty} =: \tilde{\rho}_{\text{upper}}, \\ & \left\| \tilde{U}^n \right\|_{L_x^\infty} \leq \frac{4 \bar{C}_{\delta,q-1}}{\bar{C}_{a,b} C_0^1} e^{\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa + A_{\nu,\theta} \Delta t}\right) A_{\nu,\theta} T^f} \|f_0\|_{L_q^\infty} =: \tilde{U}_{\text{upper}}, \\ & \left\| \left(\tilde{T}_\delta \right)^n \right\|_{L_x^\infty} \leq \frac{8}{3 + \delta} \frac{\bar{C}_{\delta,q-2}}{\bar{C}_{a,b} C_0^1} e^{\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa + A_{\nu,\theta} \Delta t}\right) A_{\nu,\theta} T^f} \|f_0\|_{L_q^\infty} =: \left(\tilde{T}_\delta \right)_{\text{upper}}. \end{aligned}$$

(3) We define $E^n = E_1^n \wedge E_2^n$.

Remark 4.3. The constants C_0^1 and C_0^2 are defined in (3.1). Also, the definition of $C_{\mathcal{M}}$ is given in Lemma 4.9.

Before stating the main result of this section, we define three technical constants.

Definition 4.4. We define a_1, a_2 and a_3 by

$$\begin{aligned} a_1 &:= \left(\frac{1}{2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}}} \frac{\tilde{\rho}_{\text{lower}} \left(\tilde{T}_\delta \right)_{\text{lower}} e^{-\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f}}{\|f_0\|_{L_q^\infty}} \right)^{\frac{1}{5+\delta}}, \\ a_2 &:= \left(\frac{q - \delta - 5}{2^{-\frac{2+\delta}{2}} \pi^2 (3 + \delta)^{\frac{3+\delta}{2}}} \frac{\tilde{\rho}_{\text{lower}} e^{-\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f}}{\|f_0\|_{L_q^\infty}} \right)^{\frac{1}{\delta+3-q}}, \\ a_3 &:= \left(\frac{1}{2^{\frac{8+\delta-q}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta-q}{2}}} \frac{\tilde{\rho}_{\text{lower}} \left(\tilde{T}_\delta \right)_{\text{lower}}^q e^{-\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f}}{\|f_0\|_{L_q^\infty}} \right)^{\frac{1}{3+\delta+q}}. \end{aligned}$$

Now, we state the main stability estimate of this section, which will be crucially used when we estimate the discrepancy between the continuous ellipsoidal Gaussian and discrete one in Proposition 6.4.

Theorem 4.5. Choose $l > 0$ small enough so that $\Delta v, \Delta I < l$ satisfies

$$\begin{aligned} \frac{1}{2} \bar{C}_{a,b} &< \sum_{j,k} e^{-C_0^2 (|v_j|^a + I_k^b)} (\Delta v)^3 \Delta I < 2 \bar{C}_{a,b}, \\ \frac{1}{2} \bar{C}_{a,b,q,\delta} &< \sup_{j,k} e^{-C_0^2 (|v_j|^a + I_k^b)} \left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}} \right)^{\frac{q}{2}} < 2 \bar{C}_{a,b,q,\delta}, \\ \frac{1}{2} \bar{C}_{\delta,q-m} &< \sum_{j,k} \frac{1}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}} \right)^{\frac{q-m}{2}}} (\Delta v)^3 \Delta I < 2 \bar{C}_{\delta,q-m}, \end{aligned} \tag{4.1}$$

and

$$\begin{aligned} \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R + \Delta v + \Delta I} (\Delta v)^3 \Delta I &\leq \int_{\mathcal{A}(v, \tilde{U}_i^n, I) \leq 2(R + \Delta v + \Delta I)} dv dI, \\ \sum_{\mathcal{A}(v_j, 0, I_k) > R + 2\Delta v + 2\Delta I} \frac{1}{|\mathcal{A}(v_j, 0, I_k)|^{q-2}} (\Delta v)^3 \Delta I &\leq \int_{\mathcal{A}(v, 0, I) > R + \Delta v + \Delta I} \frac{1}{|\mathcal{A}(v, 0, I)|^{q-2}} dv dI, \end{aligned} \tag{4.2}$$

where

$$\mathcal{A}(a, b, c) := \left(\frac{1}{3 + \delta} |a - b|^2 + \frac{2}{3 + \delta} c^{\frac{2}{\delta}} \right)^{\frac{1}{2}}.$$

Also, assume that Δv and ΔI satisfies

$$\Delta v + \Delta I < \min \left(a_1, a_2, a_3, l, \frac{1}{2} \right) =: r_{\Delta v, \Delta I}, \tag{4.3}$$

where a_1, a_2, a_3 are defined in Definition 4.4. Then, $f_{i,j,k}^n$ satisfies E^n for all $n \geq 0$.

Since several technical lemmas have to be established, we postpone the proof of this theorem to the end of this section.

In the following Lemmas 4.6–4.8, we provide series of estimates for discrete macroscopic quantities.

Lemma 4.6. Assume $f_{i,j,k}^n$ satisfies E^n and the condition (4.3) holds. Then,

$$\tilde{\rho}_i^n \leq C_\delta \|f^n\|_{L_q^\infty} \left(\left(\tilde{T}_\delta \right)_i^n \right)^{\frac{3+\delta}{2}},$$

where

$$C_\delta = 2^{\frac{13+2\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}}.$$

Proof. We first divide the macroscopic density $\tilde{\rho}_i^n$ into two parts:

$$\begin{aligned} \tilde{\rho}_i^n &= \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) > R + \Delta v + \Delta I} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I + \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R + \Delta v + \Delta I} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I \\ &\equiv \mathcal{I}_{11} + \mathcal{I}_{12}. \end{aligned}$$

The first term \mathcal{I}_{11} is bounded by

$$\begin{aligned} \mathcal{I}_{11} &= \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) > R + \Delta v + \Delta I} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I \\ &\leq \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) > R + \Delta v + \Delta I} \tilde{f}_{i,j,k}^n \frac{\frac{1}{3+\delta} |v_j - \tilde{U}_i^n|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}}}{(R + \Delta v + \Delta I)^2} (\Delta v)^3 \Delta I \\ &\leq \frac{1}{(R + \Delta v + \Delta I)^2} \tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n. \end{aligned}$$

Since Δv and ΔI satisfy (4.2), we can bound \mathcal{I}_{12} by

$$\mathcal{I}_{12} = \sum_{\frac{1}{3+\delta} |v_j - \tilde{U}_i^n|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \leq (R + \Delta v + \Delta I)^2} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I$$

$$\leq \left(\int_{\frac{1}{3+\delta} |v - \tilde{U}_i^n|^2 + \frac{2}{3+\delta} I^{\frac{2}{\delta}} \leq 4(R + \Delta v + \Delta I)^2} dv dI \right) \|\tilde{f}^n\|_{L_q^\infty}. \tag{4.4}$$

To calculate the definite integral in (4.4), we use a change of variable:

$$\left(\sqrt{\frac{1}{3+\delta}} (v - \tilde{U}_i^n), \sqrt{\frac{2}{3+\delta}} I^{\frac{1}{\delta}} \right) = (r \sin \varphi \cos \theta \sin k, r \sin \varphi \sin \theta \sin k, r \cos \varphi \sin k, r \cos k),$$

where

$$0 \leq r \leq 2(R + \Delta v + \Delta I), \quad 0 \leq \varphi \leq \pi, \quad 0 \leq \theta \leq 2\pi, \quad 0 \leq k \leq \frac{\pi}{2}.$$

Then, the Jacobian is given by

$$\left| \frac{\partial \left(v^1 - (\tilde{U}_i^n)^1, v^2 - (\tilde{U}_i^n)^2, v^3 - (\tilde{U}_i^n)^3, I \right)}{\partial(r, \varphi, \theta, k)} \right| = 2^{-\frac{\delta}{2}} (3 + \delta)^{\frac{3+\delta}{2}} \delta r^{\delta+2} |\sin \varphi \cos^{\delta-1} k \sin^2 k|,$$

and we have

$$\mathcal{I}_{12} \leq \|\tilde{f}^n\|_{L_q^\infty} 2^{-\frac{\delta}{2}} (3 + \delta)^{\frac{3+\delta}{2}} \int_0^{\frac{\pi}{2}} \int_0^\pi \int_0^{2\pi} \int_0^{2(R + \Delta v + \Delta I)} \delta r^{\delta+2} |\sin \varphi \cos^{\delta-1} k \sin^2 k| dr d\theta d\varphi dk.$$

Using

$$\begin{aligned} \int_0^{\frac{\pi}{2}} \delta |\cos^{\delta-1} k \sin^2 k| dk &\leq \int_0^{\frac{\pi}{2}} \delta \cos^{\delta-1} k \sin k dk = 1, \\ \int_0^\pi |\sin \varphi| d\varphi &\leq \pi, \quad \int_0^{2\pi} d\theta \leq 2\pi, \\ \int_0^{2(R + \Delta v + \Delta I)} r^{\delta+2} dr &\leq \frac{1}{3 + \delta} (2(R + \Delta v + \Delta I))^{3+\delta}, \end{aligned}$$

we obtain

$$\begin{aligned} \mathcal{I}_{12} &\leq \|\tilde{f}^n\|_{L_q^\infty} \left\{ 2^{-\frac{\delta}{2}} (3 + \delta)^{\frac{3+\delta}{2}} \frac{2\pi^2}{3 + \delta} \right\} (2(R + \Delta v + \Delta I))^{3+\delta} \\ &= \|\tilde{f}^n\|_{L_q^\infty} \left\{ 2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\} (R + \Delta v + \Delta I)^{3+\delta}. \end{aligned}$$

Combining the estimates for \mathcal{I}_{11} and \mathcal{I}_{12} , we derive

$$\tilde{\rho}_i^n \leq \frac{1}{(R + \Delta v + \Delta I)^2} \tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n + \left\{ 2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\} (R + \Delta v + \Delta I)^{3+\delta} \|\tilde{f}^n\|_{L_q^\infty}.$$

Here, we equates two terms on the upper bound so that the bound can be minimized. That is, the number R is taken by

$$R + \Delta v + \Delta I = \left(\frac{\tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n}{2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \|\tilde{f}^n\|_{L_q^\infty}} \right)^{\frac{1}{5+\delta}} \geq a_1 > \Delta v + \Delta I,$$

where a_1 is given in Definition 4.4 and the last inequality holds due to (4.3). With the choice of such $R > 0$, we have

$$\tilde{\rho}_i^n \leq 2 \left\{ 2^{\frac{8+\delta}{2}} \pi^2 (3+\delta)^{\frac{1+\delta}{2}} \right\}^{\frac{2}{5+\delta}} \|\tilde{f}^n\|_{L_q^\infty}^{\frac{2}{5+\delta}} \left\{ \tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n \right\}^{\frac{3+\delta}{5+\delta}}.$$

This, together with Lemma A.1, gives

$$\tilde{\rho}_i^n \leq \left\{ 2^{\frac{13+2\delta}{2}} \pi^2 (3+\delta)^{\frac{1+\delta}{2}} \right\} \|f^n\|_{L_q^\infty} \tilde{T}_\delta^{\frac{3+\delta}{2}},$$

which completes the proof. □

Lemma 4.7. *Let $q > 5 + \delta$. Suppose further that $f_{i,j,k}^n$ satisfies E^n and $\Delta v, \Delta I$ satisfy the condition (4.3). Then,*

$$\tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i^n + \left| \tilde{U}_i^n \right|^2 \right)^{\frac{q-\delta-3}{2}} \leq C_{\delta,q,1} \|f^n\|_{L_q^\infty},$$

where

$$C_{\delta,q,1} = \left\{ \frac{2^{\frac{q-2\delta-5}{2}} \pi^2 (3+\delta)^{\frac{q}{2}}}{q-\delta-5} \right\}.$$

Proof. We start by splitting the following quantity into two parts:

$$\begin{aligned} \tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i^n + \frac{1}{3+\delta} \left| \tilde{U}_i^n \right|^2 \right) &= \sum_{\mathcal{A}(v_j, 0, I_k) > R+2\Delta v+2\Delta I} \left(\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right) \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I \\ &+ \sum_{\mathcal{A}(v_j, 0, I_k) \leq R+2\Delta v+2\Delta I} \left(\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right) \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I \\ &= \mathcal{I}_{21} + \mathcal{I}_{22}. \end{aligned} \tag{4.5}$$

The second term \mathcal{I}_{22} is bounded by

$$\mathcal{I}_{22} \leq 4(R + \Delta v + \Delta I)^2 \tilde{\rho}_i^n. \tag{4.6}$$

For \mathcal{I}_{21} , we extract $\|f^n\|_{L_q^\infty}$ out of the summation:

$$\begin{aligned} \mathcal{I}_{21} &\leq \sum_{\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} > (R+2\Delta v+2\Delta I)^2} \frac{\left(\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right)^{\frac{q}{2}}}{\left(\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right)^{\frac{q-2}{2}}} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I \\ &\leq \|\tilde{f}^n\|_{L_q^\infty} \sum_{\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} > (R+2\Delta v+2\Delta I)^2} \frac{1}{\left(\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right)^{\frac{q-2}{2}}} (\Delta v)^3 \Delta I. \end{aligned}$$

As in Lemma 4.6, the condition (4.2) makes it possible to estimate the above discrete summation by a definite integral using a change of variable:

$$\left(\sqrt{\frac{1}{3+\delta}} v, \sqrt{\frac{2}{3+\delta}} I_k^{\frac{1}{\delta}} \right) = (r \sin \varphi \cos \theta \sin k, r \sin \varphi \sin \theta \sin k, r \cos \varphi \sin k, r \cos k).$$

Then, we get

$$\begin{aligned}
 \mathcal{I}_{21} &\leq \|\tilde{f}^n\|_{L_q^\infty} \int_0^{\frac{\pi}{2}} \int_0^\pi \int_0^{2\pi} \int_{R+\Delta v+\Delta I}^\infty \frac{\delta(3+\delta)^{\frac{3}{2}} \left(\frac{3+\delta}{2}\right)^{\frac{\delta}{2}} r^{\delta+2} |\sin \varphi \cos^{\delta-1} k \sin^2 k|}{r^{q-2}} dr d\theta d\varphi dk \\
 &\leq \|\tilde{f}^n\|_{L_q^\infty} \left\{ \frac{2\pi^2(3+\delta)^{\frac{3}{2}} \left(\frac{3+\delta}{2}\right)^{\frac{\delta}{2}}}{q-\delta-5} \right\} (R+\Delta v+\Delta I)^{\delta+5-q} \\
 &= \|\tilde{f}^n\|_{L_q^\infty} \left\{ \frac{2^{\frac{2-\delta}{2}} \pi^2(3+\delta)^{\frac{3+\delta}{2}}}{q-\delta-5} \right\} (R+\Delta v+\Delta I)^{\delta+5-q}.
 \end{aligned} \tag{4.7}$$

Combining (4.6) and (4.7), we estimate (4.5) by

$$\tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i^n + \frac{1}{3+\delta} |\tilde{U}_i^n|^2 \right) \leq 4\tilde{\rho}_i^n (R+\Delta v+\Delta I)^2 + \left\{ \frac{2^{\frac{2-\delta}{2}} \pi^2(3+\delta)^{\frac{3+\delta}{2}}}{q-\delta-5} \right\} \|\tilde{f}^n\|_{L_q^\infty} (R+\Delta v+\Delta I)^{\delta+5-q}.$$

To get an optimal bound, we equate two terms on the upper bound to derive

$$R+\Delta v+\Delta I = \left(\frac{q-\delta-5}{2^{-\frac{2+\delta}{2}} \pi^2(3+\delta)^{\frac{3+\delta}{2}}} \frac{\tilde{\rho}_i^n}{\|\tilde{f}^n\|_{L_q^\infty}} \right)^{\frac{1}{\delta+3-q}} \geq a_2 > \Delta v+\Delta I,$$

where such R can be chosen due to the existence of a_2 given in Definition 4.4. Then,

$$\tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i^n + \frac{1}{3+\delta} |\tilde{U}_i^n|^2 \right) \leq 2 \left\{ \frac{2^{-\frac{2+\delta}{2}} \pi^2(3+\delta)^{\frac{3+\delta}{2}}}{q-\delta-5} \right\}^{\frac{2}{q-\delta-3}} (\tilde{\rho}_i^n)^{\frac{\delta+5-q}{\delta+3-q}} \|\tilde{f}^n\|_{L_q^\infty}^{\frac{2}{q-\delta-3}}.$$

Consequently,

$$\begin{aligned}
 \tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i^n + |\tilde{U}_i^n|^2 \right)^{\frac{q-\delta-3}{2}} &\leq \{2(3+\delta)\}^{\frac{q-\delta-3}{2}} \left\{ \frac{2^{-\frac{2+\delta}{2}} \pi^2(3+\delta)^{\frac{3+\delta}{2}}}{q-\delta-5} \right\} \|\tilde{f}^n\|_{L_q^\infty} \\
 &= \left\{ \frac{2^{\frac{q-2\delta-5}{2}} \pi^2(3+\delta)^{\frac{q}{2}}}{q-\delta-5} \right\} \|\tilde{f}^n\|_{L_q^\infty}.
 \end{aligned}$$

Combined with Lemma A.1, this gives the desired estimate. □

Lemma 4.8. Assume that $f_{i,j,k}^n$ satisfies E^n and $\Delta v, \Delta I$ satisfy the condition (4.3). Then,

$$\frac{\tilde{\rho}_i^n |\tilde{U}_i^n|^{3+\delta+q}}{\left(\left(\left(\tilde{T}_\delta \right)_i^n + |\tilde{U}_i^n|^2 \right) \left(\tilde{T}_\delta \right)_i^n \right)^{\frac{3+\delta}{2}}} \leq C_{\delta,q,2} \|f^n\|_{L_q^\infty},$$

where

$$C_{\delta,q,2} = 2^{\frac{17+3\delta+2q}{2}} \pi^2(3+\delta)^{2+\delta}.$$

Proof. We split the macroscopic momentum into two parts:

$$\left| \tilde{\rho}_i^n \tilde{U}_i^n \right| \leq \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R+\Delta v+\Delta I} \tilde{f}_{i,j}^n |v_j| (\Delta v)^3 \Delta I + \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) > R+\Delta v+\Delta I} \tilde{f}_{i,j}^n |v_j| (\Delta v)^3 \Delta I$$

$$\equiv \mathcal{I}_{31} + \mathcal{I}_{32}.$$

We first use Hölder's inequality to obtain

$$\begin{aligned} \mathcal{I}_{31} &\leq \left| \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R + \Delta v + \Delta I} \tilde{f}_{i,j}^n (\Delta v)^3 \Delta I \right|^{1 - \frac{1}{q}} \left| \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R + \Delta v + \Delta I} \tilde{f}_{i,j}^n |v_j|^q (\Delta v)^3 \Delta I \right|^{\frac{1}{q}} \\ &\leq (\tilde{\rho}_i^n)^{1 - \frac{1}{q}} \|\tilde{f}^n\|_{L_q^\infty}^{\frac{1}{q}} \left| \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R + \Delta v + \Delta I} (\Delta v)^3 \Delta I \right|^{\frac{1}{q}}. \end{aligned}$$

Then, we use the condition (4.2) to get

$$\begin{aligned} \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) \leq R + \Delta v + \Delta I} (\Delta v)^3 \Delta I &\leq \int_{\frac{3}{3+\delta}|v|^2 + \frac{2}{3+\delta}I_k^{\frac{2}{\delta}} \leq 4(R + \Delta v + \Delta I)^2} dv dI \\ &\leq \left\{ 2^{\frac{2-\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\} 2^{3+\delta} (R + \Delta v + \Delta I)^{3+\delta}, \end{aligned}$$

which gives

$$\mathcal{I}_{31} \leq (\tilde{\rho}_i^n)^{1 - \frac{1}{q}} \|\tilde{f}^n\|_{L_q^\infty}^{\frac{1}{q}} \left\{ 2^{\frac{2-\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\}^{\frac{1}{q}} 2^{\frac{3+\delta}{q}} (R + \Delta v + \Delta I)^{\frac{3+\delta}{q}}.$$

On the other hand, \mathcal{I}_{32} satisfies

$$\mathcal{I}_{32} \leq \sum_{\mathcal{A}(v_j, \tilde{U}_i^n, I_k) > R + \Delta v + \Delta I} \tilde{f}_{i,j}^n |v_j| \frac{\left(\frac{1}{3+\delta} |v_j - \tilde{U}_i^n|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right)^{\frac{1}{2}}}{R + \Delta v + \Delta I} (\Delta v)^3 \Delta I.$$

Here, we use Hölder's inequality to obtain

$$\begin{aligned} \mathcal{I}_{32} &\leq \frac{\sqrt{2(3+\delta)}}{R + \Delta v + \Delta I} \left\{ \sum_{j,k} \tilde{f}_{i,j}^n \left(\frac{1}{3+\delta} |v_j|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I \right\}^{\frac{1}{2}} \\ &\quad \times \left\{ \sum_{j,k} \tilde{f}_{i,j}^n \left(\frac{1}{3+\delta} |v_j - \tilde{U}_i^n|^2 + \frac{2}{3+\delta} I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I \right\}^{\frac{1}{2}} \\ &= \frac{\sqrt{2(3+\delta)}}{R + \Delta v + \Delta I} \left\{ \frac{1}{3+\delta} \tilde{\rho}_i^n |\tilde{U}_i^n|^2 + \tilde{\rho}_i^n (\tilde{T}_\delta)_i^n \right\}^{\frac{1}{2}} \left\{ \tilde{\rho}_i^n (\tilde{T}_\delta)_i^n \right\}^{\frac{1}{2}}. \end{aligned}$$

To sum up, we have

$$\begin{aligned} \left| \tilde{\rho}_i^n \tilde{U}_i^n \right| &\leq (\tilde{\rho}_i^n)^{1 - \frac{1}{q}} \|\tilde{f}^n\|_{L_q^\infty}^{\frac{1}{q}} \left\{ 2^{\frac{2-\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\}^{\frac{1}{q}} 2^{\frac{3+\delta}{q}} (R + \Delta v + \Delta I)^{\frac{3+\delta}{q}} \\ &\quad + \frac{\sqrt{2(3+\delta)}}{R + \Delta v + \Delta I} \left\{ \tilde{\rho}_i^n |\tilde{U}_i^n|^2 + \tilde{\rho}_i^n (\tilde{T}_\delta)_i^n \right\}^{\frac{1}{2}} \left\{ \tilde{\rho}_i^n (\tilde{T}_\delta)_i^n \right\}^{\frac{1}{2}}. \end{aligned} \tag{4.8}$$

To optimize the upper bound in (4.8), we take $R > 0$ such that

$$R + \Delta v + \Delta I = \left(\frac{\{2(3 + \delta)\}^{\frac{q}{2}} \tilde{\rho}_i^n \left\{ \left(|\tilde{U}_i^n|^2 + (\tilde{T}_\delta)_i^n \right) (\tilde{T}_\delta)_i^n \right\}^{\frac{q}{2}}}{\left\{ 2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\} \|\tilde{f}^n\|_{L_q^\infty}} \right)^{\frac{1}{3+\delta+q}} \geq a_3 > \Delta v + \Delta I.$$

The number a_3 is given in Definition 4.4. Then, the upper bound of (4.8) is simplified to

$$2 \left(\left\{ 2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\} \{2(3 + \delta)\}^{\frac{3+\delta}{2}} (\tilde{\rho}_i^n)^{2+\delta+q} \left\{ \left(|\tilde{U}_i^n|^2 + (\tilde{T}_\delta)_i^n \right) (\tilde{T}_\delta)_i^n \right\}^{\frac{3+\delta}{2}} \|\tilde{f}^n\|_{L_q^\infty} \right)^{\frac{1}{3+\delta+q}},$$

from which we conclude that

$$\begin{aligned} \frac{\tilde{\rho}_i^n |\tilde{U}_i^n|^{3+\delta+q}}{\left[\left(|\tilde{U}_i^n|^2 + (\tilde{T}_\delta)_i^n \right) (\tilde{T}_\delta)_i^n \right]^{\frac{3+\delta}{2}}} &\leq 2^{3+\delta+q} \{2(3 + \delta)\}^{\frac{3+\delta}{2}} \left\{ 2^{\frac{8+\delta}{2}} \pi^2 (3 + \delta)^{\frac{1+\delta}{2}} \right\} \|\tilde{f}^n\|_{L_q^\infty} \\ &= 2^{\frac{17+3\delta+2q}{2}} \pi^2 (3 + \delta)^{2+\delta} \|\tilde{f}^n\|_{L_q^\infty}. \end{aligned}$$

From Lemma A.1, we finally obtain the desired estimate. □

Based on the estimates in Lemmas 4.6–4.8, we now show that the ellipsoidal Gaussian is bounded by the discrete distribution in L_q^∞ -norm.

Lemma 4.9. *Let $q > 5 + \delta$. Suppose further that $f_{i,j,k}^n$ satisfies E^n and $\Delta v, \Delta I$ satisfy the condition (4.3). Then,*

$$\left\| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^n) \right\|_{L_q^\infty} \leq C_{\mathcal{M}} \|f^n\|_{L_q^\infty},$$

where $C_{\mathcal{M}}$ depending on ν, δ, θ and q .

Remark 4.10. In the proof, it will be shown that $C_{\mathcal{M}}$ blows up as θ tends to 0 because $C_{\mathcal{M}} \propto 1/\theta^{\frac{3+\delta}{2}}$.

Proof. We will show that $\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k}$, $|v_j|^q \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k}$ and $I_k^{\frac{q}{\delta}} \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k}$ are controlled by $\|f^n\|_{L_q^\infty}$, respectively.

(a) **The estimate for $\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k}$** : we first use Lemma A.2 to get

$$\frac{1}{2} (v_j - \tilde{U}_i^n)^\top \left((\tilde{T}_{\nu,\theta}_i)^n \right)^{-1} (v_j - \tilde{U}_i^n) + \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n} \geq \frac{3}{2 \lambda C_\nu \{3 + \delta(1 - \theta)\}} \frac{|v_j - \tilde{U}_i^n|^2}{(\tilde{T}_\delta)_i^n} + \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n} \geq 0. \quad (4.9)$$

Next, we recall the relation (1) in Lemma A.2, which implies that the eigenvalues of $(\tilde{T}_{\nu,\theta}_i)^n$ lie between $\lambda\theta(\tilde{T}_\delta)_i^n$ and $\frac{1}{3}\lambda C_\nu \{3 + \delta(1 - \theta)\}(\tilde{T}_\delta)_i^n$. Then, the determinant of $(\tilde{T}_{\nu,\theta}_i)^n$ satisfies

$$\left(\lambda\theta(\tilde{T}_\delta)_i^n \right)^3 \leq \det \left\{ (\tilde{T}_{\nu,\theta}_i)^n \right\}.$$

To sum up, we obtain

$$\begin{aligned}
\mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k} &\leq \frac{\tilde{\rho}_i^n \Lambda_\delta}{\sqrt{\det\left(2\pi\left(\tilde{T}_{\nu,\theta}\right)_i\right)\left(\left(\tilde{T}_\theta\right)_i\right)^{\frac{\delta}{2}}}} \\
&\leq \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \frac{1}{(2\pi)^{3/2}} \frac{\Lambda_\delta}{\theta^{\frac{3+\delta}{2}}} \frac{\tilde{\rho}_i^n}{\left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{3+\delta}{2}}} \\
&\leq \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \frac{1}{(2\pi)^{3/2}} \frac{\Lambda_\delta}{\theta^{\frac{3+\delta}{2}}} \left\{2^{\frac{13+2\delta}{2}} \pi^2 (3+\delta)^{\frac{1+\delta}{2}}\right\} \|f^n\|_{L_q^\infty}. \tag{4.10}
\end{aligned}$$

(b) **The estimate for $\mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k} |v_j|^q$:** for this, we consider two estimates $\left|\tilde{U}_i^n\right|^q \mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k}$, and $\left|v_j - \tilde{U}_i^n\right|^q \mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k}$, separately.

(b₁) $\left|\tilde{U}_i^n\right|^q \mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k}$: from the second inequality in (4.10), we obtain

$$\left|\tilde{U}_i^n\right|^q \mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k} \leq \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \frac{1}{(2\pi)^{3/2}} \frac{\Lambda_\delta}{\theta^{\frac{3+\delta}{2}}} \left|\tilde{U}_i^n\right|^q \frac{\tilde{\rho}_i^n}{\left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{3+\delta}{2}}}.$$

If $\left|\tilde{U}_i^n\right| < \left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{1}{2}}$, we have from Lemma 4.7 that

$$\left|\tilde{U}_i^n\right|^q \frac{\tilde{\rho}_i^n}{\left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{3+\delta}{2}}} \leq \tilde{\rho}_i^n \left(\left(\tilde{T}_\delta\right)_i + \left|\tilde{U}_i^n\right|^2\right)^{\frac{q-3-\delta}{2}} \leq \left\{2^{\frac{q-2\delta-5}{2}} \pi^2 (3+\delta)^{\frac{q}{2}}\right\} \|f^n\|_{L_q^\infty}.$$

On the other hand, in the case of $\left|\tilde{U}_i^n\right| \geq \left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{1}{2}}$, we use Lemma 4.8 to obtain

$$\begin{aligned}
\left|\tilde{U}_i^n\right|^q \frac{\tilde{\rho}_i^n}{\left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{3+\delta}{2}}} &= \frac{\tilde{\rho}_i^n \left|\tilde{U}_i^n\right|^{q+3+\delta}}{\left|\tilde{U}_i^n\right|^{3+\delta} \left(\left(\tilde{T}_\delta\right)_i\right)^{\frac{3+\delta}{2}}} \\
&\leq 2^{\frac{3+\delta}{2}} \frac{\tilde{\rho}_i^n \left|\tilde{U}_i^n\right|^{q+3+\delta}}{\left\{\left(\left(\tilde{T}_\delta\right)_i + \left|\tilde{U}_i^n\right|^2\right) \left(\tilde{T}_\delta\right)_i\right\}^{\frac{3+\delta}{2}}} \\
&\leq 2^{10+3\delta+q} \pi^2 (3+\delta)^{2+\delta} \|f^n\|_{L_q^\infty}.
\end{aligned}$$

Therefore,

$$\left|\tilde{U}_i^n\right|^q \mathcal{M}_{\nu,\theta,\delta}\left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n\right)_{j,k} \leq \frac{C_1}{\theta^{\frac{3+\delta}{2}}} \|f^n\|_{L_q^\infty},$$

for

$$C_1 = \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \Lambda_\delta \left\{ \frac{2^{\frac{q-2\delta-5}{2}} \sqrt{\pi} (3+\delta)^{\frac{q}{2}}}{q-\delta-5} \right\} + 2^{\frac{17+6\delta+2q}{2}} \sqrt{\pi} (3+\delta)^{2+\delta}.$$

(b₂) The estimate for $|v_j - \tilde{U}_i^n|^q \mathcal{M}_{\nu, \theta, \delta}(\tilde{f}_{i, \mathcal{J}, \mathcal{K}}^n)_{j, k}$: from (4.9) and Lemma A.2, we have

$$\begin{aligned} & |v_j - \tilde{U}_i^n|^q \mathcal{M}_{\nu, \theta, \delta}(\tilde{f}_{i, \mathcal{J}, \mathcal{K}}^n)_{j, k} \\ & \leq \frac{1}{(2\pi)^{3/2}} \frac{1}{\theta^{\frac{3+\delta}{2}}} |v_j - \tilde{U}_i^n|^q \frac{\tilde{\rho}_i^n \Lambda_\delta}{((\tilde{T}_\delta)_i)^{\frac{3+\delta}{2}}} \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \exp\left(-\frac{3}{2\lambda C_\nu \{3 + \delta(1 - \theta)\}} \frac{|v_j - \tilde{U}_i^n|^2}{(\tilde{T}_\delta)_i^n}\right) \\ & = \frac{1}{(2\pi)^{3/2}} \frac{1}{\theta^{\frac{3+\delta}{2}}} ((\tilde{T}_\delta)_i)^{\frac{q}{2}} \frac{\tilde{\rho}_i^n \Lambda_\delta}{((\tilde{T}_\delta)_i)^{\frac{3+\delta}{2}}} \left(\frac{|v_j - \tilde{U}_i^n|^2}{(\tilde{T}_\delta)_i^n}\right)^{\frac{q}{2}} \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \\ & \quad \times \exp\left(-\frac{3}{2\lambda C_\nu \{3 + \delta(1 - \theta)\}} \frac{|v_j - \tilde{U}_i^n|^2}{(\tilde{T}_\delta)_i^n}\right) \\ & \equiv \frac{C_2}{\theta^{\frac{3+\delta}{2}}} \tilde{\rho}_i^n ((\tilde{T}_\delta)_i)^{\frac{q-3-\delta}{2}}, \end{aligned}$$

where

$$C_2 = \left(\frac{1}{\lambda}\right)^{\frac{3}{2}} \frac{\Lambda_\delta}{(2\pi)^{3/2}} \sup_{x \geq 0} (x^{q/2} e^{-x}) \left\{ \frac{2\lambda C_\nu (3 + \delta(1 - \theta))}{3} \right\}^{\frac{q}{2}}.$$

Then, we use Lemma 4.7 to obtain

$$\begin{aligned} |v_j - \tilde{U}_i^n|^q \mathcal{M}_{\nu, \theta, \delta}(\tilde{f}_{i, \mathcal{J}, \mathcal{K}}^n)_{j, k} & \leq \frac{C_2}{\theta^{\frac{3+\delta}{2}}} \tilde{\rho}_i^n \left(((\tilde{T}_\delta)_i)^n + |\tilde{U}_i^n|^2 \right)^{\frac{q-\delta-3}{2}} \\ & \leq \frac{C_2}{\theta^{\frac{3+\delta}{2}}} \left\{ \frac{2^{\frac{q-2\delta-5}{2}} \pi^2 (3 + \delta)^{\frac{q}{2}}}{q - \delta - 5} \right\} \|f^n\|_{L_q^\infty} \\ & \equiv \frac{C_3}{\theta^{\frac{3+\delta}{2}}} \|f^n\|_{L_q^\infty}. \end{aligned}$$

(c) The estimate for $I_k^{\frac{q}{\delta}} \mathcal{M}_{\nu, \theta, \delta}(\tilde{f}_{i, \mathcal{J}, \mathcal{K}}^n)_{j, k}$: from (4.9), we have

$$\frac{1}{2} (v_j - \tilde{U}_i^n)^\top \left((\tilde{T}_{\nu, \theta})_i \right)^{-1} (v_j - \tilde{U}_i^n) + \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n} \geq \frac{\delta}{\delta + 3(1 - \theta)} \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n},$$

and hence

$$\begin{aligned} I_k^{\frac{q}{\delta}} \mathcal{M}_{\nu, \theta, \delta}(\tilde{f}_{i, \mathcal{J}, \mathcal{K}}^n)_{j, k} & \leq \frac{\Lambda_\delta}{\sqrt{(2\pi)^3}} I_k^{\frac{q}{\delta}} \frac{1}{\theta^{\frac{3+\delta}{2}}} \frac{\tilde{\rho}_i^n}{\tilde{T}_\delta^{\frac{3+\delta}{2}}} \exp\left(-\frac{\delta}{\delta + 3(1 - \theta)} \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n}\right) \\ & = \frac{\Lambda_\delta}{\sqrt{(2\pi)^3}} \frac{1}{\theta^{\frac{3+\delta}{2}}} ((\tilde{T}_\delta)_i)^{\frac{q}{2}} \frac{\tilde{\rho}_i^n}{((\tilde{T}_\delta)_i)^{\frac{3+\delta}{2}}} \left(\frac{I_k^{\frac{2}{\delta}}}{((\tilde{T}_\delta)_i)^n}\right)^{\frac{q}{2}} \exp\left(-\frac{\delta}{\delta + 3(1 - \theta)} \frac{I_k^{\frac{2}{\delta}}}{(\tilde{T}_\theta)_i^n}\right) \end{aligned}$$

$$\equiv \frac{C_4}{\theta^{\frac{3+\delta}{2}}} \tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i \right)^{\frac{q-3-\delta}{2}},$$

where

$$C_4 = \frac{\Lambda_\delta}{\sqrt{(2\pi)^3}} \sup_{x>0} |x^{q/2} e^{-x}| \left(\frac{\delta + 3(1-\theta)}{\delta} \right)^{q/2}.$$

Next, we use Lemma 4.7 to derive

$$\begin{aligned} I_k^{\frac{q}{2}} \mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k} &\leq \frac{C_4}{\theta^{\frac{3+\delta}{2}}} \Lambda_\delta \tilde{\rho}_i^n \left(\left(\tilde{T}_\delta \right)_i + \left| \tilde{U}_i^n \right|^2 \right)^{\frac{q-\delta-3}{2}} \\ &\leq \frac{C_4}{\theta^{\frac{3+\delta}{2}}} \Lambda_\delta \left\{ \frac{2^{\frac{q-2\delta-5}{2}} \pi^2 (3+\delta)^{\frac{q}{2}}}{q-\delta-5} \right\} \|f^n\|_{L_q^\infty} \\ &\equiv \frac{C_5}{\theta^{\frac{3+\delta}{2}}} \|f^n\|_{L_q^\infty}. \end{aligned}$$

Combining (a), (b) and (c), we finally obtain

$$\begin{aligned} \sup_{i,j,k} \left| \mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k} \left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}} \right)^{\frac{q}{2}} \right| &\leq \sup_{i,j,k} \left| \mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k} \left(1 + |v_j - \tilde{U}_i^n + \tilde{U}_i^n|^2 + I_k^{\frac{2}{\delta}} \right)^{\frac{q}{2}} \right| \\ &\leq 2 \sup_{i,j,k} \left| \mathcal{M}_{\nu,\theta,\delta} \left(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n \right)_{j,k} \left(1 + |v_j - \tilde{U}_i^n|^2 + |\tilde{U}_i^n|^2 + I_k^{\frac{2}{\delta}} \right)^{\frac{q}{2}} \right| \\ &\leq C_{\mathcal{M}} \|f^n\|_{L_q^\infty}, \end{aligned}$$

where $C_{\mathcal{M}}$ is a constant depending on ν, δ, θ and q and proportional to $1/\theta^{\frac{3+\delta}{2}}$. □

Lemma 4.11. Assume that f_0 has no initial error (2.4) and satisfies 3.1. Then, f_0 satisfies E^0 .

Proof. – (A^0) From Lemma A.1, we know

$$\left\| \tilde{f}^0 \right\|_{L_q^\infty} \leq \|f_0\|_{L_q^\infty}.$$

– (B^0) Using the lower bound assumption for f_0 in (3.1), we have

$$\tilde{f}_{i,j,k}^0 = f_0(x_i - v_j^1 \Delta t, v_j, I_k) \geq C_0^1 e^{-C_0^2 (|v_j|^a + I_k^b)} \geq e^{-\frac{A_{\nu,\theta}}{\kappa} T^f} C_0^1 e^{-C_0^2 (|v_j|^a + I_k^b)}.$$

– (C^0) We also have from (3.1) and (4.1) that

$$\begin{aligned} \tilde{\rho}_i^0 &= \int_{\mathbb{R}^3 \times \mathbb{R}_+} f_0(x_i - v^1 \Delta t, v, I) \, dv \, dI \\ &\geq C_0^1 \int_{\mathbb{R}^3 \times \mathbb{R}_+} e^{-C_0^2 (|v|^a + I^b)} \, dv \, dI \\ &= \bar{C}_{a,b} C_0^1 \\ &\geq \frac{1}{2} \bar{C}_{a,b} C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f}. \end{aligned}$$

This together with Lemma 4.6 gives

$$\left(\tilde{T}_\delta \right)_i^0 \geq \left(\frac{\tilde{\rho}_i^0}{C_\delta \|f_0\|_{L_q^\infty}} \right)^{\frac{2}{3+\delta}} \geq \left(\frac{\bar{C}_{a,b} C_0^1}{C_\delta \|f_0\|_{L_q^\infty}} \right)^{\frac{2}{3+\delta}} \geq \left(\frac{1}{2} \frac{\bar{C}_{a,b} C_0^1}{C_\delta \|f_0\|_{L_q^\infty}} e^{-\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa + A_{\nu,\theta} \Delta t} \right) A_{\nu,\theta} T^f} \right)^{\frac{2}{3+\delta}},$$

where C_δ is a constant given in Lemma 4.6.

– (D^0) Using (4.1), we obtain the upper bounds for $\tilde{\rho}_i^0, |\tilde{U}_i^0|$ and $(\tilde{T}_\delta)_i^0$ as follows:

$$\begin{aligned} \tilde{\rho}_i^0 &= \int_{\mathbb{R}^3 \times \mathbb{R}_+} f_0(x_i - v^1 \Delta t, v, I) \frac{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}}{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}} \, dv \, dI \\ &\leq \|f_0\|_{L_q^\infty} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{1}{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}} \, dv \, dI \\ &= \bar{C}_{\delta,q} \|f_0\|_{L_q^\infty}, \\ |\tilde{U}_i^0| &\leq \frac{1}{\tilde{\rho}_i^0} \left| \int_{\mathbb{R}^3 \times \mathbb{R}_+} f_0(x_i - v^1 \Delta t, v, I) \frac{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}}{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}} |v| \, dv \, dI \right| \\ &\leq \frac{\|f_0\|_{L_q^\infty}}{\tilde{\rho}_i^0} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{1}{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q-1}{2}}} \, dv \, dI \\ &\leq \frac{\bar{C}_{\delta,q-1}}{\bar{C}_{a,b} C_0^1} \|f_0\|_{L_q^\infty}, \end{aligned}$$

and

$$\begin{aligned} (\tilde{T}_\delta)_i^0 &= \frac{2}{3 + \delta} \frac{1}{\tilde{\rho}_i^0} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{1}{2} |v - \tilde{U}_i^0|^2 + I^{\frac{2}{3}} \right) f_0(x_i - v^1 \Delta t, v, I) \, dv \, dI \\ &\leq \frac{2}{3 + \delta} \left(\frac{1}{\tilde{\rho}_i^0} \int_{\mathbb{R}^3 \times \mathbb{R}_+} f_0(x_i - v^1 \Delta t, v, I) (|v|^2 + I^{\frac{2}{3}}) \, dv \, dI - |\tilde{U}_i^0|^2 \right) \\ &\leq \frac{2}{3 + \delta} \frac{1}{\tilde{\rho}_i^0} \int_{\mathbb{R}^3 \times \mathbb{R}_+} f_0(x_i - v^1 \Delta t, v, I) \frac{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}}{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q}{2}}} (|v|^2 + I^{\frac{2}{3}}) \, dv \, dI \\ &\leq \frac{2}{3 + \delta} \frac{\|f_0\|_{L_q^\infty}}{\tilde{\rho}_i^0} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{1}{(1 + |v|^2 + I^{\frac{2}{3}})^{\frac{q-2}{2}}} \, dv \, dI \\ &\leq \frac{2}{3 + \delta} \frac{\bar{C}_{\delta,q-2}}{\bar{C}_{a,b} C_0^1} \|f_0\|_{L_q^\infty}. \end{aligned}$$

□

Lemma 4.12. Assume $f_{i,j,k}^{n-1}$ satisfies E^{n-1} . Then, $f_{i,j,k}^n$ satisfies A^n :

$$(A^n) \quad \|\tilde{f}^n\|_{L_q^\infty} \leq \left(\frac{\kappa + A_{\nu,\theta} \Delta t C_{\mathcal{M}}}{\kappa + A_{\nu,\theta} \Delta t} \right)^n \|f_0\|_{L_q^\infty} \leq e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa + A_{\nu,\theta} \Delta t} T^f} \|f_0\|_{L_q^\infty}.$$

Proof. Recall (2.14) and use Lemmas A.1 and 4.9 to obtain

$$\|f^n\|_{L_q^\infty} \leq \frac{\kappa \|\tilde{f}^{n-1}\|_{L_q^\infty} + A_{\nu,\theta} \Delta t \|\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^{n-1})\|_{L_q^\infty}}{\kappa + A_{\nu,\theta} \Delta t}$$

$$\begin{aligned} &\leq \frac{\kappa + A_{\nu,\theta}\Delta t C_{\mathcal{M}}}{\kappa + A_{\nu,\theta}\Delta t} \|f^{n-1}\|_{L_{\tilde{q}}^{\infty}} \\ &\leq \left(\frac{\kappa + A_{\nu,\theta}\Delta t C_{\mathcal{M}}}{\kappa + A_{\nu,\theta}\Delta t}\right)^n \|f_0\|_{L_{\tilde{q}}^{\infty}}. \end{aligned}$$

Now, we make use of $(1+x)^n \leq e^{nx}$ to see

$$\left(\frac{\kappa + A_{\nu,\theta}\Delta t C_{\mathcal{M}}}{\kappa + A_{\nu,\theta}\Delta t}\right)^n = \left(1 + \frac{(C_{\mathcal{M}} - 1)A_{\nu,\theta}\Delta t}{\kappa + A_{\nu,\theta}\Delta t}\right)^n \leq e^{\frac{C_{\mathcal{M}}A_{\nu,\theta}}{\kappa + A_{\nu,\theta}\Delta t} T^f}.$$

Note that $C_{\mathcal{M}} > 1$ and this estimate holds uniformly for $n \geq 0$. □

Lemma 4.13. *Assume $f_{i,j,k}^{n-1}$ satisfies E^{n-1} . Then, $f_{i,j,k}^n$ satisfies B^n :*

$$(B^n) \quad \tilde{f}_{i,j,k}^n \geq \left(\frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t}\right)^n C_0^1 e^{-C_0^2(|v_j|^a + I_k^b)} \geq e^{-\frac{A_{\nu,\theta}}{\kappa} T^f} C_0^1 e^{-C_0^2(|v_j|^a + I_k^b)}.$$

Proof. From the non-negativity of $\mathcal{M}_{\nu,\theta,\delta}$ and (2.14), we have

$$f_{i,j,k}^n \geq \frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t} \tilde{f}_{i,j,k}^{n-1} = \frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t} \left(a_j f_{s,j,k}^{n-1} + (1 - a_j) f_{s+1,j,k}^{n-1}\right).$$

We recall (2.1), $0 \leq a_j \leq 1$ and use the lower bound of $f_{i,j,k}^{n-1}$ in Lemma 4.11 to obtain

$$\begin{aligned} f_{i,j,k}^n &\geq \frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t} \left(a_j f_{s,j,k}^{n-1} + (1 - a_j) f_{s+1,j,k}^{n-1}\right) \\ &\geq \frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t} \left(\frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t}\right)^{n-1} \min_i f_{i,j,k}^0 \\ &\geq \left(\frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t}\right)^n C_0^1 e^{-C_0^2(|v_j|^a + I_k^b)}. \end{aligned}$$

Using $(1+x)^{-n} \geq e^{-nx}$, we complete the proof. □

Lemma 4.14. *Assume $f_{i,j,k}^n$ satisfies $A^n \wedge B^n$. Then, $f_{i,j,k}^n$ satisfies C^n :*

$$(C^n) \quad \tilde{\rho}_i^n \geq \frac{1}{2} \bar{C}_{a,b} C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f}, \quad (\tilde{T}_{\delta})_i^n \geq \left(\frac{1}{2} \frac{\bar{C}_{a,b} C_0^1}{C_{\delta} \|f_0\|_{L_{\tilde{q}}^{\infty}}} e^{-\left(\frac{1}{\kappa} + \frac{(C_{\mathcal{M}} - 1)}{\kappa + A_{\nu,\theta}\Delta t}\right) A_{\nu,\theta} T^f}\right)^{\frac{2}{3+\delta}}.$$

Proof. Since Lemma 4.13 holds, the discrete local density $\tilde{\rho}_i^n$ satisfies

$$\tilde{\rho}_i^n = \sum_{j,k} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I \geq C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f} \sum_{j,k} e^{-C_0^2(|v_j|^a + I_k^b)} (\Delta v)^3 \Delta I \geq \frac{1}{2} \bar{C}_{a,b} C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f}.$$

This, together with Lemmas 4.6 and 4.12, gives

$$(\tilde{T}_{\delta})_i^n \geq \left(\frac{\tilde{\rho}_i^n}{C_{\delta} \|f^n\|_{L_{\tilde{q}}^{\infty}}}\right)^{\frac{2}{3+\delta}} \geq \left(\frac{1}{2} \frac{\bar{C}_{a,b} C_0^1}{C_{\delta} \|f_0\|_{L_{\tilde{q}}^{\infty}}} e^{-\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa + A_{\nu,\theta}\Delta t}\right) A_{\nu,\theta} T^f}\right)^{\frac{2}{3+\delta}}.$$

□

Lemma 4.15. *Assume $f_{i,j,k}^n$ satisfies $A^n \wedge B^n \wedge C^n$. Then, $f_{i,j,k}^n$ satisfies D^n :*

$$\begin{aligned}
 (D^n) \quad & \|\tilde{\rho}^n\|_{L^\infty} \leq 2\bar{C}_{\delta,q} e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa+A_{\nu,\theta}\Delta t} T^f} \|f_0\|_{L^\infty}, \\
 & \|\tilde{U}^n\|_{L^\infty} \leq \frac{4\bar{C}_{\delta,q-1}}{\bar{C}_{a,b} C_0^1} e^{\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa+A_{\nu,\theta}\Delta t}\right) A_{\nu,\theta} T^f} \|f_0\|_{L^\infty}, \\
 & \left\| \left(\tilde{T}_\delta\right)^n \right\|_{L^\infty} \leq \frac{8}{3+\delta} \frac{\bar{C}_{\delta,q-2}}{\bar{C}_{a,b} C_0^1} e^{\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa+A_{\nu,\theta}\Delta t}\right) A_{\nu,\theta} T^f} \|f_0\|_{L^\infty}.
 \end{aligned}$$

Proof. From the upper bound for $\|\tilde{f}^n\|_{L^q}$ in Lemma 4.12, we see that

$$\begin{aligned}
 \tilde{\rho}_i^n &= \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} (\Delta v)^3 \Delta I \\
 &\leq \|\tilde{f}^n\|_{L^q} \sum_{j,k} \frac{1}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} (\Delta v)^3 \Delta I \\
 &\leq 2\bar{C}_{\delta,q} e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa+A_{\nu,\theta}\Delta t} T^f} \|f_0\|_{L^\infty}.
 \end{aligned}$$

To estimate \tilde{U}_i^n , we use the upper bound of $\|\tilde{f}^n\|_{L^q}$ in Lemma 4.12 and the lower bound of $\tilde{\rho}_i^n$ in Lemma 4.14:

$$\begin{aligned}
 |\tilde{U}_i^n| &= \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} |v_j| (\Delta v)^3 \Delta I \\
 &\leq \frac{\|\tilde{f}^n\|_{L^q}}{\tilde{\rho}_i^n} \sum_{j,k} \frac{1}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q-1}{2}}} (\Delta v)^3 \Delta I \\
 &\leq 2\bar{C}_{\delta,q-1} \left(\frac{1}{2} \bar{C}_{a,b} C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f}\right)^{-1} e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa+A_{\nu,\theta}\Delta t} T^f} \|f_0\|_{L^\infty} \\
 &= \frac{4\bar{C}_{\delta,q-1}}{\bar{C}_{a,b} C_0^1} e^{\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa+A_{\nu,\theta}\Delta t}\right) A_{\nu,\theta} T^f} \|f_0\|_{L^\infty}.
 \end{aligned}$$

Similarly, we compute

$$\begin{aligned}
 \left(\tilde{T}_\delta\right)_i^n &= \frac{2}{3+\delta} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \left(\frac{|v_j - \tilde{U}_i^n|^2}{2} + I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I \\
 &\leq \frac{2}{3+\delta} \left(\frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \left(|v_j|^2 + I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I - |\tilde{U}_i^n|^2 \right) \\
 &\leq \frac{2}{3+\delta} \frac{1}{\tilde{\rho}_i^n} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} \left(|v_j|^2 + I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I.
 \end{aligned}$$

Then, from A^n and C^m , we have

$$\begin{aligned} \left(\tilde{T}_\delta\right)_i^n &\leq \frac{4}{3+\delta} \bar{C}_{\delta,q-2} \left(\frac{1}{2} \bar{C}_{a,b} C_0^1 e^{-\frac{A_{\nu,\theta}}{\kappa} T^f}\right)^{-1} e^{\frac{C_{\mathcal{M}} A_{\nu,\theta}}{\kappa+A_{\nu,\theta} \Delta t} T^f} \|f_0\|_{L_q^\infty} \\ &= \frac{8}{3+\delta} \frac{\bar{C}_{\delta,q-2}}{\bar{C}_{a,b} C_0^1} e^{\left(\frac{1}{\kappa} + \frac{C_{\mathcal{M}}}{\kappa+A_{\nu,\theta} \Delta t}\right) A_{\nu,\theta} T^f} \|f_0\|_{L_q^\infty}. \end{aligned}$$

□

Using the estimates that we have built up throughout this section, we now prove the Theorem 4.5 as follows:

Proof of Theorem 4.5. The proof is based on the induction argument. Lemma 4.11 implies E^0 . For $n \geq 1$, one can easily confirm that Lemmas 4.12–4.15 gives E^n . □

5. CONSISTENT FORM

In this section, we rewrite (1.1) in a consistent form to make it easily comparable with (2.6). For convenience, we introduce the following notation:

– Distribution function on $x - v^1 \Delta t$:

$$\tilde{f}(x, v, t, I) := f(x - v^1 \Delta t, v, t, I).$$

– Mass:

$$\tilde{\rho}(x, t) = \int_{\mathbb{R}^3 \times \mathbb{R}_+} \tilde{f}(x, v, t, I) \, dv \, dI.$$

– Momentum:

$$\tilde{\rho}(x, t) \tilde{U}(x, t) := \int_{\mathbb{R}^3 \times \mathbb{R}_+} v \tilde{f}(x, v, t, I) \, dv \, dI.$$

– Stress tensor:

$$\tilde{\rho}(x, t) \tilde{\Theta}(x, t) = \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(v - \tilde{U}(x, t)\right) \otimes \left(v - \tilde{U}(x, t)\right) \tilde{f}(x, v, t, I) \, dv \, dI.$$

– Polyatomic temperature:

$$\tilde{T}_\delta(x, t) = \frac{3}{3+\delta} \tilde{T}_{\text{tr}}(x, t) + \frac{\delta}{3+\delta} \tilde{T}_{I,\delta}(x, t),$$

where

$$\left(\tilde{T}_{\text{tr}}\right)(x, t) := \frac{2}{3} \frac{1}{\tilde{\rho}(x, t)} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{|v - \tilde{U}(x, t)|^2}{2} \tilde{f}(x, v, t, I) \, dv \, dI,$$

$$\tilde{T}_{I,\delta}(x, t) := \frac{2}{\delta} \frac{1}{\tilde{\rho}(x, t)} \int_{\mathbb{R}^3 \times \mathbb{R}_+} I^{\frac{2}{\delta}} \tilde{f}(x, v, t, I) \, dv \, dI.$$

– Relaxation temperature:

$$\tilde{T}_\theta(x, t) := \theta \tilde{T}_\delta(x, t) + (1 - \theta) \tilde{T}_{I,\delta}(x, t).$$

– Polyatomic temperature:

$$\tilde{T}_{\nu,\theta}(x, t) := \theta \tilde{T}_\delta(x, t) Id + (1 - \theta)(1 - \nu) \tilde{T}_{\text{tr}}(x, t) Id + (1 - \theta) \nu \tilde{\Theta}(x, t).$$

Lemma 5.1. *The equation (1.1) can be rewritten as*

$$\begin{aligned} f(x, v, t + \Delta t, I) &= \frac{\kappa}{\kappa + A_{\nu, \theta} \Delta t} \tilde{f}(x, v, t, I) + \frac{A_{\nu, \theta} \Delta t}{\kappa + A_{\nu, \theta} \Delta t} \mathcal{M}_{\nu, \theta, \delta}(\tilde{f})(x, v, t, I) \\ &\quad + \frac{A_{\nu, \theta}}{\kappa + A_{\nu, \theta} \Delta t} (R_1 + R_2), \end{aligned} \quad (5.1)$$

with

$$\begin{aligned} R_1 &= - \int_t^{t+\Delta t} \left\{ \mathcal{M}_{\nu, \theta, \delta}(\tilde{f})(x, v, t, I) - \mathcal{M}_{\nu, \theta, \delta}(f)(x, v, t, I) \right\} ds \\ &\quad - \int_t^{t+\Delta t} (t + \Delta t - s) v^1 \partial_x \mathcal{M}_{\nu, \theta, \delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) - (s - t) \partial_t \mathcal{M}_{\nu, \theta, \delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) ds, \\ R_2 &= - \frac{1}{\kappa} \int_t^{t+\Delta t} (s - t - \Delta t) A_{\nu, \theta} (\mathcal{M}_{\nu, \theta, \delta}(f) - f)(x_{\theta_2}, v, t_{\theta_2}, I) ds, \end{aligned} \quad (5.2)$$

where x_{θ_i} , $i = 1, 2$, lies between x and $x_i - v^1 \Delta t$ and t_{θ_i} between t and $t + \Delta t$.

Proof. We start by integrating (2.5) from t to $t + \Delta t$:

$$f(x, v, t + \Delta t, I) = f(x - v^1 \Delta t, v, t, I) + \frac{A_{\nu, \theta}}{\kappa} \int_t^{t+\Delta t} (\mathcal{M}_{\nu, \theta, \delta}(f) - f)(x - (t + \Delta t - s)v^1, v, s, I) ds.$$

Using Taylor's theorem, we obtain

$$\begin{aligned} \mathcal{M}_{\nu, \theta, \delta}(f)(x - (t + \Delta t - s)v^1, v, s, I) &= \mathcal{M}_{\nu, \theta, \delta}(f)(x, v, t, I) - (t + \Delta t - s) v^1 \partial_x \mathcal{M}_{\nu, \theta, \delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) \\ &\quad + (s - t) \partial_t \mathcal{M}_{\nu, \theta, \delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) \\ &= \left\{ \mathcal{M}_{\nu, \theta, \delta}(f)(x, v, t, I) - \mathcal{M}_{\nu, \theta, \delta}(\tilde{f})(x, v, t, I) \right\} \\ &\quad + \mathcal{M}_{\nu, \theta, \delta}(\tilde{f})(x, v, t, I) - (t + \Delta t - s) v^1 \partial_x \mathcal{M}_{\nu, \theta, \delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) \\ &\quad + (s - t) \partial_t \mathcal{M}_{\nu, \theta, \delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I), \end{aligned} \quad (5.3)$$

for some x_{θ_1} between x and $x - (t + \Delta t - s)v^1$ and t_{θ_1} between t and $t + \Delta t$. Similarly,

$$\begin{aligned} f(x - (t + \Delta t - s)v^1, v, s, I) &= f(x, v, t + \Delta t, I) - (t + \Delta t - s) v^1 \partial_x f(x_{\theta_1}, v, t_{\theta_1}, I) \\ &\quad + (s - t - \Delta t) \partial_t f(x_{\theta_1}, v, t_{\theta_1}, I) \\ &= f(x, v, t + \Delta t, I) + (s - t - \Delta t) \{ \partial_t + v^1 \partial_x \} f(x_{\theta_2}, v, t_{\theta_2}, I) \\ &= f(x, v, t + \Delta t, I) + (s - t - \Delta t) \frac{A_{\nu, \theta}}{\kappa} (\mathcal{M}_{\nu, \theta, \delta}(f) - f)(x_{\theta_2}, v, t_{\theta_2}, I). \end{aligned} \quad (5.4)$$

Combining (5.3) and (5.4), we can derive the desired representation. \square

In the rest of this section, we aim to estimate the remainder terms R_1 and R_2 in (5.2) using L_q^∞ -norm. As a first step, we recall the following three estimates in [34].

Proposition 5.2 ([34]). *Let f and g satisfy (A1) and (A2) in Theorem 3.1. Then $\mathcal{M}_{\nu, \theta, \delta}$ satisfies the following continuity property:*

$$\| \mathcal{M}_{\nu, \theta, \delta}(f) - \mathcal{M}_{\nu, \theta, \delta}(g) \|_{L_q^\infty} \leq C_{Lip} \| f - g \|_{L_q^\infty},$$

for some constant C_{Lip} depending on T^f, δ, θ, q and f_0 .

Proposition 5.3 ([34]). *Let $\delta > 0$, $-1/2 < \nu < 1$ and $0 < \theta \leq 1$. Suppose $\rho > 0$, $T_{tr} > 0$ and $T_{I,\delta} > 0$. Then, temperature tensor $\mathcal{T}_{\nu,\theta}$ and the relaxation temperature T_θ satisfy the following equipanlence type estimates:*

$$\begin{aligned} (1) \quad & \theta T_\delta Id \leq \mathcal{T}_{\nu,\theta} \leq C_\nu \frac{(3 + \delta - \delta\theta)}{3} T_\delta Id, \\ (2) \quad & \theta T_\delta \leq T_\theta \leq \frac{(3 + \delta - 3\theta)}{\delta} T_\delta, \end{aligned}$$

where the constants $C_\nu = \max_\nu\{1 - \nu, 1 + 2\nu\}$.

Proposition 5.4 ([34]). *Let $\delta > 0$, $-1/2 < \nu < 1$, $0 < \theta \leq 1$, $q > 5 + \delta$. Suppose $f \in \Omega_{0,q}$, there exists a constant C depending on ν, δ, θ and q such that*

$$\|\mathcal{M}_{\nu,\theta,\delta}(f)\|_{L^\infty_q} \leq C \|f\|_{L^\infty_q},$$

where C blows up as θ tends to 0.

Now, we estimate the time and spatial derivatives of polyatomic Gaussian in $L^\infty_{1,q}$ -norm. This result will play the key role in the estimate of R_1 in (5.2).

Proposition 5.5. *Let f be a smooth solution to (1.1) in $\Omega_{1,q}$ corresponding to f_0 . Then, for $q > 5 + \delta$, $\delta > 0$, we have*

$$\|\partial_t \mathcal{M}_{\nu,\theta,\delta}\|_{L^\infty}, \quad \|\nabla_x \mathcal{M}_{\nu,\theta,\delta}\|_{L^\infty} < C \left\{ \|f_0\|_{L^\infty_{1,q}} + 1 \right\},$$

where C is a positive constant which depends on $\nu, \delta, q, \theta, f_0, T^f$.

Proof. We begin by estimating the time derivative of macroscopic quantities. Using the collision invariants, $1, v_j, \frac{1}{2}|v|^2 + I^{\frac{2}{5}}$, we obtain

$$\begin{aligned} \left| \frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}^+} f \left(\begin{array}{c} 1 \\ v \\ \frac{1}{2}|v|^2 + I^{\frac{2}{5}} \end{array} \right) dv dI \right| &= \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f \left(\begin{array}{c} 1 \\ v \\ \frac{1}{2}|v|^2 + I^{\frac{2}{5}} \end{array} \right) dv dI \right| \\ &\leq C \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v| |\nabla_x f| \left(1 + |v|^2 + I^{\frac{2}{5}} \right) dv dI \right| \\ &\leq C \|f(t)\|_{L^\infty_{1,q}} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{1}{\left(1 + |v|^2 + I^{\frac{2}{5}} \right)^{\frac{q}{2}-2}} dv dI \right| \\ &\leq C \left\{ \|f_0\|_{L^\infty_{1,q}} + 1 \right\}, \end{aligned} \tag{5.5}$$

which gives $|\partial_t \rho|, |\partial_t \{\rho U\}| < C \left\{ \|f_0\|_{L^\infty_{1,q}} + 1 \right\}$. Using the lower bound for ρ and the upper bound for $\rho + |U| + T_\delta$ in Theorem 3.1, we further obtain

$$|\partial_t U| \leq \frac{1}{\rho} \left(|\partial_t \rho| |U| + C \left\{ \|f_0\|_{L^\infty_{1,q}} + 1 \right\} \right) \leq C \left\{ \|f_0\|_{L^\infty_{1,q}} + 1 \right\}. \tag{5.6}$$

To bound $|\partial_t E_\delta|$, we start from

$$\begin{aligned} |\partial_t E_\delta| &= \left| \frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}^+} f \left(\frac{1}{2} |v - U|^2 + I^{\frac{2}{5}} \right) dv dI \right| \\ &\leq \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f \left(\frac{1}{2} |v - U|^2 + I^{\frac{2}{5}} \right) dv dI \right| + \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} f (|v - U| |\partial_t U|) dv dI \right| \\ &\equiv \mathcal{I}_{41} + \mathcal{I}_{42}. \end{aligned} \tag{5.7}$$

\mathcal{I}_{41} satisfies

$$\mathcal{I}_{41} \leq \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f \left(\frac{1}{2}|v|^2 + I^{\frac{2}{\delta}} \right) dv dI \right| + \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f \left(|v||U| + \frac{|U|^2}{2} + I^{\frac{2}{\delta}} \right) dv dI \right|. \tag{5.8}$$

In (5.8), the first term of the upper bound can be estimated by (5.5). The second term is bounded by

$$\begin{aligned} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f \left(|v||U| + \frac{|U|^2}{2} + I^{\frac{2}{\delta}} \right) dv dI \right| &\leq \|\nabla_x \cdot f\|_{L_q^\infty} \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v| \frac{|v||U| + \frac{|U|^2}{2} + I^{\frac{2}{\delta}}}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} dv dI \\ &\leq \|\nabla_x \cdot f\|_{L_q^\infty} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v| \frac{\frac{|v|^2}{2} + |U|^2 + I^{\frac{2}{\delta}}}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} dv dI \right| \\ &\leq \max\{1, |U|^2\} \|\nabla_x \cdot f\|_{L_q^\infty} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{1}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2} - \frac{3}{\delta}}} dv dI \right| \\ &\leq C \left\{ \|f_0\|_{L_{1,q}^\infty} + 1 \right\}, \end{aligned} \tag{5.9}$$

where we use the boundedness of $|U|$ in Theorem 3.1 and $q > 5 + \delta$.

To estimate \mathcal{I}_{42} , we use the boundedness of f and U in Theorem 3.1 and $\partial_t U$ in (5.6):

$$\begin{aligned} \mathcal{I}_{42} &\leq |\partial_t U| \|f\|_{L_q^\infty} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{|v| + |U|}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} dv dI \right| \\ &\leq \max\{1, |U|\} |\partial_t U| \|f\|_{L_q^\infty} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{|v| + 1}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} dv dI \right| \\ &\leq C \left\{ \|f_0\|_{L_{1,q}^\infty} + 1 \right\}. \end{aligned} \tag{5.10}$$

Combining (5.7)–(5.10), we obtain

$$|\partial_t E_\delta| \leq C \left\{ \|f_0\|_{L_{1,q}^\infty} + 1 \right\}.$$

Now, we use the relation $E_\delta = \frac{3+\delta}{2} \rho T_\delta$ and the lower and upper bounds for ρ and T_δ in Theorem 3.1, which together with $|\partial_t \rho|, |\partial_t E_\delta| \leq C \left\{ \|f_0\|_{L_{1,q}^\infty} + 1 \right\}$ give

$$|\partial_t T_\delta| = \frac{1}{\rho} \left(\frac{2}{3+\delta} |\partial_t E_\delta| + |\partial_t \rho| T_\delta \right) \leq C \left\{ \|f_0\|_{L_{1,q}^\infty} + 1 \right\}.$$

Similarly, we compute

$$\begin{aligned} |\partial_t T_{I,\delta}| &= \left| \frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}^+} f I^{\frac{2}{\delta}} dv dI \right| \\ &\leq \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f I^{\frac{2}{\delta}} dv dI \right| + \frac{A_{\nu,\theta}}{\kappa} \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} (\mathcal{M}_{\nu,\theta,\delta} - f) I^{\frac{2}{\delta}} dv dI \right| \end{aligned}$$

$$= \left| \int_{\mathbb{R}^3 \times \mathbb{R}^+} v \cdot \nabla_x f I^{\frac{2}{3}} dv dI \right| + \frac{A_{\nu, \theta}}{\kappa} \left| \frac{\delta}{2} \rho T_\theta - E_{I, \delta} \right|. \quad (5.11)$$

In the last line, the first term can be bounded by (5.5). For the second term, we use

$$T_\theta = \theta T_\delta + (1 - \theta) T_{I, \delta}, \quad T_\delta = \frac{3}{3 + \delta} T_{\text{tr}} + \frac{\delta}{3 + \delta} T_{I, \delta}, \quad E_{I, \delta} = \frac{\delta}{2} \rho T_{I, \delta},$$

to obtain

$$\left| \frac{\delta}{2} \rho T_\theta - E_{I, \delta} \right| = \left| \frac{\delta}{2} \rho \theta (T_\delta - T_{I, \delta}) \right| = \left| \frac{\rho \theta}{2} \frac{3\delta}{3 + \delta} (T_{\text{tr}} - T_{I, \delta}) \right| \leq \frac{\rho \theta}{2} (3 + \delta) T_\delta. \quad (5.12)$$

Combining (5.11) and (5.12), we also derive $|\partial_t T_{I, \delta}| < C$. From $T_\delta = \frac{3}{3 + \delta} T_{\text{tr}} + \frac{\delta}{3 + \delta} T_{I, \delta}$, we further have $|\partial_t T_{\text{tr}}| < C$. It remains to estimate $|\partial_t \Theta|$. We recall the definition of stress tensor $\Theta(x, t)$:

$$\rho(x, t) \Theta(x, t) = \int_{\mathbb{R}^3 \times \mathbb{R}^+} (v - U(x, t)) \otimes (v - U(x, t)) f(x, v, t) dv dI.$$

For simplicity, we only consider two cases $|\partial_t \Theta_{11}|$ and $|\partial_t \Theta_{12}|$:

$$\begin{aligned} |\partial_t \Theta_{11}| &= \left| \frac{\partial_t \rho}{\rho^2} \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v^1 - U^1|^2 f dv dI \right| + \left| \frac{1}{\rho} \int_{\mathbb{R}^3 \times \mathbb{R}^+} 2|v^1 - U^1| |\partial_t U^1| f dv dI \right| \\ &\quad + \left| \frac{1}{\rho} \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v^1 - U^1|^2 |\partial_t f| dv dI \right| \\ &\leq \left| \frac{\partial_t \rho}{\rho^2} + \frac{2}{\rho} (1 + |\partial_t U|) \right| \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v - U|^2 (|f| + |\partial_t f|) dv dI \end{aligned}$$

and

$$\begin{aligned} |\partial_t \Theta_{12}| &= \left| \frac{\partial_t \rho}{\rho^2} \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v^1 - U^1| |v^2 - U^2| f dv dI \right| \\ &\quad + \left| \frac{1}{\rho} \int_{\mathbb{R}^3 \times \mathbb{R}^+} (|v^1 - U^1| |\partial_t U^2| + |v^2 - U^2| |\partial_t U^1|) f dv dI \right| \\ &\quad + \left| \frac{1}{\rho} \int_{\mathbb{R}^3 \times \mathbb{R}^+} |v^1 - U^1| |v^2 - U^2| \partial_t f dv dI \right| \\ &\leq \left| \frac{\partial_t \rho}{\rho^2} + \frac{2}{\rho} (1 + |\partial_t U|) \right| \int_{\mathbb{R}^3 \times \mathbb{R}^+} (|v - U|^2 + |v - U|) (|f| + |\partial_t f|) dv dI. \end{aligned}$$

In both cases, the last upper bounds can be bounded using (5.5), the lower bound of ρ and the upper bounds of ρ , U , $|\partial_t \rho|$, $|\partial_t U|$, $|\partial_t E_\delta|$. Therefore, we have $|\partial_t \Theta_{11}|, |\partial_t \Theta_{12}| < C$ for a constant $C > 0$.

Until now, we show that the following time derivatives of macroscopic quantities are bounded:

$$|\partial_t \rho|, |\partial_t U|, |\partial_t T_\delta|, |\partial_t T_{I, \delta}|, |\partial_t T_{\text{tr}}|, |\partial_t T_\theta|, |\partial_t \Theta_{ij}| \leq C.$$

From the definition of $T_{\nu, \theta}$, we further obtain that $|\partial_t (T_{\nu, \theta})_{ij}| \leq C$ for $1 \leq i, j \leq 3$.

Now, we move on to the estimate of $|\partial_t \mathcal{M}_{\nu, \theta, \delta}|$. For this, we write

$$\begin{aligned}
 \partial_t \mathcal{M}_{\nu,\theta,\delta} &= \partial_t \left\{ \frac{\rho \Lambda_\delta}{\sqrt{\det(2\pi \mathcal{T}_{\nu,\theta})} (T_\theta)^{\frac{\delta}{2}}} \exp \left(-\frac{(v-U(x,t))^\top \mathcal{T}_{\nu,\theta}^{-1} (v-U(x,t))}{2} - \frac{I^{\frac{2}{\delta}}}{T_\theta} \right) \right\} \\
 &= \left(\frac{\partial_t \rho}{\rho} - \frac{1}{2} \{ \det(2\pi \mathcal{T}_{\nu,\theta}) \}^{-1} \partial_t \{ \det(2\pi \mathcal{T}_{\nu,\theta}) \} - \frac{\delta}{2} \frac{1}{T_\theta} \partial_t T_\theta \right) \mathcal{M}_{\nu,\theta,\delta} \\
 &\quad + \left(-\frac{(\partial_t U)^\top \mathcal{T}_{\nu,\theta}^{-1} (v-U)}{2} - \frac{(v-U)^\top \mathcal{T}_{\nu,\theta}^{-1} \partial_t U}{2} + \frac{I^{\frac{2}{\delta}}}{(T_\theta)^2} \partial_t T_\theta \right) \mathcal{M}_{\nu,\theta,\delta} \\
 &\quad + \left(-\frac{(v-U)^\top \mathcal{T}_{\nu,\theta}^{-1} \partial_t \{ \mathcal{T}_{\nu,\theta}^{-1} \} \mathcal{T}_{\nu,\theta}^{-1} (v-U)}{2} \right) \mathcal{M}_{\nu,\theta,\delta}.
 \end{aligned} \tag{5.13}$$

Note that each macroscopic quantity and its time derivative are bounded, and the positivity of T_θ is also guaranteed by $T_\delta > C$. Finally, we combine Propositions 5.3, 5.4, Theorem 3.1 and (5.13) to derive

$$|\partial_t \mathcal{M}_{\nu,\theta,\delta}| \leq C(1 + |v| + |v|^2) \mathcal{M}_{\nu,\theta,\delta} \leq C \left(1 + |v|^2 + I^{\frac{2}{\delta}} \right)^{\frac{q}{2}} \mathcal{M}_{\nu,\theta,\delta} \leq C \left\{ \|f_0\|_{L_{1,q}^\infty} + 1 \right\}$$

for $q > 5 + \delta$. The estimate for spatial derivative $|\nabla_x \mathcal{M}_{\nu,\theta,\delta}|$ can be done similarly. □

Lemma 5.6. *Under the assumption of Theorem 3.1, the estimations for R_1 and R_2 in (5.2) satisfy*

$$\|R_1\|_{L_q^\infty} + \|R_2\|_{L_q^\infty} \leq C(\Delta t)^2$$

for a constant $C > 0$ depending on $T^f, q, \delta, \kappa, \theta, \nu, C_{2,1}, C_{2,2}$.

Proof. We first split R_1 in Lemma 5.1 into two parts:

$$\begin{aligned}
 R_1 &= - \int_t^{t+\Delta t} \left\{ \mathcal{M}_{\nu,\theta,\delta}(\tilde{f})(x, v, t, I) - \mathcal{M}_{\nu,\theta,\delta}(f)(x, v, t, I) \right\} ds \\
 &\quad - \left(\int_t^{t+\Delta t} (t + \Delta t - s) v^1 \partial_x \mathcal{M}_{\nu,\theta,\delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) \right. \\
 &\quad \left. - (s - t) \partial_t \mathcal{M}_{\nu,\theta,\delta}(f)(x_{\theta_1}, v, t_{\theta_1}, I) \right) ds \\
 &= \mathcal{I}_{51} + \mathcal{I}_{52}.
 \end{aligned}$$

For \mathcal{I}_{51} , we use Proposition 5.2 to get

$$\left\| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}) - \mathcal{M}_{\nu,\theta,\delta}(f) \right\|_{L_q^\infty} \leq C_{Lip} \left\| \tilde{f} - f \right\|_{L_q^\infty}.$$

Next, we use the mean value theorem to obtain

$$\left\| \tilde{f} - f \right\|_{L_q^\infty} = \left\| \Delta t v^1 \partial_x f \right\|_{L_q^\infty} \leq \|f\|_{L_{1,q+1}^\infty} \Delta t \leq C_{2,1} e^{C_{2,2} T^f} \left(\|f_0\|_{L_{1,q+1}^\infty} + 1 \right) \Delta t.$$

In the last line, we use Theorem 3.1. Then,

$$|\mathcal{I}_{51}| \leq C_{2,1} e^{C_{2,2} T^f} \left(\|f_0\|_{L_{1,q+1}^\infty} + 1 \right) (\Delta t)^2.$$

To estimate \mathcal{I}_{52} , we use Proposition 5.5:

$$\|v^1 \partial_x \mathcal{M}_{\nu,\theta,\delta}(f)\|_{L^\infty}, \quad \|\partial_t \mathcal{M}_{\nu,\theta,\delta}(f)\|_{L^\infty} \leq C \left(\|f_0\|_{L_{1,q+1}^\infty} + 1 \right),$$

then

$$|\mathcal{I}_{52}| \leq 2C \left(\|f_0\|_{L^\infty_{1,q+1}} + 1 \right) (\Delta t)^2.$$

Therefore, R_1 is estimated by

$$|R_1| \leq C(\Delta t)^2.$$

For R_2 , we use Proposition 5.4 Theorem 3.1 to obtain

$$\|(\mathcal{M}_{\nu,\theta,\delta}(f) - f)\|_{L^\infty_q} \leq \|\mathcal{M}_{\nu,\theta,\delta}(f)\|_{L^\infty_q} + \|f\|_{L^\infty_q} \leq C \left\{ \|f_0\|_{L^\infty_q} + 1 \right\},$$

from which we have

$$\begin{aligned} |R_2| &\leq \left| \frac{1}{\kappa} \int_t^{t+\Delta t} (s-t-\Delta t) A_{\nu,\theta}(\mathcal{M}_{\nu,\theta,\delta}(f) - f)(x_{\theta_2}, v, t_{\theta_2}, I) \, ds \right| \\ &\leq \frac{A_{\nu,\theta}}{\kappa} \|(\mathcal{M}_{\nu,\theta,\delta}(f) - f)\|_{L^\infty_q} \int_t^{t+\Delta t} (s-t-\Delta t) A_{\nu,\theta} \, ds \\ &\leq C \left\{ \|f_0\|_{L^\infty_q} + 1 \right\} (\Delta t)^2. \end{aligned}$$

This completes the proof. □

6. ESTIMATE OF $\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}(t^n)) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^n)$

The goal of this section is to establish the discrepancy estimate of the continuous ellipsoidal Gaussian $\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}(t^n))$ in (1.2) and the discrete one $\mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^n)$ in (2.2).

Lemma 6.1. *Let $\tilde{f}(t^n)$ and \tilde{f}^n denote the continuous and the discrete solutions at t^n . Then,*

$$\left\| \tilde{f}(t^n) - \tilde{f}^n \right\|_{L^\infty_q} \leq \|f(t^n) - f^n\|_{L^\infty_q} + \frac{C_{2,1}}{2} e^{C_{2,2}T^f} \left\{ \|f_0\|_{L^\infty_{2,q}} + 1 \right\} (\Delta x)^2,$$

where $C_{2,1}, C_{2,2}$ are defined in Theorem 3.1.

Proof. Recalling (2.1), we compute $\tilde{f}^n_{i,j,k}$ as

$$\tilde{f}^n_{i,j,k} := a_j f^n_{s,j,k} + (1 - a_j) f^n_{s+1,j,k}, \quad a_j = (x_{s+1} - x(i, j)) / \Delta x.$$

Also, we use Taylor’s theorem to obtain

$$\begin{aligned} \tilde{f}(x_i, v_j, t^n, I_k) &= f(x_i - v_j^1 \Delta t, v_j, t^n, I_k) \\ &= a_j \left(f(x_s, v_j, t^n, I_k) + \frac{(x_i - \Delta t v_j^1 - x_s)^2}{2} \partial_{xx} f(x_{\xi_1}, v_j, t^n, I_k) \right) \\ &\quad + (1 - a_j) \left(f(x_{s+1}, v_j, t^n, I_k) + \frac{(x_i - \Delta t v_j^1 - x_{s+1})^2}{2} \partial_{xx} f(x_{\xi_2}, v_j, t^n, I_k) \right), \end{aligned} \tag{6.1}$$

where x_{ξ_1} lies between x_s and $x_i - v_j^1 \Delta t$, and x_{ξ_2} lies between x_{s+1} and $x_i - v_j^1 \Delta t$. Now, we estimate the discrepancy of $\tilde{f}(x_i, v_j, t^n, I_k)$ and $\tilde{f}^n_{i,j,k}$ as

$$\begin{aligned} \left| \tilde{f}(t^n) - \tilde{f}^n \right| &\leq a_j |f(x_s, v_j, t^n, I_k) - f_{s,j,k}^n| + (1 - a_j) |f(x_{s+1}, v_j, t^n, I_k) - f_{s+1,j,k}^n| \\ &\quad + a_j \frac{(\Delta x)^2}{2} |\partial_{xx} f(x_{\xi_1}, v, t^n, I)| + (1 - a_j) \frac{(\Delta x)^2}{2} |\partial_{xx} f(x_{\xi_2}, v_j, t^n, I_k)|. \end{aligned} \tag{6.2}$$

We also note that Theorem 3.1 imposes

$$\|\partial_{xx} f(t^n)\|_{L_q^\infty} \leq \|f(t^n)\|_{L_{2,q}^\infty} \leq C_{2,1} e^{C_{2,2} T^f} \left(\|f_0\|_{L_{2,q}^\infty} + 1 \right).$$

This, combined with (6.2), gives

$$\begin{aligned} \left\| \tilde{f}(t^n) - \tilde{f}^n \right\|_{L_q^\infty} &\leq a_j \|f(t^n) - f^n\|_{L_q^\infty} + (1 - a_j) \|f(t^n) - f^n\|_{L_q^\infty} + \frac{(\Delta x)^2}{2} \|\partial_{xx} f\|_{L_q^\infty} \\ &\leq \|f(t^n) - f^n\|_{L_q^\infty} + 2 \|f(t^n)\|_{L_{2,q}^\infty} (\Delta x)^2 \\ &\leq \|f(t^n) - f^n\|_{L_q^\infty} + \frac{C_{2,1}}{2} e^{C_{2,2} T^f} \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\} (\Delta x)^2, \end{aligned}$$

which completes the proof. □

Lemma 6.2. *Suppose that $q > 5 + \delta$ and $\Delta v, \Delta I$ satisfies the condition (4.3). Let $\Phi(v, I)$ denote one of $1, v, |v|^2, I^{\frac{2}{5}}, v^m v^n$ ($1 \leq m, n \leq 3$) and $\Phi_{j,k} := \Phi(v_j, I_k)$, then we have*

$$\begin{aligned} &\left| \sum_{j,k} \tilde{f}_{i,j,k}^n \Phi_{j,k} (\Delta v)^3 \Delta I - \int_{\mathbb{R}^3 \times \mathbb{R}_+} \tilde{f}(x_i, v, t^n, I) \Phi(v, I) \, dv \, dI \right| \\ &\leq \bar{C}_1 \left\| \tilde{f}(t^n) - \tilde{f}^n \right\|_{L_q^\infty} + \bar{C}_2 \left(\|f_0\|_{L_{2,q}^\infty} + 1 \right) \left((\Delta x)^2 + \Delta v \Delta t + \Delta v + \Delta I \right) \end{aligned}$$

for some positive constants \bar{C}_1 and \bar{C}_2 which depend on $\delta, q, C_{2,1}, C_{2,2}, T^f$.

Proof. Let $\Delta_{j,k}$ denotes a domain such that

$$(v_j, I_k) \in \Delta_{j,k} = [v_j^1, v_j^1 + \Delta v) \times [v_j^2, v_j^2 + \Delta v) \times [v_j^3, v_j^3 + \Delta v) \times [I_k, I_{k+1}).$$

With this, we have

$$\begin{aligned} &\sum_{j,k} \tilde{f}_{i,j,k}^n \Phi_{j,k} (\Delta v)^3 \Delta I - \int_{\mathbb{R}^3 \times \mathbb{R}_+} \tilde{f}(x_i, v, t^n, I) \Phi(v, I) \, dv \, dI \\ &= \sum_{j,k} \tilde{f}_{i,j,k}^n \Phi_{j,k} (\Delta v)^3 \Delta I - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \Phi(v, I) \, dv \, dI \\ &= \left(\sum_{j,k} \tilde{f}_{i,j,k}^n \Phi_{j,k} (\Delta v)^3 \Delta I - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \Phi_{j,k} \, dv \, dI \right) \\ &\quad + \left(\sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \Phi_{j,k} \, dv \, dI - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \Phi(v, I) \, dv \, dI \right) \\ &= \mathcal{I}_{61} + \mathcal{I}_{62}. \end{aligned}$$

From (6.1) and Taylor's theorem, we have

$$\begin{aligned}
 \tilde{f}(x_i, v, t^n, I) &= f(x_i - v^1 \Delta t, v, t^n, I) \\
 &= f(x_i - v_j^1 \Delta t, v_j, t^n, I_k) + (v_j^1 - v^1) \Delta t \partial_x f(z_{\theta_1}) \\
 &\quad + (v - v_j) \cdot \nabla_v f(z_{\theta_2}) + (I - I_k) \partial_I f(z_{\theta_3}) \\
 &= a_j f(x_s, v_j, t^n, I_k) + (1 - a_j) f(x_{s+1}, v_j, t^n, I_k) + R,
 \end{aligned}$$

where R is given by

$$\begin{aligned}
 R &= (v_j^1 - v^1) \Delta t \partial_x f(z_{\theta_1}) + (v - v_j) \cdot \nabla_v f(z_{\theta_2}) + (I - I_k) \partial_I f(z_{\theta_3}) \\
 &\quad + a_j \frac{(x_i - \Delta t v_j^1 - x_s)^2}{2} \partial_{xx} f(x_{\xi_1}, v_j, t^n, I_k) \\
 &\quad + (1 - a_j) \frac{(x_i - \Delta t v_j^1 - x_{s+1})^2}{2} \partial_{xx} f(x_{\xi_2}, v_j, t^n, I_k),
 \end{aligned}$$

where $x_{\xi_1}, x_{\xi_2} \in [x_s, x_{s+1})$ and $z_{\theta_\ell} := (x_s + \theta_{\ell x} \Delta x, v_j + \theta_{\ell v} \Delta v, t^n, I_k + \theta_{\ell I} \Delta I)$ for some $\theta_{\ell x}, \theta_{\ell I} \in [0, 1)$, $\theta_{\ell v} \in [0, 1)^3$, ($\ell = 1, 2, 3$). To estimate \mathcal{I}_{61} , we first separate it into two parts:

$$\begin{aligned}
 \mathcal{I}_{61} &= \sum_{j,k} \tilde{f}_{i,j,k}^n \Phi_{jk} (\Delta v)^3 \Delta I - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \Phi_{jk} \, dv \, dI \\
 &= \sum_{j,k} \int_{\Delta_{j,k}} a_j (f_{s,j,k}^n - f(x_s, v_j, t^n, I_k)) + (1 - a_j) (f_{s+1,j,k}^n - f(x_{s+1}, v_j, t^n, I_k)) \Phi_{jk} \, dv \, dI \\
 &\quad - \sum_{j,k} \int_{\Delta_{j,k}} R \Phi_{jk} \, dv \, dI \\
 &= \mathcal{I}_{611} + \mathcal{I}_{612}.
 \end{aligned}$$

We bound \mathcal{I}_{611} as follows:

$$\begin{aligned}
 |\mathcal{I}_{611}| &\leq \sum_{j,k} (a_j |f_{s,j,k}^n - f(x_s, v_j, t^n, I_k)| + (1 - a_j) |f_{s+1,j,k}^n - f(x_{s+1}, v_j, t^n, I_k)|) |\Phi_{jk}| (\Delta v)^3 \Delta I \\
 &\leq \left\| \tilde{f}(t^n) - \tilde{f}^n \right\|_{L^q} \sum_{j,k} \frac{|\Phi_{jk}|}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} (\Delta v)^3 \Delta I \\
 &\leq 2\bar{C}_{\delta, q-2} \left\| \tilde{f}(t^n) - \tilde{f}^n \right\|_{L^q}. \tag{6.3}
 \end{aligned}$$

In the last line, the inequality comes from Theorem 4.5. For \mathcal{I}_{612} , we bound R using Theorem 3.1 and the following inequality:

$$\begin{aligned}
 |\partial_x f(z_{\theta_\ell})|, |\partial_{xx} f(z_{\theta_\ell})|, |\nabla_v f(z_{\theta_\ell})|, |\partial_I f(z_{\theta_\ell})| &\leq \frac{\|f\|_{L_{2,q}^\infty}}{\left(1 + |v_j + \theta_{\ell v} \Delta v|^2 + (I_k + \theta_{\ell I} \Delta I)^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} \\
 &\leq \frac{\|f\|_{L_{2,q}^\infty}}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}}.
 \end{aligned}$$

That is,

$$|R| \leq C_{2,1} e^{C_{2,2} T^f} \left((\Delta x)^2 + \Delta v \Delta t + \Delta v + \Delta I \right) \left(\frac{\|f_0\|_{L_{2,q}^\infty} + 1}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} \right).$$

Using this, we have

$$\begin{aligned} |\mathcal{I}_{612}| &\leq \sum_{j,k} \int_{\Delta_{j,k}} |R| |\Phi_{jk}| \, dv \, dI \\ &\leq C_{2,1} e^{C_{2,2} T^f} ((\Delta x)^2 + \Delta v \Delta t + \Delta v + \Delta I) \left(\|f_0\|_{L_{2,q}^\infty} + 1 \right) \sum_{j,k} \int_{\Delta_{j,k}} \frac{|\Phi_{jk}|}{\left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} \, dv \, dI \\ &\leq 2\bar{C}_{\delta,q-2} C_{2,1} e^{C_{2,2} T^f} ((\Delta x)^2 + \Delta v \Delta t + \Delta v + \Delta I) \left(\|f_0\|_{L_{2,q}^\infty} + 1 \right), \end{aligned}$$

where the last inequality holds as in (6.3). For \mathcal{I}_{62} , we consider $(v, I) \equiv (v_j + \xi \Delta v, I_k + \eta \Delta I) \in \Delta_{j,k}$, for $\xi, \eta \in [0, 1)$. Then, we have from $\Delta v \leq \frac{1}{2}$ that

$$|v_j - v| \leq \sqrt{3} \Delta v, \quad \left| |v_j|^2 - |v|^2 \right| \leq \sqrt{3} \Delta v (|v_j| + |v|) \leq \sqrt{3} \Delta v (\sqrt{3} \Delta v + 2|v|) \leq 6 \Delta v (1 + |v|^2)$$

and, for $1 \leq m, n \leq 3$,

$$\begin{aligned} |v_j^m v_j^n - v^m v^n| &\leq |v_j^m v_j^n - v_j^m v^n + v_j^m v^n - v^m v^n| \\ &\leq |v_j^m v_j^n - v_j^m v^n| + |v_j^m v^n - v^m v^n| \\ &\leq \Delta v |v_j^m| + \Delta v |v^n| \\ &\leq 3 \Delta v (1 + |v|^2). \end{aligned}$$

Moreover, for $I \in [I_k, I_{k+1})$, the mean-value theorem implies

$$\left| I_k^{\frac{2}{\delta}} - I^{\frac{2}{\delta}} \right| \leq |I_k - I| \frac{2}{\delta} (I + \Delta I)^{\frac{2}{\delta} - 1} \leq \frac{2 \Delta I}{\delta} (I + \Delta I)^{\frac{2}{\delta} - 1}, \quad 0 < \delta \leq 2.$$

This, together with the assumption $\Delta I < \frac{1}{2}$ in (4.3), gives

$$\left| I_k^{\frac{2}{\delta}} - I^{\frac{2}{\delta}} \right| \leq \frac{2 \Delta I}{\delta} (I + 1)^{\frac{2}{\delta} - 1} \leq \frac{2 \Delta I}{\delta} \left(2^{\frac{2}{\delta} - 1} + (2I)^{\frac{2}{\delta} - 1} \right) \leq 2^{\frac{2}{\delta}} \frac{\Delta I}{\delta} \left(1 + I^{\frac{2}{\delta}} \right).$$

To sum up,

$$|\Phi_{jk} - \Phi(v, I)| \leq 6 \Delta v (1 + |v|^2) + 2^{\frac{2}{\delta}} \frac{\Delta I}{\delta} \left(1 + I^{\frac{2}{\delta}} \right).$$

Now, \mathcal{I}_{62} is estimated by

$$\begin{aligned} |\mathcal{I}_{62}| &\leq \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) |\Phi_{jk} - \Phi(v, I)| \, dv \, dI \\ &\leq \|f(t^n)\|_{L_q^\infty} \sum_{j,k} \left\{ \int_{\Delta_{j,k}} \frac{6 \Delta v (1 + |v|^2)}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} \, dv \, dI + \int_{\Delta_{j,k}} \frac{2^{\frac{2}{\delta}} \frac{\Delta I}{\delta} \left(1 + I^{\frac{2}{\delta}}\right)}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q}{2}}} \, dv \, dI \right\} \\ &\leq \|f(t^n)\|_{L_q^\infty} \left(6 \Delta v + 2^{\frac{2}{\delta}} \frac{\Delta I}{\delta} \right) \sum_{j,k} \int_{\Delta_{j,k}} \frac{1}{\left(1 + |v|^2 + I^{\frac{2}{\delta}}\right)^{\frac{q-2}{2}}} \, dv \, dI \\ &\leq \left(6 + 2^{\frac{2}{\delta}} \frac{1}{\delta} \right) (\Delta v + \Delta I) \bar{C}_{\delta,q-2} C_{2,1} e^{C_{2,2} T^f} \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\}. \end{aligned}$$

where $\bar{C}_{\delta,q-2}$ is given in Definition 4.1. Combining \mathcal{I}_{61} and \mathcal{I}_{62} , we obtain the desired result. □

Lemma 6.3. *Suppose that $q > 5 + \delta$ and $\Delta v, \Delta I$ satisfy the condition (4.3). Then,*

$$\begin{aligned} & \left| \tilde{\rho}_i - \tilde{\rho}(x_i, t^n) \right|, \left| \tilde{U}_i - \tilde{U}(x_i, t^n) \right|, \left| \left(\tilde{T}_{\nu, \theta}^{\alpha, \beta} \right)_i^n - \tilde{T}_{\nu, \theta}^{\alpha, \beta}(x_i, t^n) \right| \\ & \leq C \|f(t^n) - f^n\|_{L^\infty_q} + C \left\{ \|f_0\|_{L^\infty_{2,q}} + 1 \right\} \left\{ (\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t \right\}. \end{aligned}$$

where $C > 0$ is a constant and the (α, β) element of $\tilde{T}_{\nu, \theta}$ is denoted by $\tilde{T}_{\nu, \theta}^{\alpha, \beta}$ for $1 \leq \alpha, \beta \leq 3$.

Proof. Consider the case $\Phi_{jk} \equiv 1$ in Lemma 6.2, then

$$\begin{aligned} \left| \tilde{\rho}_i^n - \tilde{\rho}(x_i, t^n) \right| &= \left| \sum_{j,k} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \, dv \, dI \right| \\ &\leq \bar{C}_1 \|f(t^n) - f^n\|_{L^\infty_q} + \bar{C}_2 \left\{ \|f_0\|_{L^\infty_{2,q}} + 1 \right\} \left\{ (\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t \right\}. \end{aligned}$$

The number \bar{C}_1 and \bar{C}_2 are constants in Lemma 6.2. For the second estimate, we begin with

$$\left| \tilde{U}_i^n - \tilde{U}(x_i, t^n) \right| = \left| \frac{\tilde{\rho}_i^n \tilde{U}_i^n - \tilde{\rho}(x_i, t^n) \tilde{U}(x_i, t^n)}{\tilde{\rho}_i^n} + \frac{\tilde{\rho}(x_i, t^n) \tilde{U}(x_i, t^n) - \tilde{\rho}_i^n \tilde{U}(x_i, t^n)}{\tilde{\rho}_i^n} \right|.$$

From C^n in Definition 4.2, we have

$$\frac{1}{\tilde{\rho}_i^n} \leq \frac{2}{\bar{C}_{a,b} C_0^1} e^{\frac{A_{\nu, \theta}}{\kappa} T^f},$$

which together with Lemma 6.2 gives

$$\left| \tilde{\rho}_i^n \tilde{U}_i^n - \tilde{\rho} \tilde{U}(x_i, t^n) \right| \leq \bar{C}_1 \left\| \tilde{f}(t^n) - \tilde{f}^n \right\|_{L^\infty_q} + \bar{C}_2 \left(\|f_0\|_{L^\infty_{2,q}} + 1 \right) \left((\Delta x)^2 + \Delta v \Delta t + \Delta v + \Delta I \right).$$

Moreover, we have

$$\begin{aligned} \left| \tilde{\rho} \tilde{U}(x_i, t^n) \right| &= \left| \int_{\mathbb{R}^3 \times \mathbb{R}_+} v \tilde{f}(x_i, v, t^n, I_k) \, dv \, dI \right| \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}_+} |v| f(x_i - v^1 \Delta t, v, t^n, I) \frac{\left(1 + |v|^2 + I^{\frac{2}{3}} \right)^{\frac{q}{2}}}{\left(1 + |v|^2 + I^{\frac{2}{3}} \right)^{\frac{q}{2}}} \, dv \, dI \\ &\leq \|f(t^n)\|_{L^\infty_q} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \frac{1}{\left(1 + |v|^2 + I^{\frac{2}{3}} \right)^{\frac{q-1}{2}}} \, dv \, dI \\ &= \bar{C}_{\delta, q-1} C_{2,1} e^{C_{2,2} T^f} \left\{ \|f_0\|_{L^\infty_{2,q}} + 1 \right\}. \end{aligned}$$

Therefore,

$$\begin{aligned} \left| \tilde{U}_i^n - \tilde{U}(x_i, t^n) \right| &= \left| \frac{\tilde{\rho}_i^n \tilde{U}_i^n - \tilde{\rho}(x_i, t^n) \tilde{U}(x_i, t^n)}{\tilde{\rho}_i^n} + \frac{\tilde{\rho}(x_i, t^n) \tilde{U}(x_i, t^n) - \tilde{\rho}_i^n \tilde{U}(x_i, t^n)}{\tilde{\rho}_i^n} \right| \\ &= \frac{1}{\tilde{\rho}_i^n} \left| \sum_{j,k} \tilde{f}_{i,j,k}^n v_j (\Delta v)^3 \Delta I - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) v \, dv \, dI \right| \end{aligned}$$

$$\begin{aligned}
 & + \frac{\tilde{U}(x_i, t^n)}{\tilde{\rho}_i^n} \left| \sum_{j,k} \tilde{f}_{i,j,k}^n (\Delta v)^3 \Delta I - \sum_{j,k} \int_{\Delta_{j,k}} \tilde{f}(x_i, v, t^n, I) \, dv \, dI \right| \\
 & \leq C \|f(t^n) - f^n\|_{L_q^\infty} + C \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\} \{(\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t\},
 \end{aligned}$$

for a constant $C > 0$.

For the estimate of $\tilde{T}_{\nu,\theta}$, we recall its definition in to get

$$\begin{aligned}
 \tilde{\rho}_i^n \left(\tilde{T}_{\nu,\theta} \right)_i^n - \tilde{\rho} \tilde{T}_{\nu,\theta} &= (1 - \theta) \tilde{\rho}_i^n \left\{ (1 - \nu) \left(\tilde{T}_{\text{tr}} \right)_i^n Id + \nu \tilde{\Theta}_i^n \right\} + \theta \tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n Id \\
 & + \tilde{\rho}_i^n \left[\frac{(1 - \theta) \nu \Delta t A_{\nu,\theta} \theta}{\Delta t + \kappa} \left(\tilde{T}_\delta \right)_i^n Id + \frac{(1 - \theta) \nu \Delta t (1 - A_{\nu,\theta} \theta)}{\Delta t + \kappa} \left(\tilde{T}_{\text{tr}} \right)_i^n Id - (1 - \theta) \nu \frac{\Delta t}{\Delta t + \kappa} \tilde{\Theta}_i^n \right] \\
 & - (1 - \theta) \tilde{\rho} \left\{ (1 - \nu) \tilde{T}_{\text{tr}} Id + \nu \tilde{\Theta} \right\} - \theta \tilde{\rho} \tilde{T}_\delta Id \\
 & = (1 - \theta) \sum_{j,k} \tilde{f}_{i,j,k}^n \left\{ \frac{(1 - \nu)}{3} |v_j - \tilde{U}_i^n|^2 Id + \nu (v_j - \tilde{U}_i^n) \otimes (v - \tilde{U}_i^n) \right\} (\Delta v)^3 \Delta I \\
 & + \frac{\theta}{3 + \delta} \sum_{j,k} \tilde{f}_{i,j,k}^n \left\{ |v_j - \tilde{U}_i^n|^2 + 2I^{\frac{2}{3}} \right\} Id (\Delta v)^3 \Delta I \\
 & - (1 - \theta) \int_{\mathbb{R}^3 \times \mathbb{R}^+} \tilde{f} \left\{ \frac{(1 - \nu)}{3} |v - \tilde{U}|^2 Id + \nu (v - \tilde{U}) \otimes (v - \tilde{U}) \right\} \, dv \, dI \\
 & - \frac{\theta}{3 + \delta} \int_{\mathbb{R}^3 \times \mathbb{R}^+} \tilde{f} \left\{ |v - \tilde{U}|^2 + 2I^{\frac{2}{3}} \right\} Id \, dv \, dI \\
 & + \tilde{\rho}_i^n \left[\frac{(1 - \theta) \nu \Delta t A_{\nu,\theta} \theta}{\Delta t + \kappa} \left(\tilde{T}_\delta \right)_i^n Id + \frac{(1 - \theta) \nu \Delta t (1 - A_{\nu,\theta} \theta)}{\Delta t + \kappa} \left(\tilde{T}_{\text{tr}} \right)_i^n Id - (1 - \theta) \nu \frac{\Delta t}{\Delta t + \kappa} \tilde{\Theta}_i^n \right],
 \end{aligned}$$

which can be rewritten as

$$\begin{aligned}
 & \tilde{\rho}_i^n \left(\tilde{T}_{\nu,\theta} \right)_i^n - \tilde{\rho} \tilde{T}_{\nu,\theta} \\
 & = \left\{ (1 - \theta) \frac{1 - \nu}{3} + \frac{\theta}{3 + \delta} \right\} \left(\sum_{j,k} \tilde{f}_{i,j,k}^n |v_j - \tilde{U}_i^n|^2 (\Delta v)^3 \Delta I - \int_{\mathbb{R}^3 \times \mathbb{R}^+} \tilde{f} |v - \tilde{U}|^2 \, dv \, dI \right) Id \\
 & + (1 - \theta) \nu \left(\sum_{j,k} \tilde{f}_{i,j,k}^n (v_j - \tilde{U}_i^n) \otimes (v_j - \tilde{U}_i^n) (\Delta v)^3 \Delta I - \int_{\mathbb{R}^3 \times \mathbb{R}^+} \tilde{f} (v - \tilde{U}) \otimes (v - \tilde{U}) \, dv \, dI \right) \\
 & + \frac{2\theta}{3 + \delta} \left(\sum_{j,k} \tilde{f}_{i,j,k}^n I_k^{\frac{2}{3}} (\Delta v)^3 \Delta I - \int_{\mathbb{R}^3 \times \mathbb{R}^+} \tilde{f} I^{\frac{2}{3}} \, dv \, dI \right) Id \\
 & + \tilde{\rho}_i^n \left[\frac{(1 - \theta) \nu \Delta t A_{\nu,\theta} \theta}{\Delta t + \kappa} \left(\tilde{T}_\delta \right)_i^n Id + \frac{(1 - \theta) \nu \Delta t (1 - A_{\nu,\theta} \theta)}{\Delta t + \kappa} \left(\tilde{T}_{\text{tr}} \right)_i^n Id - (1 - \theta) \nu \frac{\Delta t}{\Delta t + \kappa} \tilde{\Theta}_i^n \right] \\
 & \equiv \mathcal{I}_{71} + \mathcal{I}_{72} + \mathcal{I}_{73} + \mathcal{I}_{74}.
 \end{aligned}$$

For \mathcal{I}_{71} , we use Lemma 6.2 to obtain

$$\begin{aligned}
 & \sum_{j,k} \tilde{f}_{i,j,k}^n |v_j - \tilde{U}_i^n|^2 (\Delta v)^3 \Delta I - \int_{\mathbb{R}^3 \times \mathbb{R}^+} \tilde{f} |v_j - \tilde{U}|^2 \, dv \, dI \\
 & \leq C \|f(t^n) - f^n\|_{L_q^\infty} + C \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\} \{(\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t\}.
 \end{aligned}$$

Similar estimates hold for \mathcal{I}_{72} and \mathcal{I}_{73} . Together with

$$\left| \frac{(1-\theta)\nu\Delta t A_{\nu,\theta}}{\Delta t + \kappa} \right|, \quad \left| \frac{(1-\theta)\nu\Delta t(1-A_{\nu,\theta})}{\Delta t + \kappa} \right|, \quad \left| (1-\theta)\nu \frac{\Delta t}{\Delta t + \kappa} \right| \leq C \frac{\Delta t}{\Delta t + \kappa},$$

the macroscopic quantities in \mathcal{I}_{74} are also bounded by D^n in Definition 4.2. Therefore, for $1 \leq \alpha, \beta \leq 3$, we have

$$\begin{aligned} \left| \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n - \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n) \right| &= \left| \frac{\tilde{\rho}_i^n \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n - \tilde{\rho}(x_i, t^n) \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n)}{\tilde{\rho}_i^n} + \frac{\tilde{\rho}(x_i, t^n) \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n) - \tilde{\rho}_i^n \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n)}{\tilde{\rho}_i^n} \right| \\ &\leq \frac{1}{\tilde{\rho}_i^n} \left| \tilde{\rho}_i^n \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n - \tilde{\rho}(x_i, t^n) \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n) \right| + \frac{\left| \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n) \right|}{\tilde{\rho}_i^n} \left| \tilde{\rho}(x_i, t^n) - \tilde{\rho}_i^n \right| \\ &\leq C \|f(t^n) - f^n\|_{L_q^\infty} + C \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\} \left\{ (\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t \right\}, \end{aligned}$$

for a constant $C > 0$. This completes the proof. \square

The following is the main result of this section.

Proposition 6.4. *Suppose that $q > 5 + \delta$ and $\Delta v, \Delta I$ satisfy the condition (4.3). Then,*

$$\left\| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}(t^n)) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^n) \right\|_{L_q^\infty} \leq C \|f(t^n) - f^n\|_{L_q^\infty} + C \left\{ \|f_0\|_{L_{2,q}^\infty} + 1 \right\} \left\{ (\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t \right\}.$$

Proof. We begin by writing

$$\begin{aligned} &\mathcal{M}_{\nu,\theta,\delta}(\tilde{f})(x_i, v_j, I_k, t^n) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k} \\ &= \mathcal{M}_{\nu,\theta,\delta}(\tilde{\rho}(x_i, t^n), \tilde{U}(x_i, t^n), \tilde{\mathcal{T}}_{\nu,\theta}(x_i, t^n))(v_j, I_k) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{\rho}_i^n, \tilde{U}_i^n, (\tilde{\mathcal{T}}_{\nu,\theta})_i^n)(v_j, I_k). \end{aligned}$$

Then,

$$\begin{aligned} &\mathcal{M}_{\nu,\theta,\delta}(\tilde{\rho}(x_i, t^n), \tilde{U}(x_i, t^n), \tilde{\mathcal{T}}_{\nu,\theta}(x_i, t^n))(v_j, I_k) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{\rho}_i^n, \tilde{U}_i^n, (\tilde{\mathcal{T}}_{\nu,\theta})_i^n)(v_j, I_k) \\ &= (\tilde{\rho}(x_i, t^n) - \tilde{\rho}_i^n) \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial \rho}(\eta) d\eta + (\tilde{U}(x_i, t^n) - \tilde{U}_i^n) \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial U}(\eta) d\eta \\ &\quad + \sum_{1 \leq \alpha, \beta \leq 3} \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n) - (\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta})_i^n \right) \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) d\eta \\ &\quad + \left(\tilde{\mathcal{T}}_\theta(x_i, t^n) - (\tilde{\mathcal{T}}_\theta)_i^n \right) \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial T_\theta}(\eta) d\eta \\ &\equiv J_1 + J_2 + J_3 + J_4, \end{aligned}$$

where

$$\frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial X}(\eta) := \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial X} \Big|_{X \equiv (\rho, U, \mathcal{T}_{\nu,\theta}, T_\theta) = (\tilde{\rho}_i^n(\eta), \tilde{U}_i^n(\eta), (\tilde{\mathcal{T}}_{\nu,\theta})_i^n(\eta), (\tilde{\mathcal{T}}_\theta)_i^n(\eta))}$$

and

$$\begin{aligned} &\left(\tilde{\rho}_i^n(\eta), \tilde{U}_i^n(\eta), (\tilde{\mathcal{T}}_{\nu,\theta})_i^n(\eta), (\tilde{\mathcal{T}}_{I,\delta})_i^n(\eta), (\tilde{\mathcal{T}}_\theta)_i^n(\eta), (\tilde{\mathcal{T}}_\delta)_i^n(\eta) \right) \\ &:= (1-\eta) \left(\tilde{\rho}(x_i, t^n), \tilde{U}(x_i, t^n), \tilde{\mathcal{T}}_{\nu,\theta}(x_i, t^n), (\tilde{\mathcal{T}}_{I,\delta})(x_i, t^n), (\tilde{\mathcal{T}}_\theta)(x_i, t^n), (\tilde{\mathcal{T}}_\delta)(x_i, t^n) \right) \end{aligned}$$

$$+ \eta \left(\tilde{\rho}_i^n, \tilde{U}_i^n, \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n, \left(\tilde{\mathcal{T}}_{I,\delta} \right)_i^n, \left(\tilde{\mathcal{T}}_{\theta} \right)_i^n, \left(\tilde{\mathcal{T}}_{\delta} \right)_i^n \right)$$

for $\eta \in [0, 1]$. Since each macroscopic quantity is given by the convex combination of continuous and discrete macroscopic fields, its estimate can be directly obtained by combining the estimates of continuous solution in Theorem 3.1 and those of discrete solution in Theorem 4.5 as follows:

$$\begin{aligned} \tilde{\rho}_i^n(\eta), \tilde{U}_i^n(\eta), \left(\tilde{\mathcal{T}}_{\delta} \right)_i^n(\eta), \left(\tilde{\mathcal{T}}_{\theta} \right)_i^n(\eta) &\leq C_{Tf} \\ \tilde{\rho}_i^n(\eta), \left(\tilde{\mathcal{T}}_{\delta} \right)_i^n(\eta), \left(\tilde{\mathcal{T}}_{\theta} \right)_i^n(\eta) &\geq C_{Tf} e^{-C_{Tf}} \\ k^\top \left\{ \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right\} k &\geq C_{Tf} e^{-C_{Tf}} |k|^2, \quad k \in \mathbb{R}^3. \end{aligned} \tag{6.4}$$

On the other hand, Brum-Minkowski inequality implies that

$$\begin{aligned} \det \left\{ \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right\} &= \det \left\{ (1 - \eta) \tilde{\mathcal{T}}_{\nu,\theta}(x_i, t^n) + \eta \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n \right\} \\ &\geq \det \left\{ \tilde{\mathcal{T}}_{\nu,\theta}(x_i, t^n) \right\}^{1-\eta} \det \left\{ \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n \right\}^\eta \\ &\geq \{ C_{Tf} e^{-C_{Tf}} \}^{1-\eta} \{ C_{Tf} e^{-C_{Tf}} \}^\eta \\ &\geq C_{Tf} e^{-C_{Tf}}, \end{aligned}$$

from which we have

$$\begin{aligned} \mathcal{M}_{\nu,\theta,\delta}(\eta)(v_j, I_k) &= \frac{\tilde{\rho}_i^n(\eta) \Lambda_\delta}{\sqrt{\det \left(2\pi \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right) \left(\left(\tilde{\mathcal{T}}_{\theta} \right)_i^n(\eta) \right)^{\frac{\delta}{2}}}} \\ &\times \exp \left(- \frac{(v_j - \tilde{U}_i^n(\eta))^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} (v_j - \tilde{U}_i^n(\eta))}{2} - \frac{I_k^{\frac{2}{\delta}}}{\left(\tilde{\mathcal{T}}_{\theta} \right)_i^n(\eta)} \right) \\ &\leq C_{Tf} \exp \left(-C_{Tf} \left(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{\frac{2}{\delta}} \right) \right). \end{aligned}$$

Now, we return to the estimate of J_i for $i = 1, 2, 3, 4$. We bound J_1 with

$$\left| \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial \rho}(\eta) d\eta \right| = \int_0^1 \frac{\mathcal{M}_{\nu,\theta,\delta}}{\tilde{\rho}_i^n(\eta)} d\eta \leq \int_0^1 C_{Tf} \exp \left(-C_{Tf} \left(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{\frac{2}{\delta}} \right) \right) d\eta.$$

For J_2 , we recall from Lemma A.2 that

$$\lambda \theta \left(\tilde{\mathcal{T}}_{\delta} \right)_i^n Id \leq \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n.$$

This, combined with Proposition 5.3, gives

$$C \theta \left(\tilde{\mathcal{T}}_{\delta} \right)_i^n(\eta) Id \leq \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta).$$

Now, we consider the following inequality:

$$\left| \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial U}(\eta) \right| \leq \left(\left| \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} (v_j - \tilde{U}_i^n(\eta)) \right| + \left| (v_j - \tilde{U}_i^n(\eta))^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} \right| \right) \mathcal{M}_{\nu,\theta,\delta}(\eta).$$

To estimate the upper bound, we introduce $X = v_j - \tilde{U}_i^n(\eta)$ and obtain

$$\begin{aligned}
 & \left| X^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} \right| \\
 & \leq \sup_{|Y| \leq 1} \left| X^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} Y \right| \\
 & \leq \sup_{|Y| \leq 1} \left| (X + Y)^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} (X + Y) - X^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} X - Y^\top \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} Y \right| \\
 & \leq \frac{C}{\theta} \sup_{|Y| \leq 1} \left| \frac{|X + Y|^2 - |X|^2 - |Y|^2}{\left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1}} \right| \\
 & \leq \frac{C}{\theta} \left(1 + |v_j - \tilde{U}(\eta)|^2 \right). \tag{6.5}
 \end{aligned}$$

In the last line, we use Lemma A.2. Similarly, we compute

$$\left| \left(\left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \right)^{-1} X \right| \leq \frac{C}{\theta} \left(1 + |v_j - \tilde{U}(\eta)|^2 \right). \tag{6.6}$$

Consequently,

$$\left| \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial U}(\eta) \, d\eta \right| \leq \int_0^1 \frac{C_{Tf}}{\theta} \left(1 + |v_j - \tilde{U}(\eta)|^2 \right) \exp \left(-C_{Tf} \left(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{\frac{2}{\beta}} \right) \right) \, d\eta.$$

To estimate J_3 , for $1 \leq \alpha, \beta \leq 3$, we compute

$$\begin{aligned}
 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) &= \frac{1}{2} \left[- \frac{1}{\det \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta)} \frac{\partial \det(\mathcal{T}_{\nu,\theta})}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \right. \\
 & \quad \left. + \left(v_j - \tilde{U}_i^n(\eta) \right)^\top \tilde{\mathcal{T}}_{\nu,\theta}^{-1}(\eta) \left(\frac{\partial(\mathcal{T}_{\nu,\theta})}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \right) \tilde{\mathcal{T}}_{\nu,\theta}^{-1}(\eta) \left(v_j - \tilde{U}(\eta) \right) \right] \mathcal{M}_{\nu,\theta,\delta}(\eta),
 \end{aligned}$$

where

$$\frac{\partial \det(\mathcal{T}_{\nu,\theta})}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) := \frac{\partial \det(\mathcal{T}_{\nu,\theta})}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}} \Big|_{\mathcal{T}_{\nu,\theta} = (\tilde{\mathcal{T}}_{\nu,\theta})_i^n(\eta)}, \quad \frac{\partial(\mathcal{T}_{\nu,\theta})}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) := \frac{\partial(\mathcal{T}_{\nu,\theta})}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}} \Big|_{\mathcal{T}_{\nu,\theta} = (\tilde{\mathcal{T}}_{\nu,\theta})_i^n(\eta)}.$$

Now, we prove the following estimates:

$$\begin{aligned}
 (\mathcal{F}_1) : & \left| \left(v_j - \tilde{U}(\eta) \right)^\top \tilde{\mathcal{T}}_{\nu,\theta}^{-1}(\eta) \left(\frac{\partial \mathcal{T}_{\nu,\theta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \right) \tilde{\mathcal{T}}_{\nu,\theta}^{-1}(\eta) \left(v_j - \tilde{U}(\eta) \right) \right| \leq \left(\frac{C}{\theta} \left(1 + |v_j - \tilde{U}(\eta)|^2 \right) \right)^2, \\
 (\mathcal{F}_2) : & \det \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \geq \theta^3 C, \\
 (\mathcal{F}_3) : & \left| \frac{\partial \det(\mathcal{T}_{\nu,\theta})_i^n}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \right| \leq C.
 \end{aligned}$$

– (\mathcal{F}_1) : we use that $\tilde{\mathcal{T}}_{\nu,\theta}^{-1}$ is symmetric matrix and $\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} = \tilde{\mathcal{T}}_{\nu,\theta}^{\beta,\alpha}$ to obtain

$$\left| X^\top \left(\frac{\partial \mathcal{T}_{\nu,\theta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \right) Y \right| = |X^\alpha Y^\beta + X^\beta Y^\alpha| \leq |X| |Y|.$$

This gives

$$\begin{aligned} & \left| (v_j - \tilde{U}(\eta))^\top \tilde{\mathcal{T}}_{\nu,\theta}^{-1}(\eta) \left(\frac{\partial \mathcal{T}_{\nu,\theta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \right) \tilde{\mathcal{T}}_{\nu,\theta}^{-1}(\eta) (v_j - \tilde{U}(\eta)) \right| \\ & \leq \left| (v_j - \tilde{U}(\eta))^\top \left((\tilde{\mathcal{T}}_{\nu,\theta})_i^n(\eta) \right)^{-1} \right| \left| \left((\tilde{\mathcal{T}}_{\nu,\theta})_i^n(\eta) \right)^{-1} (v_j - \tilde{U}(\eta)) \right| \\ & \leq \left(\frac{C}{\theta} \left(1 + |v_j - \tilde{U}(\eta)|^2 \right) \right)^2, \end{aligned}$$

where we use (6.5) and (6.6).

– (\mathcal{F}_2) : by (6.4), we have

$$\det \left(\tilde{\mathcal{T}}_{\nu,\theta} \right)_i^n(\eta) \geq \left(C\theta \left(\tilde{T}_\delta \right)_i^n(\eta)^3 \right) = \theta^3 C.$$

– (\mathcal{F}_3) : recalling the definition of $\tilde{\Theta}$, \tilde{T}_{tr} , \tilde{T}_δ and $\tilde{\mathcal{T}}_{\nu,\theta}$, for $1 \leq \alpha, \beta \leq 3$, we have

$$\begin{aligned} & \left| \tilde{\Theta}^{\alpha,\beta}(x_i, t^n) \right| \leq 3\tilde{T}_{\text{tr}}(x_i, t^n), \\ & \tilde{T}_\delta(x_i, t^n) = \frac{3}{3+\delta}\tilde{T}_{\text{tr}}(x_i, t^n) + \frac{\delta}{3+\delta}\tilde{T}_{L,\delta}(x_i, t^n) \geq \frac{3}{3+\delta}\tilde{T}_{\text{tr}}(x_i, t^n). \end{aligned}$$

and

$$\begin{aligned} \left| \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta}(x_i, t^n) \right| & \leq \theta \tilde{T}_\delta(x_i, t^n) + (1-\theta) \left\{ (1-\nu)\tilde{T}_{\text{tr}}(x_i, t^n) + \nu \left| \tilde{\Theta}^{\alpha,\beta}(x_i, t^n) \right| \right\} \\ & \leq \theta \tilde{T}_\delta(x_i, t^n) + (1-\theta)(1+2\nu)\tilde{T}_{\text{tr}}(x_i, t^n) \\ & \leq \theta \tilde{T}_\delta(x_i, t^n) + (1-\theta)(1+2\nu)\frac{3+\delta}{3}\tilde{T}_\delta(x_i, t^n) \\ & \leq (1+2\nu)\frac{3+\delta}{3}\tilde{T}_\delta(x_i, t^n). \end{aligned}$$

That is,

$$\left| \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n \right| \leq C \left(\tilde{T}_\delta \right)_i^n,$$

which implies

$$\left| \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n(\eta) \right| \leq C \left(\tilde{T}_\delta \right)_i^n(\eta) \leq C.$$

For simplicity, we only cover the case: $(\alpha, \beta) = (1, 2)$. A direct calculation gives

$$\frac{\partial \det \mathcal{T}_{\nu,\theta}}{\partial \mathcal{T}_{\nu,\theta}^{1,2}}(\eta) = \tilde{\mathcal{T}}_{\nu,\theta}^{2,3}(\eta)\tilde{\mathcal{T}}_{\nu,\theta}^{3,1}(\eta) - \tilde{\mathcal{T}}_{\nu,\theta}^{3,3}(\eta)\tilde{\mathcal{T}}_{\nu,\theta}^{2,1}(\eta),$$

which is a second order polynomial of $\left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n(\eta)$ for $1 \leq \alpha, \beta \leq 3$. Therefore,

$$\left| \frac{\partial \det \mathcal{T}_{\nu,\theta}}{\partial \mathcal{T}_{\nu,\theta}^{1,2}}(\eta) \right| \leq C,$$

for some constant C . This completes the proof for claims.

Using (\mathcal{F}_1) , (\mathcal{F}_2) and (\mathcal{F}_3) , we can bound the integral J_3 as

$$\left| \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \, d\eta \right| \leq \int_0^1 \left[\frac{C}{\theta^3} + \left(\frac{C}{\theta} \left(1 + |v_j - \tilde{U}(\eta)|^2 \right) \right)^2 \right] \mathcal{M}_{\nu,\theta,\delta}(\eta) \, d\eta.$$

Then,

$$\left| \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial \mathcal{T}_{\nu,\theta}^{\alpha,\beta}}(\eta) \, d\eta \right| \leq C \left(\frac{1}{\theta^2} + \frac{1}{\theta^3} \right) \int_0^1 \left(1 + |v_j - \tilde{U}(\eta)|^2 \right)^2 \exp \left(-C_{Tf} \left(|v_j - \tilde{U}(\eta)|^2 + I_k^{2/\delta} \right) \right) \, d\eta.$$

For J_4 , we begin with

$$\frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial T_\theta}(\eta) = \left(\frac{2I_k^{2/\delta} - \delta \tilde{T}_\theta(\eta)}{2(\tilde{T}_\theta(\eta))^2} \right) \mathcal{M}_{\nu,\theta,\delta} \leq \left(\frac{1}{(\tilde{T}_\theta(\eta))^2} + \frac{\delta}{\tilde{T}_\theta(\eta)} \right) \left(1 + I_k^{2/\delta} \right) \mathcal{M}_{\nu,\theta,\delta}.$$

Since there exist a lower bound for $\tilde{T}_\theta(\eta)$, we have

$$\left| \int_0^1 \frac{\partial \mathcal{M}_{\nu,\theta,\delta}}{\partial T_\theta}(\eta) \, d\eta \right| \leq C \left(1 + I_k^{2/\delta} \right) \exp \left(-C_{Tf} \left(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta} \right) \right).$$

Combining all the estimates for J_i , $i = 1, 2, 3, 4$, we finally obtain

$$\begin{aligned} & \left| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f})(x_i, v_j, I_k, t^n) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k} \right| \\ & \leq C \left(1 + \frac{1}{\theta} + \frac{1}{\theta^2} + \frac{1}{\theta^3} \right) \left\{ |\tilde{\rho} - \tilde{\rho}_i^n| + |\tilde{U} - \tilde{U}_i^n| + \sum_{1 \leq \alpha, \beta \leq 3} |\tilde{T}_{\nu,\theta}^{\alpha,\beta} - (\tilde{T}_{\nu,\theta}^{\alpha,\beta})_i^n| + |\tilde{T}_\theta - (\tilde{T}_\theta)_i^n| \right\} \\ & \quad \times \left(1 + |v_j - \tilde{U}(\eta)|^2 + |v_j - \tilde{U}(\eta)|^4 + I_k^{2/\delta} \right) e^{-C(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta})}. \end{aligned} \tag{6.7}$$

Now, recall that $\tilde{U}_i^n(\eta) \leq C_{Tf}$ to derive

$$\left(1 + |v_j|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}} = \left(1 + |v_j - \tilde{U}_i^n(\eta) + \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}} \leq C \left(1 + |v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}},$$

which further gives

$$\begin{aligned} & \left(1 + |v_j|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}} \left(1 + |v_j - \tilde{U}(\eta)|^2 + |v_j - \tilde{U}(\eta)|^4 + I_k^{2/\delta} \right) e^{-C(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta})} \\ & \leq C \left(1 + |v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}} \left(1 + |v_j - \tilde{U}(\eta)|^2 + |v_j - \tilde{U}(\eta)|^4 + I_k^{2/\delta} \right) e^{-C(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta})} \\ & \leq C \left(1 + |v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}+3} e^{-C(|v_j - \tilde{U}_i^n(\eta)|^2 + I_k^{2/\delta})}. \end{aligned} \tag{6.8}$$

Note that the last upper bound can be understood as the form of $C(1+x)^{\frac{q}{2}+3}e^{-Cx}$, hence it is uniformly bounded for $x \geq 0$. To obtain desired estimate, we multiply $\left(1 + |v_j|^2 + I_k^{2/\delta} \right)^{\frac{q}{2}}$ on both sides of (6.7) and take supremum, then we have from (6.8) that

$$\begin{aligned} & \left\| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f})(x_i, v_j, I_k, t^n) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}_{i,\mathcal{J},\mathcal{K}}^n)_{j,k} \right\|_{L_q^\infty} \\ & \leq C \left(1 + \frac{1}{\theta} + \frac{1}{\theta^2} + \frac{1}{\theta^3} \right) \left\{ |\tilde{\rho} - \tilde{\rho}_i^n| + |\tilde{U} - \tilde{U}_i^n| + \sum_{1 \leq \alpha, \beta \leq 3} \left| \tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} - \left(\tilde{\mathcal{T}}_{\nu,\theta}^{\alpha,\beta} \right)_i^n \right| + \left| \tilde{T}_\theta - \left(\tilde{T}_\theta \right)_i^n \right| \right\}. \end{aligned}$$

This, together with Lemma 6.3, gives the desired estimate. □

7. PROOF OF THEOREM 3.2

Here, we prove our main theorem. We first subtract (5.1) from (2.14) and take L_q^∞ -norm:

$$\begin{aligned} \|f^{n+1} - f(t^{n+1})\|_{L_q^\infty} &= \frac{\kappa}{\kappa + A_{\nu,\theta}\Delta t} \|\tilde{f}^n - \tilde{f}(t^n)\|_{L_q^\infty} + \frac{A_{\nu,\theta}\Delta t}{\kappa + A_{\nu,\theta}\Delta t} \left\| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^n) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f})(t^n) \right\|_{L_q^\infty} \\ &+ \frac{A_{\nu,\theta}}{\kappa + A_{\nu,\theta}\Delta t} \|R_1\|_{L_q^\infty} + \frac{A_{\nu,\theta}}{\kappa + A_{\nu,\theta}\Delta t} \|R_2\|_{L_q^\infty}. \end{aligned}$$

Next, we recall Lemmas 5.6, 6.1 and Proposition 6.4:

$$\begin{aligned} \|R_1\|_{L_q^\infty} + \|R_2\|_{L_q^\infty} &\leq C(\Delta t)^2, \\ \|\tilde{f}(t^n) - \tilde{f}^n\|_{L_q^\infty} &\leq \|f(t^n) - f^n\|_{L_q^\infty} + C(\Delta x)^2, \\ \left\| \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}(t^n)) - \mathcal{M}_{\nu,\theta,\delta}(\tilde{f}^n) \right\|_{L_q^\infty} &\leq C \left(\|f(t^n) - f^n\|_{L_q^\infty} + \{(\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t\} \right), \end{aligned}$$

where C is a constant which can be bounded regardless of the values of Δt . From these estimates, we obtain

$$\begin{aligned} \|f^{n+1} - f(t^{n+1})\|_{L_q^\infty} &\leq \frac{\kappa + CA_{\nu,\theta}\Delta t}{\kappa + A_{\nu,\theta}\Delta t} \|f(t^n) - f^n\|_{L_q^\infty} \\ &+ \frac{C}{\kappa + A_{\nu,\theta}\Delta t} (\kappa(\Delta x)^2 + A_{\nu,\theta}\Delta t((\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t + \Delta t)). \end{aligned} \tag{7.1}$$

For the sake of simplicity, we introduce

$$\Gamma_n := \|f^n - f(t^n)\|_{L_q^\infty}$$

and

$$P(\Delta x, \Delta v, \Delta I, \Delta t) := \frac{C}{\kappa + A_{\nu,\theta}\Delta t} (\kappa(\Delta x)^2 + A_{\nu,\theta}\Delta t((\Delta x)^2 + \Delta v + \Delta I + \Delta v \Delta t + \Delta t)).$$

Then, using

$$\frac{\kappa + CA_{\nu,\theta}\Delta t}{\kappa + A_{\nu,\theta}\Delta t} = 1 + \frac{(C-1)A_{\nu,\theta}\Delta t}{\kappa + A_{\nu,\theta}\Delta t} \leq 1 + \frac{CA_{\nu,\theta}\Delta t}{\kappa + A_{\nu,\theta}\Delta t} = 1 + Q\Delta t$$

we write (7.1) in a recurrence form as follows:

$$\Gamma_{n+1} \leq (1 + Q\Delta t)\Gamma_n + P(\Delta x, \Delta v, \Delta I, \Delta t)$$

where $Q := \frac{CA_{\nu,\theta}}{\kappa + A_{\nu,\theta}\Delta t}$. Since it is assumed that there is no error in the initial step:

$$\Gamma_0 = \|f^0 - f(t^0)\|_{L_q^\infty} = 0,$$

we have from $n\Delta t \leq N_t\Delta t = T^f$ that

$$\begin{aligned} \Gamma_{n+1} &\leq (1 + Q\Delta t)^{n+1}\Gamma_0 + \sum_{k=0}^n (1 + Q\Delta t)^k P(\Delta x, \Delta v, \Delta I, \Delta t) \\ &\leq \frac{(1 + Q\Delta t)^{N_t} - 1}{(1 + Q\Delta t) - 1} P(\Delta x, \Delta v, \Delta I, \Delta t) \\ &\leq \frac{1}{Q\Delta t} e^{QT^f} P(\Delta x, \Delta v, \Delta I, \Delta t). \end{aligned}$$

In the last line, we use $(1 + x)^n \leq e^{nx}$. Using $\Delta v < \frac{1}{2}$ and

$$\frac{P(\Delta x, \Delta v, \Delta I, \Delta t)}{\Delta t} \leq \frac{C(\kappa + A_{\nu,\theta})}{\kappa + A_{\nu,\theta}\Delta t} \left(\frac{(\Delta x)^2}{\Delta t} + (\Delta x)^2 + \Delta v + \Delta I + \Delta v\Delta t + \Delta t \right),$$

we derive

$$\Gamma_{n+1} \leq \frac{2}{Q} e^{QT^f} \frac{C(\kappa + A_{\nu,\theta})}{\kappa + A_{\nu,\theta}\Delta t} \left(\frac{(\Delta x)^2}{\Delta t} + (\Delta x)^2 + \Delta v + \Delta I + \Delta t \right).$$

This completes the proof.

8. CONCLUSION

In this paper, we present an implicit semi-Lagrangian scheme for the ES-BGK model for polyatomic gases. The main result is the convergence estimate of the scheme using argument previously adopted in [41] for BGK model and [42] for ES-BGK model for monatomic gas. For the proof of convergence estimate, the lower bound estimate for polyatomic temperature is crucially used to prevent the discrete polyatomic ellipsoidal Gaussian from degenerating into Dirac delta. The restriction of our result is that convergence estimate holds for fixed value of Knudsen number and relaxation parameter θ . Our proof covers the biatomic molecules with no vibrational degree of freedom. In future work we shall try to remove some of these restrictions, in particular we plan to make use of the asymptotic preserving property of the method to obtain a convergence estimate which is uniform in the Knudsen number.

APPENDIX A. TECHNICAL LEMMAS

Here, we present several technical lemmas.

Lemma A.1. *The discrete solution f^n and \tilde{f}^n satisfies*

$$\begin{aligned} \|\tilde{f}^0\|_{L_q^\infty} &\leq \|f_0\|_{L_q^\infty}, \quad \text{for } n = 0, \\ \|\tilde{f}^n\|_{L_q^\infty} &\leq \|f^n\|_{L_q^\infty}, \quad \text{for } n \geq 1. \end{aligned}$$

Proof. For $n = 0$, we recall that no initial errors are assumed. Then,

$$\begin{aligned} \|\tilde{f}^0\|_{L_q^\infty} &= \sup_{i,j,k} \left| \tilde{f}_{i,j,k}^0 \left(1 + |v_j|^2 + I_k^{\frac{2}{\theta}} \right)^{\frac{q}{2}} \right| \\ &= \sup_{i,j,k} \left| f_0(x_i - v_j^1 \Delta t, v_j, I_k) \left(1 + |v_j|^2 + I_k^{\frac{2}{\theta}} \right)^{\frac{q}{2}} \right| \\ &\leq \sup_{x,v,I} \left| f_0(x - v^1 \Delta t, v, I) \left(1 + |v|^2 + I^{\frac{2}{\theta}} \right)^{\frac{q}{2}} \right| \\ &= \|f_0\|_{L_q^\infty}. \end{aligned}$$

For $n \geq 1$, we use (2.1) to obtain

$$\begin{aligned} \|\tilde{f}^n\|_{L_q^\infty} &= \sup_{i,j,k} \left| \tilde{f}_{i,j,k}^n \left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}} \right| \\ &= \sup_{i,j,k} \left| (a_j f_{s,j,k}^n + (1 - a_j) f_{s+1,j,k}^n) \left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}} \right| \\ &\leq \sup_{i,j,k} \left| f_{i,j,k}^n \left(1 + |v_j|^2 + I_k^{\frac{2}{\delta}}\right)^{\frac{q}{2}} \right|, \end{aligned}$$

where the index s is determined as in (2.1) for each i, j , and the last inequality follows from the inequalities $0 < a_j \leq 1$. This completes the proof. \square

In the following lemma, we establish the equivalent relations for $(\tilde{\mathcal{T}}_{\nu,\theta})_i^n$ and $(\tilde{T}_\theta)_i^n$.

Lemma A.2. *Let $\delta > 0$, $-1/2 < \nu < 1$ and $0 < \theta \leq 1$. Suppose $\tilde{f}_{i,j,k}^n > 0$ and $\tilde{\rho}_i^n > 0$. Then, the discrete temperature tensor $(\tilde{\mathcal{T}}_{\nu,\theta})_i^n$ and relaxation temperature $(\tilde{T}_\theta)_i^n$ satisfy the following estimates:*

$$\begin{aligned} (1) \quad &\lambda\theta(\tilde{T}_\delta)_i^n Id \leq (\tilde{\mathcal{T}}_{\nu,\theta})_i^n \leq \frac{1}{3}\lambda C_\nu\{3 + \delta(1 - \theta)\}(\tilde{T}_\delta)_i^n Id, \\ (2) \quad &\theta(\tilde{T}_\delta)_i^n \leq (\tilde{T}_\theta)_i^n \leq \frac{1}{\delta}\{\delta + 3(1 - \theta)\}(\tilde{T}_\delta)_i^n, \end{aligned}$$

where $C_\nu = \max\{1 - \nu, 1 + 2\nu\}$ and $\lambda \equiv \frac{\kappa + A_{\nu,\theta}\Delta t}{\Delta t + \kappa}$.

Remark A.3. In the inequalities (1), the relation $A \leq B$ for 3×3 matrices A and B means that $B - A$ is positive definite, i.e., $k^\top(B - A)k \geq 0$ for all $k \equiv (k^1, k^2, k^3)^\top \in \mathbb{R}^3$. That is,

$$\lambda\theta(\tilde{T}_\delta)_i^n \leq \min_{|k|=1} k^\top (\tilde{\mathcal{T}}_{\nu,\theta})_i^n k \leq \max_{|k|=1} k^\top (\tilde{\mathcal{T}}_{\nu,\theta})_i^n k \leq \frac{1}{3}\lambda C_\nu\{3 + \delta(1 - \theta)\}(\tilde{T}_\delta)_i^n.$$

This further imposes that eigenvalues of $(\tilde{\mathcal{T}}_{\nu,\theta})_i^n$ lie between $\lambda\theta(\tilde{T}_\delta)_i^n$ and $\frac{1}{3}\lambda C_\nu\{3 + \delta(1 - \theta)\}(\tilde{T}_\delta)_i^n$, hence,

$$\left(\lambda\theta(\tilde{T}_\delta)_i^n\right)^3 \leq \det(\tilde{\mathcal{T}}_{\nu,\theta})_i^n \leq \left(\frac{1}{3}\lambda C_\nu\{3 + \delta(1 - \theta)\}(\tilde{T}_\delta)_i^n\right)^3.$$

Proof. (1) **The estimate for $(\tilde{\mathcal{T}}_{\nu,\theta})_i^n$:** for $k \in \mathbb{R}^3$, recall the definition of $(\tilde{\mathcal{T}}_{\nu,\theta})_i^n$ in (2.12) to have

$$\begin{aligned} k^\top \left\{ \tilde{\rho}_i^n (\tilde{\mathcal{T}}_{\nu,\theta})_i^n \right\} k &= k^\top \left\{ \lambda\theta \left[\frac{2}{3 + \delta} \sum_{j,k} \tilde{f}_{i,j,k}^n \left(\frac{|v_j - \tilde{U}_i^n|^2}{2} + I_k^{\frac{2}{\delta}} \right) (\Delta v)^3 \Delta I \right] Id \right\} k \\ &\quad + k^\top \left\{ \lambda(1 - \theta)(1 - \nu) \left[\frac{2}{3} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{|v_j - \tilde{U}_i^n|^2}{2} (\Delta v)^3 \Delta I \right] Id \right\} k \\ &\quad + k^\top \left\{ (1 - \theta)\bar{\nu} \sum_{j,k} \tilde{f}_{i,j,k}^n (v_j - \tilde{U}_i^n) \otimes (v_j - \tilde{U}_i^n) (\Delta v)^3 \Delta I \right\} k \\ &\equiv R_1 + R_2 + R_3. \end{aligned} \tag{A.1}$$

Depending on the range of ν , we respectively estimate the upper and lower bounds of $k^\top \left\{ \tilde{\rho}_i^n (\tilde{\mathcal{T}}_{\nu,\theta})_i^n \right\} k$ in (A.1) as follows:

(1-1) Upper bound estimate of (A.1):

(1-1-1) $0 < \nu < 1$: we first simplify R_3 by using the following identity:

$$k^\top \left(v_j - \tilde{U}_i^n \right) \otimes \left(v_j - \tilde{U}_i^n \right) k = \left(k \cdot \left(v_j - \tilde{U}_i^n \right) \right)^2,$$

and use the Cauchy–Schwartz inequality as follows:

$$\sum_{j,k} \tilde{f}_{i,j,k}^n \left(k \cdot \left(v_j - \tilde{U}_i^n \right) \right)^2 (\Delta v)^3 \Delta I \leq \sum_{j,k} \tilde{f}_{i,j,k}^n \left| v_j - \tilde{U}_i^n \right|^2 (\Delta v)^3 \Delta I |k|^2 \leq 3 \tilde{\rho}_i^n \left(\tilde{T}_{\text{tr}} \right)_i^n |k|^2.$$

Then, the upper bound of (A.1) is given by

$$\begin{aligned} k^\top \left\{ \tilde{\rho}_i^n \left(\tilde{T}_{\nu,\theta} \right)_i^n \right\} k &\leq \lambda \theta \tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n |k|^2 + \lambda (1 - \theta) (1 - \nu) \tilde{\rho}_i^n \left(\tilde{T}_{\text{tr}} \right)_i^n |k|^2 + 3(1 - \theta) \bar{\nu} \tilde{\rho}_i^n \left(\tilde{T}_{\text{tr}} \right)_i^n |k|^2 \\ &\leq \lambda (1 + 2\nu) \tilde{\rho}_i^n \left\{ \theta \left(\tilde{T}_\delta \right)_i^n + (1 - \theta) \left(\tilde{T}_{\text{tr}} \right)_i^n \right\} |k|^2. \end{aligned} \quad (\text{A.2})$$

In the last line, we use $0 < \bar{\nu} = \frac{\kappa \nu}{\Delta t + \kappa} \leq \nu$ and $\lambda > 1$.

(1-1-2) $-1/2 < \nu \leq 0$: in this case, we have $\bar{\nu} \leq 0$. Then, (A.1) becomes

$$\begin{aligned} k^\top \left\{ \tilde{\rho}_i^n \left(\tilde{T}_{\nu,\theta} \right)_i^n \right\} k &\leq \lambda \left\{ \theta \tilde{\rho}_i^n \left(\tilde{T}_\delta \right)_i^n |k|^2 + (1 - \theta) (1 - \nu) \tilde{\rho}_i^n \left(\tilde{T}_{\text{tr}} \right)_i^n |k|^2 \right\} \\ &\leq \lambda (1 - \nu) \tilde{\rho}_i^n \left\{ \theta \left(\tilde{T}_\delta \right)_i^n + (1 - \theta) \left(\tilde{T}_{\text{tr}} \right)_i^n \right\} |k|^2. \end{aligned} \quad (\text{A.3})$$

Combine (A.2) and (A.3) and divide both sides of (A.1) by $\tilde{\rho}_i^n > 0$ to derive

$$k^\top \left(\tilde{T}_{\nu,\theta} \right)_i^n k \leq \max\{1 - \nu, 1 + 2\nu\} \lambda \left\{ (1 - \theta) \left(\tilde{T}_{\text{tr}} \right)_i^n + \theta \left(\tilde{T}_\delta \right)_i^n \right\} |k|^2. \quad (\text{A.4})$$

Now, we recall the definition of $\left(\tilde{T}_\delta \right)_i^n$ in (2.3) to obtain

$$\left(\tilde{T}_\delta \right)_i^n = \frac{3}{3 + \delta} \left(\tilde{T}_{\text{tr}} \right)_i^n + \frac{\delta}{3 + \delta} \left(\tilde{T}_{I,\delta} \right)_i^n \geq \frac{3}{3 + \delta} \left(\tilde{T}_{\text{tr}} \right)_i^n,$$

which, together with (A.4), leads to

$$k^\top \left(\tilde{T}_{\nu,\theta} \right)_i^n k \leq \frac{1}{3} \max\{1 - \nu, 1 + 2\nu\} \lambda \{3 + \delta(1 - \theta)\} \left(\tilde{T}_\delta \right)_i^n |k|^2.$$

(1-2) Lower bound estimate of (A.1):

(1-2-1) $0 < \nu < 1$: the summation $R_2 + R_3$ in (A.1) satisfies

$$\begin{aligned} R_2 + R_3 &= k^\top \left\{ \lambda (1 - \theta) (1 - \nu) \left[\frac{2}{3} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{\left| v_j - \tilde{U}_i^n \right|^2}{2} (\Delta v)^3 \Delta I \right] Id \right\} k \\ &\quad + (1 - \theta) \bar{\nu} \sum_{j,k} \tilde{f}_{i,j,k}^n \left(k \cdot \left(v_j - \tilde{U}_i^n \right) \right)^2 (\Delta v)^3 \Delta I \\ &\geq k^\top \left\{ \lambda (1 - \theta) (1 - \nu) \tilde{\rho}_i^n \left(\tilde{T}_{\text{tr}} \right)_i^n Id \right\} k \\ &\geq \frac{\kappa}{\Delta t + \kappa} (1 - \theta) (1 - \nu) k^\top \left\{ \tilde{\rho}_i^n \left(\tilde{T}_{\text{tr}} \right)_i^n Id \right\} k. \end{aligned}$$

In the last line, we use $\lambda = \frac{\kappa + A_{\nu,\theta} \Delta t}{\Delta t + \kappa} \geq \frac{\kappa}{\Delta t + \kappa}$ with $A_{\nu,\theta} = 1/(1 - \nu + \nu\theta) > 0$.

(1-2-2) $-1/2 < \nu \leq 0$: In this range of ν , we have $\lambda > 0$. Then,

$$\begin{aligned} R_2 + R_3 &= k^\top \left\{ (\lambda(1-\theta)(1-\nu)) \left[\frac{2}{3} \sum_{j,k} \tilde{f}_{i,j,k}^n \frac{|v_j - \tilde{U}_i^n|^2}{2} (\Delta v)^3 \Delta I \right] Id \right\} k \\ &\quad + k^\top \left\{ (1-\theta)\bar{\nu} \sum_{j,k} \tilde{f}_{i,j,k}^n (v_j - \tilde{U}_i^n) \cdot (v_j - \tilde{U}_i^n) (\Delta v)^3 \Delta I \right\} k \\ &\geq k^\top \left\{ \left(\frac{\kappa}{\Delta t + \kappa} (1-\theta)(1-\nu) \right) \tilde{\rho}_i^n (\tilde{T}_{tr})_i^n Id \right\} k + k^\top \left\{ \frac{3\kappa}{\Delta t + \kappa} (1-\theta)\nu \tilde{\rho}_i^n (\tilde{T}_{tr})_i^n Id \right\} k \\ &= \frac{\kappa}{\Delta t + \kappa} (1-\theta)(1+2\nu) \tilde{\rho}_i^n (\tilde{T}_{tr})_i^n |k|^2. \end{aligned}$$

Since $R_2 + R_3 \geq 0$ for $-1/2 < \nu < 1$, we can conclude that

$$k^\top \left\{ \tilde{\rho}_i^n (\tilde{T}_{\nu,\theta})_i^n \right\} k \geq \lambda \theta \tilde{\rho}_i^n (\tilde{T}_\delta)_i^n |k|^2 + R_2 + R_3 \geq \lambda \theta \tilde{\rho}_i^n (\tilde{T}_\delta)_i^n |k|^2.$$

(2) **The estimate for $(\tilde{T}_\theta)_i^n$** : note that $(\tilde{T}_{tr})_i^n \geq 0$, which gives

$$(\tilde{T}_\delta)_i^n = \frac{3}{3+\delta} (\tilde{T}_{tr})_i^n + \frac{\delta}{3+\delta} (\tilde{T}_{I,\delta})_i^n \geq \frac{\delta}{3+\delta} (\tilde{T}_{I,\delta})_i^n.$$

Then,

$$\begin{aligned} (\tilde{T}_\theta)_i^n &= (1-\theta) (\tilde{T}_{I,\delta})_i^n + \theta (\tilde{T}_\delta)_i^n \\ &\leq (1-\theta) \left(\frac{3+\delta}{\delta} (\tilde{T}_\delta)_i^n \right) + \theta (\tilde{T}_\delta)_i^n = \frac{1}{\delta} \{ \delta + 3(1-\theta) \} (\tilde{T}_\delta)_i^n. \end{aligned}$$

Also, from $(\tilde{T}_{I,\delta})_i^n > 0$, we have

$$(\tilde{T}_\theta)_i^n = (1-\theta) (\tilde{T}_{I,\delta})_i^n + \theta (\tilde{T}_\delta)_i^n \geq \theta (\tilde{T}_\delta)_i^n.$$

This completes the proof. □

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