Entropy Decay Rates for Conservative Spectral Schemes Modeling Fokker-Planck-Landau Type Flows in the Mean Field Limit

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Abstract

Expanding upon the conservative spectral method for solving the Vlasov-Poisson Landau system, developed by Zhang and Gamba for Coulomb interactions, the deterministic scheme has been extended to model Vlasov-Poisson Fokker-Planck-Landau type equations with Maxwell type and hard sphere interactions. The original case, corresponding to the classical physical problem of Coulomb interactions, is also included and the stability for all three scenarios investigated. Simulations are presented, both for the space-homogeneous case of just particle potential interactions and the space-inhomogeneous case for the mean field coupling through the Poisson equation for total charges. The strength of the method is exemplified by the qualitative decay of relative entropy for both Coulomb, Maxwell type and hard sphere interactions. The Coulomb case shows that there is a degenerate spectrum, with the relative entropy decaying at a rate close to the law of two thirds as predicted by upper estimates in a work of Strain and Guo in 2006, while the Maxwell type and hard sphere examples both exhibit a spectral gap. This behaviour indicates that Strain and Guo’s estimate for the Coulomb case is sharp while, still to this date, there is no analytical proof of such sharp degenerate spectral behavior for the classical Fokker-Planck-Landau operator, for either space-homogeneous or space-inhomogeneous mean field limit flows.

1 Introduction

An important model for plasmas is the Landau equation, which results from the grazing collision limit of the Boltzmann equation. This limit, first derived by Landau [15], assumes that colliding particles are travelling almost parallel to each other due to repulsive Coulomb forces. A more mathematical description of the limit was detailed by Villani [20], Desvillettes and Villani [8] and
more recently Desvillettes [7], even for extended potential rates higher than Coulomb interactions and up to hard spheres. When rates different to Coulomb interactions are used, the equation is referred to as being of Fokker-Planck-Landau type. Computationally, the limiting problem has been studied by Bobylev and Potapenko [4], using Monte Carlo methods, and in Fourier space by Haack and Gamba [14].

The Landau equation is rather difficult to model, either analytically or numerically, due to the high dimensionality, non-linearity and non-locality. For numerical simulations, a deterministic scheme can be used, such as the conservative spectral method, developed by Zhang and Gamba [21], which is the model of choice for the current work. Spectral methods were first considered as a model for the space-homogeneous Landau equation by Bobylev and Rjasanow [5] and Pareschi et al. [17]. The evolution of the Landau equation has also been simulated by means of a Monte-Carlo scheme for the Boltzmann equation with sufficiently singular angular cross-sections that cancel the Coulomb potential. This approach results in an expensive algorithm compared to the spectral-based methods.

The version of the spectral method in this work exploits the weak form of the Landau equation in order to calculate the Fourier transform of the collision operator. It does so in just $O(N^3 \log N)$ operations, where the number of Fourier modes $N$ in each velocity dimension can be small, thanks to the conservation enforcement. For computational purposes, a cut-off domain in velocity space is used, within which the majority of the solution’s mass should be supported, based on a result by Gamba et al. [12] for the Boltzmann equation. This general construction of a spectral method was first applied to the Boltzmann equation by Gamba and Tharkabhushaman [13] and the details for the derivation of the Landau equation scheme can be found in [21].

Pareschi’s construction of a spectral method involved extending the solution periodically, which did not respect the decay of the solution toward infinity in velocity space. As a result, aliasing effects were noticed in their solution. Subsequently, Filbet and Pareschi [9] applied this idea to the space-inhomogeneous Landau equation by using a finite volume method in space but this scheme did not preserve the conservation properties of the Landau equation. A conservative method was later proposed by Crouseilles and Filbet [6], using centered finite differences, but this only conserved mass and energy, not momentum, and required certain symmetry properties of the initial data.

One particular attraction to the current method is its ability to yield the correct decay of entropy. The conservation enforcement is essential in the proof of convergence of the spectral method applied to the Boltzmann equation [3] and it is believed that the same should be true for Fokker-Planck-Landau type equations. The entropy decay rate is also a consequence of this fact. To the best of the authors’ knowledge, this is the first time that the convergence rate of two thirds, proven analytically by Strain and Guo [19], has been seen through a numerical approximation of the relative entropy.
The method described in [21] is in fact a solver for the space-inhomogeneous Landau equation, coupled to Poisson’s equation, where the advection is modeled by a discontinuous Galerkin scheme. Some results for the space-homogeneous version of the equation have already been described by the present authors [18]. The current work improves these results slightly to the space-inhomogeneous case. As in [18], this paper also contains calculations for Fokker-Planck-Landau type equations associated to Maxwell molecules and hard spheres, expanding upon the previous work of [21].

The layout of this work is as follows. First, the setup of the problem is described in Section 2, along with any required definitions. The expressions for the Fourier transform of the Fokker-Planck-Landau type operators corresponding to Coulomb interactions, Maxwell molecules and hard spheres are derived in Section 3 and the stability results given in Section 4. Finally, Section 5 contains the numerical results. There the correct decay rate to equilibrium is demonstrated for the space-homogeneous problem associated to Coulomb interactions, Maxwell molecules and hard spheres, as well as the space-inhomogeneous Landau equation. All work here is part of a PhD thesis by the first author, under advisorship of the second.

2 Description of Problem

A space-inhomogeneous Fokker-Planck-Landau type equation for the probability density function (pdf) $f(t, x, v)$, where $(t, x, v) \in (\mathbb{R}^+, \Omega_x, \Omega_v)$, with $\Omega_x \subseteq \mathbb{R}$ and $\Omega_v \subseteq \mathbb{R}^3$, is of the form

$$f_t(t, x, v) + v \cdot \nabla_x f(t, x, v) - E(t, x) \cdot \nabla_v f(t, x, v) = \frac{1}{\varepsilon} Q(f, f)(t, x, v),$$

(1)

where $\varepsilon$ is the Knudsen number and $Q(f, f)$ is the collision operator given by

$$Q(f, f) = \nabla_v \cdot \int_{\Omega_v} S(v - v_s)(f, \nabla_v f - f \nabla_v f_s) \, dv_s,$$

for $S(u) = |u|^\gamma + 2 \left( I - \frac{uu^T}{|u|^2} \right)$,

with $-3 \leq \gamma \leq 1$, $I \in \mathbb{R}^{3 \times 3}$ the identity matrix and the subscript notation $f_s$ meaning evaluation at $v_s$ (the velocity of a colliding particle). In general, $\gamma > 0$ corresponds to hard potentials and $\gamma < 0$ to soft potentials. More precisely, $\gamma = 1$ model hard spheres; $\gamma = 0$ are known as Maxwell molecules; and $\gamma = -3$ model Coulomb interactions between particles.

In addition, $E$ is the electric field found by solving Poisson’s equation, namely

$$E(t, x) = -\nabla_x \Phi(t, x),$$

where $\Phi$ is the potential solved from

$$-\Delta_x \Phi(t, x) = 1 - \int_{\Omega_v} f(t, x, v) \, dv.$$

(2)
Note that the right hand side of (2) is the density of positively charged ions (assumed here to be a constant background density) minus the density of electrons (due to the negative charge). Also, in this context where \( \mathbf{v} \) is a vector but \( x \) is a scalar, \( \mathbf{E}(t, x) = (E(t, x), 0, 0) \) and the gradient in \( x \) is treated as \( \nabla_x = (\frac{\partial}{\partial x}, 0, 0) \).

In the current work, boundary conditions for both the Fokker-Planck-Landau type and Poisson equations are taken as periodic in space. Furthermore, since the Poisson equation is an ordinary differential equation for any given \( t \geq 0 \) with periodic boundary conditions, if \( \Omega_x = [0, L_x] \) then it has explicit solution given by

\[
\Phi(t, x) = \int_0^L \int_0^L \int_{\Omega_V} f(t, z, \mathbf{v}) \, d\mathbf{v} \, dz \, ds - \frac{1}{2} x^2 - C_E x + \Phi(t, 0),
\]

where

\[
C_E = -\frac{1}{2} L_x + \frac{1}{L_x} \int_0^{L_x} \int_0^L \int_{\Omega_V} f(t, z, \mathbf{v}) \, d\mathbf{v} \, dz \, ds.
\]

Since the potential \( \Phi \) is never explicitly used and it is in fact the derivative that is more relevant for the Landau equation, the value of \( \Phi(t, 0) \) is irrelevant and so it is chosen as \( \Phi(t, 0) = 0 \).

It should also be noted here that the space-homogeneous version of (1) is simply to find the pdf \( f(t, \mathbf{v}) \), where \( (t, \mathbf{v}) \in (\mathbb{R}^+, \Omega_V) \), with \( \Omega_V \subseteq \mathbb{R}^3 \), such that

\[
f_t(t, \mathbf{v}) = \frac{1}{\varepsilon} Q(f, f)(t, \mathbf{v}).
\]

Since Fokker-Planck-Landau type equations are a limit of the Boltzmann equation, they enjoy the same conservation laws. In particular, for the set of collision invariants \( \{ \phi_k(\mathbf{v}) \}_{k=0}^4 = \{ 1, v_1, v_2, v_3, |\mathbf{v}|^2 \} \),

\[
\int_{\mathbb{R}^3} Q(f, f)(\mathbf{v}) \phi_k(\mathbf{v}) \, d\mathbf{v} = 0, \quad \text{for } k = 0, 1, \ldots, 4. \tag{3}
\]

This is important because it leads to the conservation of mass \( \rho \), average velocity \( \mathbf{V} \) and total energy \( T_{\text{tot}} \), where each of these quantities are found via

\[
\rho = \int_{\Omega_x} \int_{\mathbb{R}^3} f(t, x, \mathbf{v}) \, d\mathbf{v} \, dx, \quad \mathbf{V} = \frac{1}{\rho} \int_{\Omega_x} \int_{\mathbb{R}^3} f(t, x, \mathbf{v}) \mathbf{v} \, d\mathbf{v} \, dx
\]

and

\[
T_{\text{tot}}(t) = \frac{3}{2} \rho T^K(t) + T^E(t), \tag{4}
\]

where

\[
T^K = \frac{1}{3\rho} \int_{\Omega_x} \int_{\Omega_V} f(t, x, \mathbf{v}) |\mathbf{v}|^2 \, d\mathbf{v} \, dx \quad \text{and} \quad T^E = \frac{1}{2} \int_{\Omega_x} |\Phi'(t, x)|^2 \, dx \tag{5}
\]
are the kinetic energy $T^K$ and the electric energy $T^E$.

These moments will always be conserved for the single-species space-inhomogeneous Landau equation (1) when solved with appropriate boundary conditions (including the periodic ones considered here). If the initial mass, average velocity and total energy are denoted by $\rho_0$, $V_0$ and $T_{0_{\text{tot}}}$, respectively, the equilibrium solution of the Landau equation is a Gaussian distribution with the same moments. This is referred to as the equilibrium Maxwellian, denoted $M_{\text{eq}}$, and is the specific Maxwellian distribution with moments equal to those of the initial condition, given by

$$
M_{\text{eq}}(x,v) = \frac{\rho_0}{(2\pi T_{0_{\text{eq}}})^{3/2}} \int e^{\frac{\Phi_{\text{eq}}(x)}{T_{0_{\text{eq}}}}} e^{-\frac{|v-V_0|^2}{2T_{0_{\text{eq}}}}} \, dx,
$$

where $\Phi_{\text{eq}}$ is the equilibrium potential and $T_{0_{\text{eq}}}$ is such that using $M_{\text{eq}}$ in expression (4) returns $T_{0_{\text{tot}}} = T_{0_{\text{tot}}}$.

In the space-homogeneous setting there is no integration with respect to $x$ to evaluate the moments $\rho$, $V$ and $T^K$; $T_{0_{\text{tot}}} = T^K$; there is no field $\Phi$; and the equilibrium Maxwellian reduces to

$$
M_{\text{eq}}(v) = \frac{\rho_0}{(2\pi T_0)^{3/2}} e^{-\frac{|v-V_0|^2}{2T_0}},
$$

where $T_0 = T^K(0)$.

Similarly, the H-theorem holds for Fokker-Planck-Landau type equations, which states that the entropy decays throughout time.

The entropy is defined as

$$
\mathcal{H}[f](t) = \int_{\Omega} \int_{\mathbb{R}^3} f \log(f) \, dv \, dx
$$

and so the H-theorem gives that

$$
\frac{d}{dt}(\mathcal{H}[f]) \leq 0.
$$

At this point it is also useful to define the entropy relative to the equilibrium Maxwellian $M_{\text{eq}}$ as

$$
\mathcal{H}[f|M_{\text{eq}}](t) = \int_{\Omega} \int_{\mathbb{R}^3} f \log(f) \, dv \, dx - \int_{\Omega} \int_{\mathbb{R}^3} M_{\text{eq}} \log(M_{\text{eq}}) \, dv \, dx
$$

$$
= \int_{\Omega} \int_{\mathbb{R}^3} f \log \left( \frac{f}{M_{\text{eq}}} \right) \, dv \, dx.
$$

Again, in the space-homogeneous case, there is no integration with respect to $x$ when considering the entropy.

Initially $f(0,x,v) = f_0(x,v)$ and it is assumed that $\text{supp} f \subset \Omega_v$, since $f$ should have sufficient decay in velocity-space [12] and $\Omega_v$ is chosen depending on the initial data (see [3], Section 2).
In fact, $v \in \mathbb{R}^3$ but values of $f$ are negligible outside a sufficiently large ball. The initial data is then extended by zero outside the computational domain, which means it can be controlled by $e^{-c|v|^2}$, for $c > 0$ depending on the moments of $f_0$. Under such conditions, it is expected that the computational solution will remain supported on $\Omega_v$ up to a fixed small error that depends on the initial data (more details can be seen in the proof for the conservative spectral method applied to the Boltzmann equation in [3]).

For computational purposes, the space-inhomogeneous Fokker-Planck-Landau type equation (1) is broken down into two smaller problems in a process known as time splitting. To describe this, let time be discretised by $t_n = t_0 + n\Delta t$, for some time-step $\Delta t$, and let $f_n(x, v) = f(t_n, x, v)$. First, given the solution $f_n$, a collisionless advection problem is solved for $g$, namely

$$g_t(t, x, v) + v \cdot \nabla_x g(t, x, v) - \nabla_v g(t, x, v) = 0,$$

along with Poisson’s equation (2), with $g(0, x, v) = f_n(x, v)$. Then a space-homogeneous collision problem is solved for $\tilde{f}$ at each $x \in \Omega_x$, namely

$$\tilde{f}_t(t, x, v) = Q(\tilde{f}, \tilde{f})(t, x, v),$$

with $\tilde{f}(0, x, v) = g(\Delta t, x, v)$. Finally, the solution at time $t = t_{n+1}$ is given by

$$f_{n+1}(x, v) = \tilde{f}(\Delta t, x, v).$$

Equation (9) is solved by a discontinuous Galerkin (D.G.) method, with piecewise linear polynomials in $x$ and piecewise quadratic polynomials in $v$, and third order Runge-Kutta in time. Proofs of how the choice of quadratic basis functions in $v$-space ensure moment conservation at this stage are given in [21].

Then, equation (10) is solved by the conservative spectral method with fourth order Runge-Kutta for time-stepping. Conservation is enforced by considering a constrained minimisation problem. Given a collection of discrete values of the collision operator, resulting from the spectral method, a new set of values must be found which are as close as possible to the original values in $\ell^2$-norm but satisfy the discrete form of (3), where the integrals are replaced with quadrature sums. The solution to this problem is a matrix multiplication of the original values, where the matrix is identical for both the Boltzmann and Landau equations. The complete derivation can be found in [13] and [21] for the Boltzmann and Landau equations, respectively.

As will be seen in the current work, the method also respects the correct decay rate of entropy. The spectral method will be described in the next section and is extended from the Landau equation with Coulomb interactions to Fokker-Planck-Landau type equations with Maxwell molecule and hard sphere interactions.
3 The Fourier Transform of the Collision Operator

As is shown in [21], when using a ball of radius $R > 0$ as the cut-off domain for computational purposes, the Fourier transform of the collision operator $Q$ is

$$
\hat{Q}(\hat{f}, \hat{f})(\xi) = \int_{B_R(0)} \hat{f}(\xi - \omega) \hat{f}(\omega) \left( \omega^T \hat{S}(\omega) \omega - (\xi - \omega)^T \hat{S}(\omega)(\xi - \omega) \right) d\omega,
$$

where

$$
\hat{S}(\omega) = (2\pi)^{-\frac{3}{2}} \int_{B_R(0)} S(u)e^{-i\omega \cdot u} du,
$$

for

$$
S(u) = |u|^{\gamma+2} \left( 1 - \frac{uu^T}{|u|^2} \right), \quad \text{with} \quad -3 \leq \gamma \leq 1.
$$

This means that evaluating $\hat{Q}$ is performed by a fast Fourier transform (FFT) of the pdf $f$ and then a weighted convolution with itself. The FFT requires $O(N^3\log N)$ operations and multiplication by the weight and quadrature to calculate the convolution requires $O(N^3)$ operations. The weights can also be pre-computed and stored at the beginning of the code run, where the bulk of the calculation is in evaluation of $\hat{S}$. This has different forms depending on the value of $\gamma$ but the results are found through the same general method.

First, the entries of $\hat{S}$ can be decomposed as

$$
\hat{S}_{i,j}(\omega) = \hat{S}_{i,j}^1(\omega) - \hat{S}_{i,j}^2(\omega), \quad \text{for} \quad i, j = 1, 2, 3,
$$

with

$$
\hat{S}_{i,j}^1(\omega) = (2\pi)^{-\frac{3}{2}} \int_{B_R(0)} |u|^{\gamma+2}\delta_{i,j}e^{-i\omega \cdot u} du
$$

and

$$
\hat{S}_{i,j}^2(\omega) = (2\pi)^{-\frac{3}{2}} \int_{B_R(0)} |u|^{\gamma}u_iu_je^{-i\omega \cdot u} du.
$$

Then, for a given $\omega = (\omega_1, \omega_2, \omega_3)$, it should be noted that when $j = i$, there is only one value of $\hat{S}_{i,i}^1(\omega)$, for each $i = 1, 2, 3$, and that $\hat{S}_{i,i}^1(\omega) = 0$ when $i \neq j$ (thanks to the Kronecker delta). Also note that, for $i = j$,

$$
\hat{S}_{1,1}^2(\omega_1, \omega_2, \omega_3) = \hat{S}_{3,3}^2(\omega_2, \omega_3, \omega_1) \quad \text{and} \quad \hat{S}_{2,2}^2(\omega_1, \omega_2, \omega_3) = \hat{S}_{3,3}^2(\omega_1, \omega_3, \omega_2)
$$

and, for $i \neq j$,

$$
\hat{S}_{1,2}^2(\omega_1, \omega_2, \omega_3) = \hat{S}_{1,3}^2(\omega_1, \omega_3, \omega_2) \quad \text{and} \quad \hat{S}_{2,3}^2(\omega_1, \omega_2, \omega_3) = \hat{S}_{1,3}^2(\omega_2, \omega_1, \omega_3).
$$

The sub-diagonal entries are then also known since $\hat{S}$ is a symmetric matrix (because $S$ is). This means that only $\hat{S}_{1,1}, \hat{S}_{3,3}$ and $\hat{S}_{1,3}$ need to be calculated. The explicit formulae for these
quantities, evaluated at $\omega$ such that $|\omega| \neq 0$, are found to be

$$\hat{S}_{1,1}(\omega) = \begin{cases} 
\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^2} \left(1 - \cos(R|\omega|)\right), & \text{when } \gamma = -3, \\
\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^5} \left(- (R|\omega|)^3 \cos(R|\omega|) + 3(R|\omega|)^2 \sin(R|\omega|) + 6(R|\omega|) \cos(R|\omega|) - 6 \sin(R|\omega|)\right), & \text{when } \gamma = 0, \\
\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^6} \left(- (R|\omega|)^4 \cos(R|\omega|) + 4(R|\omega|)^3 \sin(R|\omega|) + 12(R|\omega|)^2 \cos(R|\omega|) - 24(R|\omega|) \sin(R|\omega|) - 24 \cos(R|\omega|) + 24\right), & \text{when } \gamma = 1,
\end{cases}$$

$$S_{3,3}^2(\omega) = \begin{cases} 
\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^4} \left(\omega_1^2 + \omega_2^2\right) \left(R|\omega| - \sin(R|\omega|) \right) \left(- \omega_3 \frac{R|\omega| + (R|\omega|) \cos(R|\omega|) - 2 \sin(R|\omega|)}{R|\omega|}\right), & \text{when } \gamma = -3, \\
\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^7} \left(\omega_1^2 + \omega_2^2\right) \left(- (R|\omega|)^2 \sin(R|\omega|) - 3(R|\omega|) \cos(R|\omega|) + 3 \sin(R|\omega|)\right) \\
\quad + \omega_3^2 \left(- (R|\omega|)^3 \cos(R|\omega|) + 5(R|\omega|)^2 \sin(R|\omega|) + 12(R|\omega|) \cos(R|\omega|) - 12 \sin(R|\omega|)\right), & \text{when } \gamma = 0, \\
\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^8} \left(\omega_1^2 + \omega_2^2\right) \left(- (R|\omega|)^3 \sin(R|\omega|) - 4(R|\omega|)^2 \cos(R|\omega|) + 8(R|\omega|) \sin(R|\omega|) + 8 \cos(R|\omega|) - 8\right) \\
\quad + \omega_3^2 \left(- (R|\omega|)^4 \cos(R|\omega|) + 6(R|\omega|)^3 \sin(R|\omega|) + 20(R|\omega|)^2 \cos(R|\omega|) - 40(R|\omega|) \sin(R|\omega|) - 40 \cos(R|\omega|) + 40\right), & \text{when } \gamma = 1.
\end{cases}$$
and

\[ S^2_{1,3}(\omega) = \begin{cases} \sqrt{\frac{2}{\pi}} \frac{2 R|\omega| + R|\omega| \cos(R|\omega|)}{|\omega|} - 3 \sin(R|\omega|), & \text{when } \gamma = -3, \\ \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^4} (- (R|\omega|)^3 \cos(3R|\omega|) + 6(R|\omega|)^2 \sin(R|\omega|)) + 15(R|\omega|) \cos(R|\omega|) - 15 \sin(R|\omega|), & \text{when } \gamma = 0, \\ \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^8} (- (R|\omega|)^4 \cos(R|\omega|) + 7(R|\omega|)^3 \sin(R|\omega|)) + 24(R|\omega|)^2 \cos(R|\omega|) - 48(R|\omega|) \sin(R|\omega|) - 48 \cos(R|\omega|) + 48), & \text{when } \gamma = 1. \end{cases} \]

The details leading to these expressions can be found in appendix A. In addition, by substituting \( \omega = 0 \) into the integrands found in \( \hat{S}^1_{1,1}, \hat{S}^2_{3,3} \) and \( \hat{S}^2_{1,3} \) and evaluating directly (noting that the exponential evaluated at \( \omega = 0 \) is equal to one),

\[ \hat{S}^1_{1,1}(0) = \begin{cases} \sqrt{\frac{1}{2\pi}} R^2, & \text{when } \gamma = -3, \\ \frac{2}{5} \sqrt{\frac{1}{2\pi}} R^5, & \text{when } \gamma = 0, \\ \frac{1}{3} \sqrt{\frac{1}{2\pi}} R^6, & \text{when } \gamma = 1, \end{cases} \]

\[ \hat{S}^2_{3,3}(0) = \begin{cases} \sqrt{\frac{1}{3\sqrt{2\pi}} R^2}, & \text{when } \gamma = -3, \\ \frac{15}{2} \sqrt{\frac{1}{2\pi}} R^5, & \text{when } \gamma = 0, \\ \frac{1}{9\sqrt{2\pi}} R^6, & \text{when } \gamma = 1 \end{cases} \]

and

\[ \hat{S}^2_{1,3}(0) = 0, \text{ for all } \gamma. \]

4 Stability of the Space-homogeneous Spectral Method

In order to consider the stability of the spectral method, first note that the integral (11) to calculate \( \hat{Q} \) is approximated using quadrature. The current code uses the composite trapezoidal rule
but, in general, for $M$ equally spaced quadrature nodes $\{\xi_m\}_{m=1}^M$ in Fourier space, corresponding weights $\{w_m\}_{m=1}^M$ and Fourier space stepsize $h_\xi$,

$$
\hat{Q}(\xi_k) = h_\xi^2 \sum_{m=1}^{M} w_m \hat{f}(\xi_k - \xi_m) \hat{\xi}(\xi_m) \left( \xi_m^T \hat{S}_{\xi} (\xi_m) \xi_m - (\xi_k - \xi_m)^T \hat{S}_{\xi} (\xi_m) (\xi_k - \xi_m) \right). \tag{12}
$$

Now, according to Lebedev [16], the criterion for stability of a numerical method of the form

$$
\frac{d}{dt} \left( \hat{f}(\xi_k) \right) = F(\hat{f}(\xi_k))
$$

is that the time-step $\Delta t$ must satisfy

$$
\Delta t \leq \frac{1}{\text{Lip}(F)},
$$

for the Lipschitz norm of $F$, $\text{Lip}(F)$. If an upper bound can be found on $\text{Lip}(F)$, this will in turn give a lower bound on $(\text{Lip}(F))^{-1}$, which $\Delta t$ must be below for the numerical method to remain stable. To find the upper bound, note that

$$
\text{Lip}(F) \leq |J_{k,l}|,
$$

for the Jacobian $J_{k,l}$ of $F(\hat{f}(\xi_k))$, given by

$$
J_{k,l} = \frac{\partial}{\partial \hat{f}(\xi_l)} \left( F(\hat{f}(\xi_k)) \right).
$$

Here, $F(\hat{f}(\xi_k)) = \frac{1}{2} \hat{Q}(\hat{f}, \hat{f})(\xi_k)$ and, to calculate the derivative of $\hat{Q}(\hat{f}, \hat{f})(\xi_k)$ with respect to $\hat{f}(\xi_l)$, it should be noted that there are two chances for $\hat{f}(\xi_l)$ to appear in the quadrature sum [12]. These are when $m = l$ and in general (depending on the choice of quadrature nodes) at another index, say $m = n$, where $\xi_k - \xi_n = \xi_l$. Assuming that there are indeed two indices which give rise to non-zero derivatives in the sum, and considering that $\xi_k - \xi_n = \xi_l$ is equivalent to $\xi_n = \xi_k - \xi_l$, the derivative is given by

$$
\frac{\partial}{\partial \hat{f}(\xi_l)} \left( \hat{Q}(\hat{f}, \hat{f})(\xi_k) \right) = h_\xi^2 w_l \hat{f}(\xi_k - \xi_l) \left( \xi_l^T \hat{S}_{\xi} (\xi_l) \xi_l - (\xi_k - \xi_l)^T \hat{S}_{\xi} (\xi_l) (\xi_k - \xi_l) \right) + h_\xi^2 w_n \hat{f}(\xi_n) \left( \xi_n^T \hat{S}_{\xi} (\xi_n) \xi_n - (\xi_k - \xi_n)^T \hat{S}_{\xi} (\xi_n) (\xi_k - \xi_n) \right) = h_\xi^2 w_l \hat{f}(\xi_k - \xi_l) \left( \xi_l^T \hat{S}_{\xi} (\xi_l) \xi_l - (\xi_k - \xi_l)^T \hat{S}_{\xi} (\xi_l) (\xi_k - \xi_l) \right) + h_\xi^2 w_n \hat{f}(\xi_k - \xi_l) \left( \xi_n^T \hat{S}_{\xi} (\xi_n) \xi_n - (\xi_k - \xi_n)^T \hat{S}_{\xi} (\xi_n) (\xi_k - \xi_n) \right) = h_\xi^2 w_l \hat{f}(\xi_k - \xi_l) \left( \xi_l^T \hat{S}_{\xi} (\xi_l) \xi_l - (\xi_k - \xi_l)^T \hat{S}_{\xi} (\xi_l) (\xi_k - \xi_l) \right) + h_\xi^2 w_n \hat{f}(\xi_k - \xi_l) \left( \xi_n^T \hat{S}_{\xi} (\xi_n) \xi_n - (\xi_k - \xi_n)^T \hat{S}_{\xi} (\xi_n) (\xi_k - \xi_n) \right), \tag{13}
$$
Then, since $h_{\xi} = \frac{\pi}{L_0}$ and $|w_l| \leq 1$ for any $l$, by the triangle inequality,

$$
\left| \frac{\partial}{\partial f(\xi_l)} \left( \hat{Q}(\hat{f}, \hat{f})(\xi_k) \right) \right| 
\leq \frac{\pi^3}{L_0^3} \left| \hat{f}(\xi_k - \xi_l) \right| \left( |\xi_l^T \hat{S} (\xi_l) \xi_l| + |(\xi_k - \xi_l)^T \hat{S} (\xi_l) (\xi_k - \xi_l)| \right. 
\left. + |(\xi_k - \xi_l)^T \hat{S} (\xi_k - \xi_l) (\xi_k - \xi_l)| + |\xi_l^T \hat{S} (\xi_k - \xi_l) \xi_l| \right). 
$$

Note that if there had been no such $\xi_n$ then the final two terms would be omitted here and the bound would only be smaller. This means the assumption that there are two appearances of $\hat{f}(\xi_l)$ in the quadrature sum (12) is more general.

Also, by definition of the Fourier transform,

$$
|\hat{f}(\xi_k - \xi_l)| \leq (2\pi)^{-\frac{3}{2}} \int_{B_R(0)} |f(u)||e^{-i(\xi_k - \xi_l) \cdot u}| du = (2\pi)^{-\frac{3}{2}} \|f\|_{L_1(B_R(0))},
$$

since $|e^{-i(\xi_k - \xi_l) \cdot u}| = 1$, and so

$$
\left| \frac{\partial}{\partial f(\xi_l)} \left( \hat{Q}(\hat{f}, \hat{f})(\xi_k) \right) \right| 
\leq \frac{\pi^3}{2\sqrt{2}L_0^3} \|f\|_{L_1(B_R(0))} \left( |\xi_l^T \hat{S} (\xi_l) \xi_l| + |(\xi_k - \xi_l)^T \hat{S} (\xi_l) (\xi_k - \xi_l)| \right. 
\left. + |(\xi_k - \xi_l)^T \hat{S} (\xi_k - \xi_l) (\xi_k - \xi_l)| + |\xi_l^T \hat{S} (\xi_k - \xi_l) \xi_l| \right). \quad (14)
$$

Now, for the terms involving $\hat{S}$, note that for a general matrix $A \in \mathbb{R}^{3 \times 3}$ and vectors $y, z \in \mathbb{R}^3$,

$$
y^T Az = \sum_{i,j=1}^{3} A_{i,j} y_i z_j \quad \text{and so} \quad |y^T Az| \leq (3)^2 \max_{i,j=1,2,3} A_{i,j} \left( \max_{i=1,2,3} y_i \right) \left( \max_{i=1,2,3} z_i \right). \quad (15)
$$

This means that a bound must be found on $|\hat{S}_{i,j}(\xi)|$, which is achieved by using the expressions in Section 3 for $\hat{S}_{1,1}^1$, $\hat{S}_{2,3}^2$ and $\hat{S}_{1,3}^2$, for $\gamma = -3$, 0 and 1. As is shown in Appendix B for any
\(k = 1, 2, \ldots, M\),

\[
|\hat{S}_{i,j}(\xi_k)| \leq \begin{cases} 
\left(\sqrt{\frac{1}{2\pi}} + \frac{3}{\pi^3} (\pi + 1) \sqrt{\frac{2}{\pi}}\right) L_v^2, & \text{when } \gamma = -3, \\
\frac{2}{\pi \pi^5} \left(2\pi^3 + 9\pi^2 + 21\pi + 21\right) L_v^5, & \text{when } \gamma = 0, \\
\frac{2}{\pi \pi^6} \left(2\pi^6 + 11\pi^3 + 36\pi^2 + 72\pi + 144\right) L_v^6, & \text{when } \gamma = 1 
\end{cases}
\]

\(\wedge \begin{cases} 
L_v^2, & \text{when } \gamma = -3, \\
L_v^5, & \text{when } \gamma = 0, \\
L_v^6, & \text{when } \gamma = 1. 
\end{cases}\)

Then, by using the identity (15) and noting that \(|(\xi_k)_i| \leq \xi = \frac{\pi}{h_v}\), for any \(k, l, n = 1, 2, \ldots, M\),

\[
|\xi_k^T \hat{S}(\xi_l) \xi_n| \lesssim \frac{9\pi^2}{h_v^2} \times \begin{cases} 
L_v^2, & \text{when } \gamma = -3, \\
L_v^5, & \text{when } \gamma = 0, \\
L_v^6, & \text{when } \gamma = 1. 
\end{cases}
\]

Now, since \(\xi_k - \xi_l = \xi_n\), each mixed \(\xi_k - \xi_l\) and \(\xi_l\) term in inequality (14) has the same upper bound. This gives

\[
\left| \frac{\partial}{\partial f(\xi_l)} \left(\hat{Q}(f, \hat{f}) (\xi_k)\right) \right| \lesssim 4 \left(\frac{\pi^2}{2\sqrt{2}h_v^2 L_v^3} ||f||_{L_1(B_R(0))}\right) \times \begin{cases} 
L_v^2, & \text{when } \gamma = -3, \\
L_v^5, & \text{when } \gamma = 0, \\
L_v^6, & \text{when } \gamma = 1, 
\end{cases}
\]

and so

\[
|J_{k,l}| \leq \frac{1}{\varepsilon} \left| \frac{\partial}{\partial f(\xi_l)} \left(\hat{Q}(f, \hat{f}) (\xi_k)\right) \right| \lesssim \frac{18\pi^2}{2\sqrt{2}h_v^2 ||f||_{L_1(B_R(0))}} \times \begin{cases} 
1, & \text{when } \gamma = -3, \\
L_v^2, & \text{when } \gamma = 0, \\
L_v^3, & \text{when } \gamma = 1, 
\end{cases}
\]

which means

\[
\frac{1}{|J_{k,l}|} \geq \begin{cases} 
\frac{\sqrt{2\varepsilon} L_v h_v^2}{18\pi^2 ||f||_{L_1(B_R(0))}}, & \text{when } \gamma = -3, \\
\frac{\sqrt{2\varepsilon} h_v^2}{18\pi^2 L_v^2 ||f||_{L_1(B_R(0))}}, & \text{when } \gamma = 0, \\
\frac{\sqrt{2\varepsilon} h_v^2}{18\pi^2 L_v^3 ||f||_{L_1(B_R(0))}}, & \text{when } \gamma = 1. 
\end{cases}
\]
Therefore, to ensure that $\Delta t \leq \frac{1}{|J_k,l|}$, choose $\Delta t$ such that

$$\Delta t \leq \begin{cases} \sqrt{2} \varepsilon L_v h_v^2, & \text{ when } \gamma = -3, \\ \frac{\sqrt{2} \varepsilon h_v^2}{18 \pi^2 \|f\|_{L_1(B_R(0))}}, & \text{ when } \gamma = 0, \\ \frac{\sqrt{2} \varepsilon L_v^2 \|f\|_{L_1(B_R(0))}}{18 \pi^2}, & \text{ when } \gamma = 1 \\ \frac{2 \sqrt{2} \varepsilon L_v^3}{9 \pi^2 N^2 \|f\|_{L_1(B_R(0))}}, & \text{ when } \gamma = -3, \\ \frac{2 \sqrt{2} \varepsilon}{9 \pi^2 N^2 \|f\|_{L_1(B_R(0))}} & \text{ when } \gamma = 0, \\ \frac{18 \pi^2 \|f\|_{L_1(B_R(0))}}{9 \pi^2 N^2 L_v \|f\|_{L_1(B_R(0))}} & \text{ when } \gamma = 1. \end{cases}$$

5 Numerical Results and Entropy Decay

5.1 Space Homogeneous Results

In the previous work by the current authors [18], simulations were already run to demonstrate the entropy decay rates for both Coulomb and hard sphere interactions using only $N = 16$ Fourier modes in each velocity direction. The results were satisfactory but it has since been discovered that the decay rates are even more convincing when increasing to $N = 32$. In addition, simulations have now been run for Maxwell molecules, which had caused some difficulty to produce at first.

The Coulomb Case ($\gamma = -3$)

When $-3 \leq \gamma < 0$, there is no spectral gap for Fokker-Planck-Landau type equations. This was proven analytically by Strain and Guo [19] where they showed that, if the initial condition is bounded by $e^{-c|v|^2}$, for some $c > 0$, the rate of convergence to a Maxwellian close to equilibrium is given by

$$e^{-kt^p}, \quad \text{with } p = -\frac{2}{\gamma} \text{ and some } k > 0. \quad (16)$$

For Coulomb interactions, with $\gamma = -3$, this gives the law of two thirds. In [18], the current authors showed this rate of convergence to equilibrium numerically by plotting the natural log.
of the relative entropy on a log-log scale against time. In particular, as the solution approaches equilibrium, it should be that
\[
\log\left(\log\left(\|H[f,M_{eq}]\|\right)\right) \sim \frac{2}{3} \log(t).
\]

The rate was captured by choosing an initial condition far from equilibrium, which is a sum of four Maxwellians with shifted centers, namely
\[
f_0(v) = \frac{1}{4} \sum_{l=0}^{3} M_v\left(v + \left((-1)^{\frac{l}{2}}, (-1)^l, (-1)^l\right)\right),
\]
for the Maxwellian \(M_v(v) = (2\pi T)^{-\frac{3}{2}} e^{-\frac{|v|^2}{2T}}\). The temperature used was \(T = 0.4\); the Knudsen number was \(\varepsilon = 20\); the velocity domain had \(L_v = 5.25\); \(N = 16\) Fourier modes were chosen; and the time-stepsize used was \(\Delta t = 0.01\). With these parameters, the rate was seen to be 0.634. This result is improved in the current simulation, however, where the number of Fourier modes has been increased to \(N = 32\) (so that \(\Delta t = 0.01\) is still below the new upper bound of approximately 0.0162 calculated for stability with these parameters for \(\gamma = -3\) in Section 4).

The marginal in \((v_1, v_2)\)-space of the initial condition (17) is plotted in Fig. 1(a), where it can be seen that this has the form of four humps. Subsequent marginals of the approximation to the Landau equation starting at this initial condition are plotted at mean-free times \(t = 2.8, 20\) and 100 in Fig. 1(b)-(d). This shows that the four humps merge together into one, before eventually taking shape as the space-homogeneous equilibrium Maxwellian (7) (see Fig. 1(d)) which, in this case with \(T = 0.4\) in (17), has equilibrium temperature \(T_{eq} = 1.4\) and is given by
\[
M_{eq}(v) = \frac{1}{(2.8\pi)^{\frac{3}{2}}} e^{-\frac{|v|^2}{2(2.8)^2}}.
\]

In Fig. 2, the relative entropy has been plotted. When natural logarithms have been taken, the curve does indeed become a straight line when close to equilibrium. It can be seen that, when \(t = 2.8\) (corresponding to Fig. 1(b)), the curve is not yet straight but that is because the solution is still far from a Maxwellian. At around \(t = 20\) (corresponding to Fig. 1(c)), however, the four humps have disappeared and the solution is becoming close to that of a Maxwellian. This is part of the entropy plot which is a straight line, with a slope of approximately 0.664. It should be noted that this is much closer to two thirds than the value of 0.634 attained with the parameters in [18].

At this point, it should be mentioned that the numerical scheme does not preserve positivity. There is potential for negativity to occur when conservation is enforced. The good news, however,
Figure 1: Marginals of $f$ in the variables $v_1$ and $v_2$ at various times during the simulation of the Landau equation starting with the initial condition (17), with $T = 0.4$, $\varepsilon = 20$, $L_v = 5.25$, $N = 32$ and $\Delta t = 0.01$, showing cells in the domain where the solution is negative (in red, near the boundary) and positive (in blue, in the interior).
Figure 2: Plot of $\log\left(\left|\log\left(\log(\mathcal{H}[f|M_{eq}])\right)\right|\right)$ against $\log(t)$ for the numerical approximation $f$ to the Landau equation, given initial condition (17), with $T = 0.4$, $\varepsilon = 20$, $L_v = 5.25$, $N = 32$ and $\Delta t = 0.01$, which has equilibrium solution $M_{eq}$ given by (18). A straight line has been added to show that the slope near equilibrium is close to two thirds, exhibiting the lack of spectral gap, but a degenerate spectrum corresponding to a stretch-time exponential decay given by $e^{-k t^p}$, with $p = \frac{2}{3}$ and some $k > 0$. The labels correspond to the marginal plots in Fig. 1.

is that the negative parts of the solution only appear as a result of tiny oscillations near the tails. The negative regions are shown underneath the marginal plots in Fig. 1 on the $(v_1, v_2)$-axes, as red cells which are indeed next to the boundary near the tails. In these regions, the solution is negligible anyway and so the effects of the negative values are not noticed. Furthermore, calculating the natural log in expression (8) for the relative entropy requires only positive values. Since the negative values are so tiny though (and the parts of the solution so close to zero give negligible influence on any bulk quantities anyway), these are just discarded when calculating the entropy. More precisely, the entropy is calculated through a quadrature method and any point for which $f$ has a negative value is considered a zero contribution to the overall sum.

The simulations are carried out with C++ code run on the Texas Advanced Computing Center’s Stampede2 supercomputer [2], utilising all sixty eight cores on 24 of the Intel Xeon Phi 7250 1.4GHz Knights Landing processors using hybrid OpenMP [11] and MPI [10]. Any procedure that requires a loop over the grid-cells in velocity space distributes the cells amongst the OpenMP threads then recombines the individual values calculated at the end of the loop. In addition,
when calculating the Fourier transform of $Q$, the evaluations at the $N^3$ many Fourier modes are evenly distributed across the MPI nodes. This means that only the values of $\hat{Q}$ are calculated on the modes associated to the current MPI node and so time is saved by evaluating at multiple Fourier modes concurrently across MPI nodes.

In [18], there was a table to show the performance increase when using more OpenMP threads was almost linear. In this work, where MPI has also been added to the space-homogeneous code, the performance increase with more MPI processes is recorded and it also appears to be close to linear. Table 1 records the times taken for 100 time-steps of the current simulation with various number of MPI processes, each with 68 OpenMP threads (averaged over three runs).

| No. of MPI processes | 1    | 2    | 4    | 8    | 16   | 24   |
|----------------------|------|------|------|------|------|------|
| Average time for 100 time-steps (s) | 18,643 | 9,391 | 4,757 | 2,439 | 1,276 | 890  |

Table 1: Average times after three runs of 100 time-steps with various number Intel Xeon Phi 7250 1.4GHz Knights Landing processors, each running one MPI task with 68 OpenMP threads in TACC’s Stampede2 supercomputer

**The Hard Sphere Case** ($\gamma = 1$)

Unlike when $\gamma < 0$, there is a spectral gap when $\gamma = 1$. This means the rate of convergence to a Maxwellian close to equilibrium is in fact exponential, of the form $e^{-kt}$, for some $k > 0$. Similar to the previous example, when close to equilibrium, the relative entropy should behave like $\log\left(\log\left(|\mathcal{H}[f|\mathcal{M}_{eq}]|\right)\right) \sim \log(t)$.

Trying to simulate hard spheres introduced a fair amount of difficulty, which shed light on an issue that should be considered for modeling hard potentials with the current spectral method. In particular, when choosing an initial condition for which the bulk of the mass is supported in too small a region near the center of the domain, the tails of the solution start to ripple after a small number of time-steps, causing an instability which leads to a blow-up. It is believed that this problem stems from the fact that collisions are more significant for hard potentials than soft ones, with more weight being given to larger relative velocities. The relative velocity becomes larger when closer to the tails in velocity-space.

At first, it may seem like a more compactly supported initial solution may help. The problem, however, is that collisions are computed in Fourier space. The Fourier transform will take a solution with small support in the original space and spread it out in the Fourier domain (consider,
for example, that a Gaussian with large peak and small variance has a Gaussian with small peak and large variance as its Fourier transform). This means that the Fourier transform of such an initial condition actually has tails with rather large magnitude near the boundaries. When multiplied by the hard sphere weights calculated in Section 3, this causes a problem computationally. This issue did not exist for $\gamma = -3$ as the weights near the tails for Coulomb interactions are smaller in magnitude. As a result, any part of the solution that turns negative is emphasized, which introduces the ripples as the conservation routine attempts to compensate.

This logic was followed for the simulations in [18] and a larger variance relative to the computational domain was chosen to fix the problem. This worked to combat the instabilities but as mass started to spread out of the domain, any bulk quantities calculated were affected. A better approach to this problem, which has been used in the current work, is to simply reduce the mass of the initial condition. This has the same result of reducing the magnitude of the tails but allows the variance to be reduced in the process.

For the hard sphere simulation, a very similar initial condition was chosen to (17), namely

$$f_0(v) = \rho_0 \sum_{l=0}^{3} \mathcal{M}_v \left( v + 0.016 \left( (-1)^{\lfloor \frac{l}{2} \rfloor}, (-1)^l, (-1)^{l+1} \right) \right),$$  

(19)

for the Maxwellian $\mathcal{M}_v(v) = \left( \frac{2\pi T}{3} \right)^{-\frac{3}{2}} e^{-\frac{|v|^2}{2T}}$, with a smaller temperature of $T = 0.00015$ than for the Coulomb interactions example. Also, in the initial condition (17), there was no $\rho_0$ factor but here $\rho_0 = 0.01$, which reduces the mass. Again, the Knudsen number is $\varepsilon = 20$ and $N = 32$ Fourier modes are used, but a much smaller velocity domain is chosen here, with boundary $L_v = 0.1$. This allows the time-step size to be increased slightly, as the stability results from Section 4 show that a smaller value of $L_v$ and smaller mass is less restrictive. In particular, the time-step size chosen is $\Delta t = 0.1$ (below the upper bound of approximately 0.1117 calculated for stability with these parameters for $\gamma = 1$ in Section 4).

The increased time-step size helps because when the mass is reduced there are fewer collisions and so simulations are slower on this time-scale. In order for the results to be comparable to those from the Coulomb interaction simulations in Sub-section 5.1, the time-scale should be adjusted to match that used for solutions with larger mass. An explanation of how the timescales differ for two simulations with different masses is given in Appendix C. In particular, in those calculations, let $t^a = t^C$ be the time-scale from the Coulomb interaction simulations; $t^b = t^H$ the time-scale from the current hard sphere simulations; and $\tau = \rho_0 = 0.01$ the mass ratio. Then, the entropy results in this sections are plotted on the scales $t = t^C = \rho_0 t^H$ and $H[f](t) = H'^C[f] = \frac{1}{\rho_0} H^H[f]$. As implied here, the superscripts are dropped in any plots.

A plot of the relative entropy for hard sphere on these scaled variables is shown in Fig. 3. When logarithms are taken, the curve is close to a straight line with slope 0.92103 which is less than the
slope of one that is expected for a spectral gap. Nevertheless, this is still larger than the slope of two thirds for Coulomb interactions and the slope of one is merely an upper bound, so this result is still satisfactory. Once again, by considering the marginals, when \( t = 9 \) (corresponding to position (b), or \( t^H = 900 \) in the original scaling), the curve is not yet straight but that is because the solution has too flat a peak and so is still relatively far from a Maxwellian. At around \( t = 30 \) (corresponding to position (c), or \( t^H = 3000 \) in the original scaling), however, the shape of the marginal is closer to that of a Maxwellian and this is much more near to the part of the entropy plot which is a straight line.

**The Maxwell Molecule Case (\( \gamma = 0 \))**

When \( \gamma = 0 \), there is still a spectral gap for the Focker-Planck-Landau type equation but this can be seen as a borderline case before \( \gamma \) drops below zero and starts to obey Strain and Guo’s

---

**Figure 3:** Plot of \( \log(\log(\mathcal{H}[f|\mathcal{M}_{eq}])) \) against \( \log(t) \) for the numerical approximation \( f \) to the Fokker-Planck-Landau type equation with \( \gamma = 1 \) and weights calculated by the exact formulae in Section [3], given initial condition [19], with \( T = 0.00015, \varepsilon = 20, L_v = 0.1, N = 32 \) and \( \Delta t = 0.1 \), which has equilibrium solution given by a Maxwellian with temperature \( T_{eq} = 0.000406 \). A straight line has been added to show that the slope near equilibrium is now approximately 0.92103, slightly below the value of one expected for the existence of a spectral gap. The \((v_1, v_2)\)-marginals are included at times (a) \( t = 0 \), (b) \( t = 9 \), (c) \( t = 30 \) and (d) \( t = 48 \).
law of stretch-time exponential decay with exponent given by formula (16). This means that a straight line in the relative entropy plot may be a little harder to detect.

For the Maxwell molecule simulation, the same initial condition (19) was used as for hard sphere interactions, with the same parameters $T = 0.00015$, $\rho_0 = 0.01$, $\varepsilon = 20$, $N = 32$, $L_v = 0.1$ and $\Delta t = 0.1$. Due to the mass being smaller again, the same scaled variables for time and entropy are used, as in the discussion from the hard sphere results. The relative entropy for this case is plotted in these scaled variables on a log-log scale in Fig. 4 where there is still a straight line forming near the end of the simulation. The slope of this line is approximately 0.92142, which is close to the value calculated for the hard sphere simulations.

![Figure 4: Plot of $\log \left( \left\| \log \left( \left| \mathcal{H} [f | M_{eq}] \right| \right) \right\| \right)$ against $\log(t)$ for the numerical approximation $f$ to the Fokker-Planck-Landau type equation with $\gamma = 0$ and weights calculated by the exact formulae in Section 3, given initial condition (19), with $T = 0.00015$, $\varepsilon = 20$, $L_v = 0.1$, $N = 32$ and $\Delta t = 0.1$, which has equilibrium solution given by a Maxwellian with temperature $T_{eq} = 0.000406$. A straight line has been added to show that the slope near equilibrium is now approximately 0.92142, slightly below the value of one expected for the existence of a spectral gap. The ($v_1$, $v_2$)-marginals are included at times (a) $t = 0$, (b) $t = 0.52$, (c) $t = 2.2$ and (d) $t = 4$.](image)

Finally, all three of the plots have been included on the same set of axes in Fig. 5. Here it can be seen that simulations associated to the Coulomb interactions (i.e. the Landau equation) give the strongest result. Not only does the straight line persist for the longest time but the slope is closest
to the predicted value. This is perhaps indicative of the fact that the Focker-Planck-Landau type equation with Coulomb interactions is the most physically realisable case. On the other hand, the fact that the slopes captured by both the hard sphere and Maxwell molecule simulations are so similar demonstrates that they are both capturing the same phenomenon, namely, the existence of the spectral gap.

![Graph](image)

**Figure 5:** Plot of $\log\left(\log\left(\frac{1}{\log(t)}\right)\right)$ against $\log(t)$ for the numerical approximation $f$ to the Fokker-Planck-Landau type equations with potentials $\gamma = -3$, 0 and 1, with weights calculated by the exact formulae in Section 3. The initial conditions and parameters used are the same as in Fig. 2-4. Straight lines are also added to show the decay rates approached by each simulation.

5.2 Space-inhomogeneous Results for the Coulomb Case ($\gamma = -3$)

Results from $N = 32$ Fourier Modes

Trying to recover Strain and Guo’s entropy decay rate of two thirds is a little more complicated in the space-inhomogeneous case, which appears to be a result of accumulating numerical error. First of all, to alleviate these difficulties, a different form of initial condition is used from the four humps used in the space-homogeneous case. In particular, a small perturbation of a Maxwellian by a cosine wave in space is chosen, which is the same used to demonstrate the phenomenon of
Landau damping, namely
\[ f_0(x, v) = (1 + A \cos(kx))M_v(v), \quad (20) \]
again for the Maxwellian
\[ M_v(v) = \frac{1}{(2\pi T)^{3/2}} e^{-\frac{|v|^2}{2T}}. \]
Here, \( T = 1.2 \), \( k = 0.5 \) and \( A = 0.05 \) are used. Additionally, the space domain is chosen to have length \( L_x = 4\pi \), so that there is exactly one period of the cosine wave and \( \int_0^{L_x} f_0(x, v) \, dx = M_v(v) \). This means the solution converges to the Maxwellian \( M_v(v) \), uniformly in space, as \( t \to \infty \).

When the simulations were first run, it became clear that the choice of \( N = 16 \) Fourier modes and \( N_v = 24 \) velocity grid cells in each dimension used originally in the space-homogeneous case in [18] were not enough to accurately calculate the space-inhomogeneous entropy. This problem can easily be fixed, however, by increasing the number of D.G. grid-cells in velocity spaces to \( N_v = 48 \) and the number of Fourier modes to \( N = 32 \), as in the space-homogeneous results in Sub-section 5.1. These parameters are used along with the Knudsen number \( \varepsilon = 20 \); velocity domain width \( L_v = 5.25 \); \( N_x = 24 \) D.G. cells in space; and time-stepsize \( \Delta t = 0.01 \). Note that increasing the number of D.G. cells in space has little effect on accuracy because the initial condition (20) leads to simulations with very small variations in space.

When the natural log of the relative entropy is then plotted on a log-log scale as a result of using these parameters, as in Fig. 6, it once again approaches a straight line. This time the slope of that line is approximately 0.6537 which is again close to the slope of two thirds that is expected. Some marginal plots are also included on this plot to show how the behaviour here is similar to that in the space-homogeneous case. First, at \( t = 4.6 \) mean-free times, the log-log plot of relative entropy is not quite yet a straight line and it can be seen in the marginal plot at position (b) that the pdf is still taking a similar form to the initial condition in position (a). As soon as the plot approaches the straight line, however, like at \( t = 9.4 \) mean-free times, the p.d.f. is starting to look more like the equilibrium solution (6), which is shown at positions (c) and (d).

**Results from \( N = 16 \) Fourier Modes**

To illustrate the issues when only \( N = 16 \) Fourier modes are used, first note that, for the current perturbation initial condition (20), \( \Phi_{eq}(x) = 0 \) for all \( x \) and \( \rho_0 = L_x \) in the equilibrium Maxwellian (6) so that
\[ M_{eq}(x,v) = \frac{1}{(2\pi T_{eq})^{3/2}} e^{-\frac{|v|^2}{2T_{eq}}}. \quad (21) \]
As is shown in appendix D for \( T = 1.2 \) and \( A = 0.05 \), \( T_{eq} = T + \frac{2}{3} A^2 = 1.2 + \frac{2}{3}(0.05)^2 = 1.201666 \) and the equilibrium entropy evaluates to
\[ \mathcal{H}[M_{eq}] = -6\pi (\ln(2\pi(1.201666\ldots)) + 1) = -56.955565 \quad (\text{to 6 d.p.}). \quad (22) \]
Figure 6: Plot of $\log\left(\log(\mathcal{H}[f|\mathcal{M}_{eq}])\right)$ against $\log(t)$ for the numerical approximation $f$ to the space-inhomogeneous Landau equation, given initial condition (20), with $T = 1.2$, $k = 0.5$, $A = 0.05$, $\varepsilon = 20$, $L_v = 5.25$, $N = 32$, $N_v = 48$, $N_x = 24$ and $\Delta t = 0.01$, which has equilibrium solution $\mathcal{M}_{eq}$ given by (21). A straight line has been added to show that the slope near equilibrium is close to two thirds, exhibiting the lack of spectral gap, but a degenerate spectrum corresponding to a stretch-time exponential decay given by $e^{-kt^p}$, with $p = \frac{2}{3}$ and some $k > 0$. Marginals in $(x,v_1)$-space are also shown at times (a) $t = 0$ (b) $t = 4.6$, (c) $t = 9.4$ and (d) $t = 12$, to demonstrate that solution is only near equilibrium when close to the stretch-time exponential decay.

When $N = 16$ Fourier modes, $N_v = 24$ velocity and $N_x = 24$ space D.G. grid cells are used in each dimension, however, the decreasing values of entropy pass the equilibrium value as early as the 342nd time-step, where it jumps from $\mathcal{H}[f](3.41) = -56.955547$ to $\mathcal{H}[f](3.42) = -56.955658$.

Initially, as a workaround for this issue, the idea was to run the simulation for long enough that the solution should reach a numerical approximation to equilibrium and then use the value of the entropy calculated from this long-time solution as the equilibrium entropy. When running the simulations for so long, however, the numerical error begins to accumulate and an instability appears to be introduced. Figure 7(a) shows that the entropy does seem to exhibit a type of exponential decay up until around $t = 200$ but then, instead of converging to some steady state value, decreases further and starts to oscillate. A similar trend can be seen in the total energy.
This should be held constant throughout, but it is common for a slight deviation to occur in the energy of the space-inhomogeneous simulations of the order of roughly $10^{-4}$. This can be seen up to about $t = 200$ in Fig. 7(b) and is expected to result from the time-splitting used. What should not happen, however, is the faster increased deviation and oscillations that occur around the same time that the entropy is also oscillating.

**Figure 7:** Results from a simulation of the space-inhomogeneous Landau equation, starting with the initial condition (20), with $T = 1.2$, $k = 0.5$, $A = 0.05$, $\varepsilon = 20$, $L_v = 5.25$, $N = 16$, $N_v = 24$, $N_x = 24$ and $\Delta t = 0.01$. (a) Plot of $H[f|M_{eq}]$ for the numerical approximation $f$, which has equilibrium solution taken from the final time-step, namely $M_{eq} = f(800)$. (b) Plot of the error in the total energy from the initial value $T_{tot}(0) = 1.201666...$

It should also be noted that the instabilities here are different to those that arise in the Boltzmann and Landau equations associated with the issues discussed in Section 4, as the source of those errors are near the tails. Here, the issue is close to the center of the Maxwellian, around $|v| = 0$. Figure 8(a) shows a marginal in $(x,v_1)$-space of the initial condition and then in Fig. 8(b) the marginal is shown at time $t = 200$ (the time up to which the entropy and total energy are behaving themselves in Fig. 7), where the approximation seems to be near the equilibrium. Finally, Fig. 8(c) shows an example of how the Maxwellian is contorting around $|v| = 0$, with points appearing there at the $x$-boundaries and a kink in the middle of space. This indicates some sort of instability interfering with the expected behaviour.

When using the values $N = 32$ and $N_v = 48$, however, the simulation does not reach the theoretical equilibrium entropy (22) until after the 1525-th time-step, at which point the approximation appears to have reached the equilibrium solution. This suggests that the solution to the Landau equation, starting with initial condition (20), reaches equilibrium much faster than initially suspected and it was never necessary to push it to the point where the numerical error accumulates enough to cause an influence.
Figure 8: Marginals in \((x, v_1)\)-space during a simulation of the space-inhomogeneous Landau equation, starting with the initial condition (20), with \(T = 1.2\), \(k = 0.5\), \(A = 0.05\), \(\varepsilon = 20\), \(L_v = 5.25\), \(N = 16\), \(N_v = 24\), \(N_x = 24\) and \(\Delta t = 0.01\) at times (a) \(t = 0\) (the initial condition) (b) \(t = 200\) (seemingly near equilibrium) and (c) \(t = 700\) (unstable behaviour).

6 Conclusion

In this work, the conservative spectral method for solving Fokker-Planck-Landau type equations was expanded upon by extending the calculations to hard sphere and Maxwell molecule potentials. Conditions for stability were then derived for each of the three cases. Finally, examples of the numerical method for all three of these potentials were given in the space-homogenous case, in addition to results for Coulomb interactions in the space-inhomogeneous setting, to show the power of the scheme. In particular, the relative entropy during a simulation was shown to decay close to the correct rate for Coulomb interactions, in accordance with the rate of two thirds predicted by Strain and Guo. This indicates that the current numerical scheme is an excellent model for the Landau equation. When the model is applied to the Fokker-Planck-Landau type equation with hard sphere and Maxwell molecule interactions, the existence of the spectral gap is evident but the decay rate seen is slightly below the expected value of one. Nevertheless, the decay rate captured was almost the same for both potentials and the effect responsible for this was the spectral gap.

The importance of the conservation routine was also emphasised by showing that the decay rate without it is less accurate. Indeed, the method does not preserve positivity but the regions in which the solution falls below zero are always near the tails and the solution is negligible at those locations anyway. Clearly this is true as dropping those values in calculation of the entropy did not detract from the result.
In addition to the numerical evidence provided here for the power of the conservative spectral method for Fokker-Planck-Landau equations, the current authors are investigating error estimates to prove analytically that the approximations from this scheme do indeed converge to the true solutions of the equation. Work is also underway to implement the present method in a multi-species setting, based on the calculations by Gamba et al. [11] to develop an asymptotic preserving explicit-implicit numerical scheme for species with disparate masses.

Appendix A  Evaluating Integrals for $\hat{S}$

In general, to calculate an integral of the form $\left(2\pi\right)^{-\frac{3}{2}} \int_{B_R(0)} f(u)e^{-i\omega \cdot u} \, du$, first a substitution is made in order to reduce the scalar product in the exponential to a single multiplication. To do this, note that the rotation matrix $A$ given by

$$A = \begin{bmatrix}
\frac{\omega_1 \omega_3}{\sqrt{\omega_1^2 + \omega_2^2}} & \frac{\omega_2 \omega_3}{\sqrt{\omega_1^2 + \omega_2^2}} & -\sqrt{\omega_1^2 + \omega_2^2} \\
-\frac{\omega_2^2}{\sqrt{\omega_1^2 + \omega_2^2}} & \frac{\omega_1^2}{\sqrt{\omega_1^2 + \omega_2^2}} & 0 \\
\sqrt{\omega_1^2 + \omega_2^2} & \omega_3 \\
\end{bmatrix}$$

has the property that $A\omega = (0, 0, |\omega|)$. Also, since $A$ is a rotation matrix, it is orthogonal and so $A^{-1} = A^T$ and $\det A = 1$.

Then, changing variables via $u = A^T v$ and noting that $\omega \cdot u = \omega^T A^T v = |\omega| v_3$,

$$\left(2\pi\right)^{-\frac{3}{2}} \int_{B_R(0)} f(u)e^{-i\omega \cdot u} \, du = \left(2\pi\right)^{-\frac{3}{2}} \int_{B_R(0)} f(A^T v)e^{-i|\omega|v_3} \, dv.$$

Finally, by changing to spherical coordinates via

$$v = r \sigma = r(\sin(\theta) \cos(\phi), \sin(\theta) \sin(\phi), \cos(\theta)),$$

where $0 \leq r \leq R$, $-\pi \leq \phi \leq \pi$ and $0 \leq \theta \leq \pi$,

$$\left(2\pi\right)^{-\frac{3}{2}} \int_{B_R(0)} f(u)e^{-i\omega \cdot u} \, du = \left(2\pi\right)^{-\frac{3}{2}} \int_0^R \int_{\pi}^{\pi} \int_0^\infty f(r A^T \sigma)e^{-ir|\omega|\cos(\theta)} r^2 \sin(\theta) \, d\theta d\phi dr. \quad (23)$$

Now, for $\hat{S}_{1,1}^1(\omega)$, $f(u) = |u|^{\gamma + 2}$ and so $f(r A^T \sigma) = r^{\gamma + 2}$. By inserting this expression in the general integral formula (23) and evaluating integrals with respect to $\phi$, this gives

$$\hat{S}_{1,1}^1(\omega) = \left(2\pi\right)^{-\frac{3}{2}} \int_0^R \int_{\pi}^{\pi} \int_0^\infty e^{-ir|\omega|\cos(\theta)} \sin(\theta) \, d\theta dr.$$
It can be checked that
\[ \int_0^\pi e^{-i r|\omega|\cos(\theta)} \sin(\theta) \, d\theta = \frac{2}{r|\omega|} \sin(r|\omega|) \]
and so
\[ \hat{S}_{1,1}(\omega) = \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|} \int_0^R r^{\gamma+3} \sin(r|\omega|) \, dr. \]

Then, by evaluating this integral in each of the Coulomb, Maxwell molecule and hard sphere cases, if \(|\omega| \neq 0\),
\[ \hat{S}_{1,1}(\omega) = \begin{cases} \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^2} \left(1 - \cos(R|\omega|)\right), & \text{when } \gamma = -3, \\ \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^5} \left(-(R|\omega|)^3 \cos(R|\omega|) + 3(R|\omega|)^2 \sin(R|\omega|)\right) + 6(R|\omega|) \cos(R|\omega|) - 6 \sin(R|\omega|), & \text{when } \gamma = 0, \\ \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^6} \left(-(R|\omega|)^4 \cos(R|\omega|) + 4(R|\omega|)^3 \sin(R|\omega|)\right) + 12(R|\omega|)^2 \cos(R|\omega|) - 24(R|\omega|) \sin(R|\omega|) \\ - 24 \cos(R|\omega|) + 24 \right), & \text{when } \gamma = 1. \end{cases} \]

Next, for \( \hat{S}_{3,3}(\omega) \), \( f(u) = |u|^\gamma u_3^2 \) and so
\[ f(rA^T\varphi) = r^{\gamma+2} \frac{1}{|\omega|^2} \left((\omega_1^2 + \omega_2^2) \sin^2(\theta) \cos^2(\phi) \right. \]
\[ - 2\omega_3 \sqrt{\omega_1^2 + \omega_2^2} \sin(\theta) \cos(\theta) \cos(\phi) + \omega_3^2 \cos^2(\theta) \right). \]

By inserting this expression in the general integral formula (23) and evaluating integrals with respect to \( \phi \) (noting that an integral of \( \cos(\phi) \) over \(-\pi \leq \phi \leq \pi \) returns zero), this gives
\[ \hat{S}_{3,3}(\omega) = (2\pi)^{-\frac{3}{2}} \int_0^R r^{\gamma+1} \frac{1}{|\omega|^2} \left((\omega_1^2 + \omega_2^2)^2\pi \int_0^\pi (1 - \cos^2(\theta))e^{-ir|\omega|\cos(\theta)} \sin(\theta) \, d\theta \right. \]
\[ + \omega_3^2 (2\pi) \int_0^\pi \cos^2(\theta)e^{-ir|\omega|\cos(\theta)} \sin(\theta) \, d\theta \left. \right) dr. \]

It can be checked that
\[ \int_0^\pi \cos^2(\theta)e^{-ir|\omega|\cos(\theta)} \sin(\theta) \, d\theta = \frac{2}{(r|\omega|)^3} \left((r|\omega|)^2 \sin(r|\omega|) + 2(r|\omega|) \cos(r|\omega|) - 2 \sin(r|\omega|) \right) \]
and
\[ \int_0^{\pi} (1 - \cos^2(\theta)) e^{-ir|\omega|\cos(\theta)} \sin(\theta) \, d\theta = \frac{4}{(r|\omega|)^3} \left( \sin(r|\omega|) - (r|\omega|) \cos(r|\omega|) \right). \]

So,
\[ \hat{S}_{3,3}^2(\omega) = (2\pi)^{-\frac{3}{2}} \int_0^R r^{\gamma+4} \frac{1}{|\omega|^2} \left( \frac{4\pi}{|\omega|^3} \left( \sin(r|\omega|) - (r|\omega|) \cos(r|\omega|) \right) \right. \]
\[ + \left. \omega_3^2 \frac{4\pi}{(r|\omega|)^3} \left( (r|\omega|)^2 \sin(r|\omega|) + 2(r|\omega|) \cos(r|\omega|) - 2 \sin(r|\omega|) \right) \right) \, dr. \]

The easiest way to calculate these integrals is to use a substitution of \( u = r|\omega| \), allowing \( \hat{S}_{3,3}^2(\omega) \) to be written as
\[ \hat{S}_{3,3}^2(\omega) = (2\pi)^{-\frac{3}{2}} \frac{4\pi}{(|\omega|)\gamma+7} \left( \frac{4\pi}{|\omega|} \left( \int_0^{R|\omega|} u^{\gamma+1} \sin(u) \, du - \int_0^{R|\omega|} u^{\gamma+2} \cos(u) \, du \right) \right. \]
\[ + \left. \omega_3 \left( \int_0^{R|\omega|} u^{\gamma+3} \sin(u) \, du - 2 \int_0^{R|\omega|} u^{\gamma+1} \sin(u) \, du + 2 \int_0^{R|\omega|} u^{\gamma+2} \cos(u) \, du \right) \right). \]

Then, by evaluating these integrals in each of the Coulomb, Maxwell molecule and hardsphere
cases, if $|\omega| \neq 0$,

\[
\begin{align*}
\hat{S}_{3,3}^2 (\omega) &= \begin{cases} \sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^4} \left( \frac{1}{2} \left( \omega^2 + \omega^2 \right) \frac{R|\omega| - \sin(R|\omega|)}{R|\omega|} ight. \\
&\quad - \omega^2 \frac{R|\omega| + (R|\omega|) \cos(R|\omega|) - 2 \sin(R|\omega|)}{R|\omega|} \right), \quad \text{when} \quad \gamma = -3, \\
&\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^4} \left( \omega^2 + \omega^2 \right) \left( -(R|\omega|)^2 \sin(R|\omega|) - 3(R|\omega|) \cos(R|\omega|) + 3 \sin(R|\omega|) \right) \\
&\quad + \omega^2 \left( -(R|\omega|)^3 \cos(R|\omega|) + 5(R|\omega|)^2 \sin(R|\omega|) ight) \\
&\quad + 12(R|\omega|) \cos(R|\omega|) - 12 \sin(R|\omega|) \right), \quad \text{when} \quad \gamma = 0, \\
&\sqrt{\frac{2}{\pi}} \frac{1}{|\omega|^4} \left( \omega^2 + \omega^2 \right) \left( -(R|\omega|)^3 \sin(R|\omega|) - 4(R|\omega|)^2 \cos(R|\omega|) ight. \\
&\quad + 8(R|\omega|) \sin(R|\omega|) + 8 \cos(R|\omega|) - 8 \\
&\quad + \omega^2 \left( -(R|\omega|)^4 \cos(R|\omega|) + 6(R|\omega|)^3 \sin(R|\omega|) ight) \\
&\quad + 20(R|\omega|)^2 \cos(R|\omega|) - 40(R|\omega|) \sin(R|\omega|) \\
&\quad - 40 \cos(R|\omega|) + 40 \right), \quad \text{when} \quad \gamma = 1.
\end{cases}
\]

Finally, for $\hat{S}_{1,3}^2 (\omega)$, $f(x) = |x|^\gamma u_1 u_3$ and so

\[
f \left( rA^T \sigma \right) = r^{\gamma+2} \frac{1}{|\omega|^2} \left( -\omega_1 \omega_3 \sin^2(\theta) \cos^2(\phi) + \frac{\omega_1 \omega_3^2}{\sqrt{\omega_1^2 + \omega_2^2}} \sin(\theta) \cos(\theta) \cos(\phi) \\
+ \omega_2 |\omega| \sin^2(\theta) \sin(\phi) \cos(\phi) - \frac{\omega_2 \omega_3 |\omega|}{\sqrt{\omega_1^2 + \omega_2^2}} \sin(\theta) \cos(\theta) \sin(\phi) \\
- \omega_1 \sqrt{\omega_1^2 + \omega_2^2} \sin(\theta) \cos(\theta) \cos(\phi) + \omega_1 \omega_3 \cos^2(\theta) \right).
\]

By inserting this expression in the general integral formula \text{(23)} and evaluating integrals with respect to $\phi$ (noting that an integral of $\cos(\phi)$, $\sin(\phi)$ and $\sin(\theta) \cos(\phi)$) over $-\pi \leq \phi \leq \pi$ returns
zero), this gives
\[
\hat{S}_{1,3}^2(\omega) = (2\pi)^{-\frac{3}{2}} \frac{\omega_1 \omega_3}{|\omega|^2} \int_0^R r^{\gamma+4} \left( -\pi \int_0^\pi (1 - \cos^2(\theta)) e^{-ir|\omega| \cos(\theta)} \sin(\theta) \, d\theta \right. \\
\left. + 2\pi \int_0^\pi \cos^2(\theta) e^{-ir|\omega| \cos(\theta)} \sin(\theta) \, d\theta \right) \, dr.
\]

Using the results for the integrals with respect to $\theta$ from $\hat{S}_{3,3}^2$,
\[
\hat{S}_{1,3}^2(\omega) = (2\pi)^{-\frac{3}{2}} \frac{\omega_1 \omega_3}{|\omega|^2} \int_0^R r^{\gamma+4} \left( \frac{1}{(r|\omega|)^3} - \frac{3}{(r|\omega|)^3} \sin(r|\omega|) + \frac{3}{(r|\omega|)^2} \cos(r|\omega|) \right) \, dr.
\]

Again, using a substitution of $u = r|\omega|$, $\hat{S}_{1,3}^2(\omega)$ can be written as
\[
\hat{S}_{1,3}^2(\omega) = (2\pi)^{-\frac{3}{2}} \frac{\omega_1 \omega_3}{|\omega|^2} \int_0^{R|\omega|} \left( (u^{\gamma+3} - 3u^{\gamma+1}) \sin(u) + 3u^{\gamma+2} \cos(u) \right) \, du.
\]

Then, by evaluating these integrals in each of the Coulomb, Maxwell molecule and hardsphere cases, if $|\omega| \neq 0$,
\[
\hat{S}_{1,3}^2(\omega) = \left\{ \begin{array}{ll}
-\sqrt{\frac{2}{\pi}} \frac{\omega_1 \omega_3}{|\omega|^4} \frac{2R|\omega| + R|\omega| \cos(R|\omega|) - 3 \sin(R|\omega|)}{R|\omega|}, & \text{when } \gamma = -3, \\
\sqrt{\frac{2}{\pi}} \frac{\omega_1 \omega_3}{|\omega|^4} \left( -(R|\omega|)^3 \cos(R|\omega|) + 6(R|\omega|)^2 \sin(R|\omega|) \right. \\
\left. + 15(R|\omega|) \cos(R|\omega|) - 15 \sin(R|\omega|) \right), & \text{when } \gamma = 0, \\
\sqrt{\frac{2}{\pi}} \frac{\omega_1 \omega_3}{|\omega|^4} \left( -(R|\omega|)^4 \cos(R|\omega|) + 7(R|\omega|)^3 \sin(R|\omega|) \right. \\
\left. + 24(R|\omega|)^2 \cos(R|\omega|) - 48(R|\omega|) \sin(R|\omega|) \right) - 48 \cos(R|\omega|) + 48), & \text{when } \gamma = 1.
\end{array} \right.
\]

### Appendix B  Calculating Bounds for $\hat{S}$

#### B.1  The case $\gamma = -3$:

First, by the triangle inequality and noting that $|\xi_k| \geq L_v = \frac{\pi}{L_v}$ when $|\xi_k| \neq 0$,
\[
|\hat{S}_{1,1}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{|\xi_k|^2} (2) \leq \frac{2}{\pi^2} \sqrt{\frac{2}{\pi}} L_v^2.
\]
Also, since \( \hat{S}_{1,1}(0) = \sqrt{\frac{1}{2\pi}} L_v^2 \),

\[
|\hat{S}_{1,1}(\xi_k)| \leq \sqrt{\frac{1}{2\pi}} L_v^2, \quad \text{for any } k = 1, 2, \ldots, M.
\]

Then, when \( |\xi_k| \neq 0 \),

\[
|\hat{S}_{2,3}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{|\xi_k|^4} \left( |\xi_k|^2 \left( 1 + \frac{1}{L_v|\xi_k|} \right) + |\xi_k|^2 \left( 1 + 1 + \frac{2}{L_v|\xi_k|} \right) \right)
= 3 \sqrt{\frac{2}{\pi}} \frac{1}{|\xi_k|^2} \left( 1 + \frac{1}{L_v} \frac{1}{|\xi_k|} \right)
\leq 3 \sqrt{\frac{2 L_v^2}{\pi^2}} \left( 1 + \frac{1}{L_v} \frac{1}{\pi} \right)
= \frac{3}{\pi^3} (\pi + 1) \sqrt{\frac{2}{\pi}} L_v^2.
\]

Also, since \( \hat{S}_{3,3}(0) = \frac{1}{3\sqrt{2\pi}} L_v^2 \),

\[
|\hat{S}_{3,3}(\xi_k)| \leq \frac{3}{\pi^3} (\pi + 1) \sqrt{\frac{2}{\pi}} L_v^2, \quad \text{for any } k = 1, 2, \ldots, M.
\]

This then means that the diagonal terms satisfy, for each \( i = 1, 2, 3 \) and \( k = 1, 2, \ldots, M \),

\[
|\hat{S}_{i,i}(\xi_k)| \leq |\hat{S}_{i,1}(\xi_k)| + |\hat{S}_{i,3}(\xi_k)| = \left( \sqrt{\frac{1}{2\pi}} + \frac{3}{\pi^3} (\pi + 1) \sqrt{\frac{2}{\pi}} \right) L_v^2.
\]

Similarly, when \( |\xi_k| \neq 0 \),

\[
|\hat{S}_{1,3}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{|\xi_k| |\xi_k|}{|\xi_k|^4} \left( 2 + 1 + \frac{3}{L_v|\xi_k|} \right)
= 3 \sqrt{\frac{2}{\pi}} \frac{1}{|\xi_k|^2} \left( 1 + \frac{1}{L_v} \frac{1}{|\xi_k|} \right)
\leq \frac{3}{\pi^3} (\pi + 1) \sqrt{\frac{2}{\pi}} L_v^2.
\]

Also, since \( \hat{S}_{3,3}(0) = 0 \),

\[
|\hat{S}_{1,3}(\xi_k)| \leq \frac{3}{\pi^3} (\pi + 1) \sqrt{\frac{2}{\pi}} L_v^2, \quad \text{for any } k = 1, 2, \ldots, M.
\]
This a bound for any off-diagonal term and so, since it is smaller than the bound for the diagonal terms, for each \( i, j = 1, 2, 3 \) and \( k = 1, 2, \ldots, M \), when \( \gamma = -3 \),

\[
|\hat{S}_{i,j}(\xi_k)| \leq |\hat{S}_{i,i}(\xi_k)| \leq \left( \sqrt{\frac{1}{2\pi}} + \frac{3}{\pi^3}(\pi + 1)\sqrt{\frac{2}{\pi}} \right) L_v^2 \approx 0.719 L_v^2 \leq L_v^2.
\]

**B.2 The case \( \gamma = 0 \):**

Here, by factoring in the highest power of \( \xi_k \) appearing in brackets and by the triangle inequality, when \( |\xi_k| \neq 0 \),

\[
|\hat{S}_{1,1}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{|\xi_k|^2} \left( L_v^3 + 3L_v^2 \frac{1}{|\xi_k|} + 6L_v \frac{1}{|\xi_k|^2} + 6 \frac{1}{|\xi_k|^3} \right) \\
\leq \sqrt{\frac{2}{\pi}} L_v^2 \left( \frac{L_v^3}{\pi} + 3L_v^2 \frac{L_v}{\pi} + 6L_v \frac{L_v^2}{\pi^2} + 6 \frac{L_v^3}{\pi^3} \right) \\
= \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} \left( \pi^3 + 3\pi^2 + 6\pi + 6 \right) L_v^5.
\]

Similarly, when \( |\xi_k| \neq 0 \),

\[
|\hat{S}_{3,3}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} \left( (\pi^2 + 3\pi + 3) + (\pi^3 + 5\pi^2 + 12\pi + 12) \right) L_v^5 \\
= \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} \left( \pi^3 + 6\pi^2 + 15\pi + 15 \right) L_v^5
\]

and

\[
|\hat{S}_{1,3}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} \left( \pi^3 + 6\pi^2 + 15\pi + 15 \right) L_v^5.
\]

Also, since \( \hat{S}_{1,1}(\mathbf{0}) = \frac{2}{\pi} \sqrt{\frac{1}{2\pi}} L_v^2 \), \( \hat{S}_{3,3}(\mathbf{0}) = \frac{2}{15\sqrt{2\pi}} L_v^2 \) and \( \hat{S}_{3,3}(\mathbf{0}) = \mathbf{0} \), which are all less than the previous bounds, the above bounds are true for all \( k = 1, 2, \ldots, M \).

Again, since the bounds for \( |\hat{S}_{1,3}(\xi_k)| \) and \( |\hat{S}_{3,3}(\xi_k)| \) are the same, the off-diagonal terms are clearly bounded by a smaller value than the diagonal terms. So, for each \( i, j = 1, 2, 3 \) and
\( k = 1, 2, \ldots, M \), when \( \gamma = 0 \),

\[
|\hat{S}_{i,j}(\xi_k)| \leq |\hat{S}^1_{i,i}(\xi_k)| + |\hat{S}^2_{i,i}(\xi_k)| \\
\leq \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} \left( (\pi^3 + 3\pi^2 + 6\pi + 6) + (\pi^3 + 6\pi^2 + 15\pi + 15) \right) L_v^5 \\
= \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} (2\pi^3 + 9\pi^2 + 21\pi + 21) L_v^5 \\
\approx 0.620 L_v^5 \\
\leq L_v^5
\]

\textbf{B.3 The case } \gamma = 1:

Finally, by the same method as for \( \gamma = 0 \), when \( |\xi_k| \neq 0 \),

\[
|\hat{S}^1_{1,1}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{|\xi_k|^2} \left( L_v^4 + 4L_v^3 \frac{1}{|\xi_k|} + 12L_v^2 \frac{1}{|\xi_k|^2} + 24L_v \frac{1}{|\xi_k|^3} + 24 \frac{1}{|\xi_k|^4} + 24 \frac{1}{|\xi_k|^4} \right) \\
= \sqrt{\frac{2}{\pi}} \frac{1}{\pi^6} \left( \pi^4 + 4\pi^3 + 12\pi^2 + 24\pi + 48 \right) L_v^6,
\]

\[
|\hat{S}^2_{3,3}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{\pi^6} \left( \pi^4 + 7\pi^3 + 24\pi^2 + 48\pi + 96 \right) L_v^6
\]

and

\[
|\hat{S}^2_{1,3}(\xi_k)| \leq \sqrt{\frac{2}{\pi}} \frac{1}{\pi^6} \left( \pi^4 + 7\pi^3 + 24\pi^2 + 48\pi + 96 \right) L_v^6.
\]

Also, since \( \hat{S}^1_{1,1}(0) = \frac{1}{3}\sqrt{\frac{1}{2\pi}} L_v^2 \), \( \hat{S}^2_{3,3}(0) = \frac{1}{9\sqrt{2\pi}} L_v^2 \) and \( \hat{S}^2_{3,3}(0) = 0 \), which are all less than the previous bounds, the above bounds are true for all \( k = 1, 2, \ldots, M \).

Again, since the bounds for \( |\hat{S}^1_{1,3}(\xi_k)| \) and \( |\hat{S}^2_{3,3}(\xi_k)| \) are the same, the off-diagonal terms are clearly bounded by a smaller value than the diagonal terms. So, for each \( i, j = 1, 2, 3 \) and
\( k = 1, 2, \ldots, M \), when \( \gamma = 1 \),

\[
|\hat{S}_{i,j}(\xi_k)| \leq |\hat{S}_{i,i}(\xi_k)| + |\hat{S}_{i,i}(\xi_k)|
\]

\[
\leq \sqrt{\frac{2}{\pi}} \frac{1}{\pi^6} \left( \left( \pi^3 + 4\pi^3 + 12\pi^2 + 24\pi + 48 \right) + \left( \pi^4 + 7\pi^3 + 24\pi^2 + 48\pi + 96 \right) \right) L_v^6
\]

\[
= \sqrt{\frac{2}{\pi}} \frac{1}{\pi^5} \left( 2\pi^4 + 11\pi^3 + 36\pi^2 + 72\pi + 144 \right) L_v^6
\]

\[
\approx 1.047 L_v^6
\]

\( \lesssim L_v^6 \).

### Appendix C  Timescales for Simulations with Different Masses

Consider two simulations of the space-homogeneous Fokker-Planck-Landau type equation, where the solution of one has mass a factor of \( \tau > 0 \) different to the other. If the two solutions are denoted \( f^a \) and \( f^b \) then this means that \( f^b = \tau f^a \). Assume also that \( f^a \) is modeled on time-scale \( t^a \) and \( f^b \) on time-scale \( t^b \). Then, the equations which the function \( f^a \) and \( f^b \) satisfy respectively are

\[
\frac{\partial f^a}{\partial t^a} = \frac{1}{\varepsilon} Q(f^a, f^a) \quad (24)
\]

and

\[
\frac{\partial f^b}{\partial t^b} = \frac{1}{\varepsilon} Q(f^b, f^b). \quad (25)
\]

Now, using \( f^b = \tau f^a \) in equation (25) gives

\[
\frac{\partial (\tau f^a)}{\partial t^b} = \frac{1}{\varepsilon} Q(\tau f^a, \tau f^a),
\]

which is equivalent to

\[
\tau \frac{\partial f^a}{\partial t^b} = \frac{\tau^2}{\varepsilon} Q(f^a, f^a), \quad (26)
\]

by considering the bilinear property of \( Q \).

Then, if the timescales are chosen such that \( t^a = \tau t^b \), \( \frac{\partial f^a}{\partial t^a} = \tau \frac{\partial f^a}{\partial t^b} \) by the chain rule, and equation (26) becomes

\[
\tau^2 \frac{\partial f^a}{\partial t^a} = \frac{\tau^2}{\varepsilon} Q(f^a, f^a),
\]

34
which is equivalent to equation [24] after dividing through by $\tau^2$. This suggests that when $f^b$ is modeled on the time-scale $t^b = \frac{\tau}{t} t^a$ then any results will be comparable to that of modeling $f^a$ on time-scale $t^a$.

One final thing to notice here is that when $f^b = \tau f^a$ then the entropy of $f^b$ satisfies $H^b[f^b](t) = \tau H^a[f^a](t) + \tau \log(\tau)$. In this case, the equilibrium Maxwellians $M^b_{eq}$ and $M^a_{eq}$ approached by $f^a$ and $f^b$, respectively, satisfy $M^b_{eq} = \tau M^a_{eq}$ as well. This means that the relative entropy is scaled as

$$H^b[f^b|M^b_{eq}] = (\tau H^a[f^a](t) + \tau \log(\tau)) - (\tau H^a[M^a](t) + \tau \log(\tau)) = \tau H^a[f^a|M^a_{eq}].$$

Appendix D  Space-inhomoegeneous Equilibrium Energy Calculations

As explained in the introduction while discussing the space-inhomogeneous equilibrium Maxwellian [6], the equilibrium total energy $T^{eq}$ satisfies $T^{eq} = T^{tot}(0)$, for $T^{tot}$ calculated by expression [4]. Here, $T^{K}(0) = T$, for $T$ used in the Maxwellian in the initial condition (20). Also, it can easily be shown that the exact solution to Poisson’s equation associated to the initial condition (20) is $\Phi(x,0) = 4A(1 - \cos(\frac{1}{2}x)) + C$ (for some constant $C$) which, when used in formula [5] gives $T^{E}(0) = A^2 L_x$.

By using expression (21) for the equilibrium solution, as well as that $\Phi_{eq}(x) = 0$, to calculate $T^{eq} = \lim_{t \to \infty} T^{tot}(t)$,

$$T^{eq} = \int_0^{L_x} \int_{\Omega_v} \frac{1}{(2\pi T^{eq})^\frac{3}{2}} e^{-\frac{|v|^2}{2T^{eq}}} \left( \frac{1}{2} |v|^2 + \frac{1}{2} |0|^2 \right) dv dx = \frac{3}{2} \rho_0 T^{eq}.$$  

So, $T^{eq} = T^{tot}(0)$ is equivalent to

$$\frac{3}{2} \rho_0 T^{eq} = \frac{3}{2} \rho_0 T + A^2 L_x,$$

which gives

$$T^{eq} = T + \frac{2}{3} A^2,$$

since $\rho_0 = L_x$ here.

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