A conservative spectral method for the Boltzmann equation with anisotropic scattering and the grazing collisions limit

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Abstract

We present the formulation of a conservative spectral scheme for Boltzmann collision operators with anisotropic scattering mechanisms to model grazing collision limit regimes approximating the solution to the Landau equation in space homogeneous setting. The scheme is based on the conservative spectral method of Gamba and Tharkabhushanam [17, 18]. This formulation is derived from the weak form of the Boltzmann equation, which can represent the collisional term as a weighted convolution in Fourier space. Within this framework, we also study the rate of convergence of the Fourier transform for the Boltzmann collision operator in the grazing collisions limit to the Fourier transform for the Landau collision operator for a family of non-integrable angular scattering cross sections. We analytically show that the decay rate to equilibrium depends on the parameters associated with the collision cross section, and specifically study numerically the differences between the classical Rutherford scattering angular cross section, which has logarithmic error in approximating Landau, and an artificial cross section with a linear error.

Keywords: Spectral methods, Boltzmann Equation, Landau-Fokker-Plank equation, grazing collisions.

1 Introduction

The initial drive of this manuscript was based on the study of simulating the Boltzmann equation's dynamics in the grazing collision limit of anisotropic, singular angular scattering cross section by spectral methods. During the search for suitable computational schemes using basic facts of Fourier space calculations,

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we found an analytical argument that not only gives an explicit representation of the effect of angular averaging for well balanced collisional mechanisms for a family of singular grazing collision angular cross sections, but also exhibits the rate of approximation for the difference of the Boltzmann collisional and Landau operators, measured in Fourier space, when evaluated on solutions of the Boltzmann initial value problem that are assumed to have a boundedness condition in Fourier space. The bulk of this manuscript will address both the numerical and analytical aspects of the so called grazing collision limit approximations of the Boltzmann equation in physically relevant regimes that includes Rutherford-Coulombic potential scattering mechanisms.

While numerical methods for solving the classical Boltzmann equation generally use the assumption of spherical particles with 'billiard ball' like collisions, however, a more physical model is to assume that particles interact via long range two-body potentials. Under this derivation the Boltzmann equation can be formulated in a very similar manner [11], but in this case the scattering cross section is highly anisotropic. In many cases, such as the physically relevent case of Coulombic interactions between charged particles, the derivation of the Boltzmann equation breaks down completely due to the singular nature of the scattering cross section. Physical arguments by Landau [21] as well as a later derivation by Rosenbluth et al. [27] showed that the dynamics of the Boltzmann equation can approximated by a Fokker-Planck type equation when grazing collisions dominate, generally referred to as the Landau or Landau-Fokker-Planck equation. Later work [5, 13, 12, 30, 2] more rigorously justified this asymptotic limit.

Many numerical methods have been developed for solving the full Landau equation, some stochastic [29, 22] and some deterministic [25], however very few methods have been developed to compute in the transition regime between the Boltzmann and Landau equations. The small parameter used to quantify this limit is related to the physical Debye length, which quantifies the distance at which particles are screened from interaction, and a heuristic minimum interaction distance for the grazing collisions assumption to hold. Other non-grazing effects from the Boltzmann equation may remain relevant [15] which makes development of numerical methods based on the Boltzmann equation itself relevant for plasma applications. To our knowledge the only numerical method that makes this distinction explicit is the recently proposed Monte Carlo method for the Landau equation of Bobylev and Potapenko [7], which grew out of the work of Bobylev and Nanbu [6]. Pareschi, Toscani, and Villani [26] showed that the weights of their spectral Galerkin method for the Boltzmann equation converged to the weights of a similar method for the Landau equation, but no computations were done in the transition regime. This work seeks to bridge that gap using the conservative spectral method for the Boltzmann equation developed by Gamba and Tharkabhushanam [17, 18].

There are many difficulties associated with numerically solving the Boltzmann equation, most notably the dimensionality of the problem and the conservation of the collision invariants. For physically relevant three dimensional applications the distribution function is seven dimensional and the velocity domain is unbounded. In addition, the collision operator is nonlinear and requires evaluation of a five dimensional integral at each point in phase space. The collision operator also locally conserves mass, momentum, and energy, and any approximation must maintain this property to ensure that macroscopic quantities evolve correctly.

Spectral methods are a deterministic approach that compute the collision operator to high accuracy by exploiting its Fourier structure. These methods grew from the analytical works of Bobylev [8] developed for the Boltzmann equation with Maxwell type potential interactions and integrable angular cross section, where the corresponding Fourier transformed equation has a closed form. Spectral approximations for these type of models where first proposed by Pareschi and Perthame [23]. Later Pareschi and Russo [24] applied this work to variable hard potentials by periodizing the problem and its solution and implementing spectral collocation methods.

These methods require $O(N^{2d})$ operations per evaluation of the collision operator, where N is the total number of velocity grid points in each dimension. While convolutions can generally be computed in $O(N^d \log N)$ operations, the presence of the convolution weights requires the full $O(N^{2d})$ computation of the convolution, except for a few special cases such as hard spheres in 3D and Maxwell molecules in 2D. Spectral methods advantages over Direct Simulation Monte Carlo Methods (DSMC) in many applications, in particular time dependent problems, low Mach number flows, high mean velocity flows, and flows that significantly deviate from equilibrium. In addition, deterministic methods avoid the statistical fluctuations that are typical of particle based methods.

Inspired by the work of Ibragimov and Rjasanow [20], Gamba and Tharkabhushanam [17, 18] observed that the Fourier transformed collision operator takes the form of a weighted convolution and developed a spectral method based on the weak form of the Boltzmann equation that provides a general framework for computing both elastic and inelastic collisions. Macroscopic conservation is enforced by solving a numerical constrained optimization problem that finds the closest distribution function in the computational domain to the output of the collision term that conserves the macroscopic quantities. These methods do not impose periodization on the function but rather assume that solution of the underlying problem on the whole phase space is obtained by the use of the Extension Operator in Sobolev spaces [3].

The proposed computational approach, is complemented by the analysis of the approximation from the Boltzmann equation for grazing collision to the Landau operators by estimating the L^∞-difference of their Fourier transforms evaluated on the solution of the corresponding Boltzmann equation, as they both can be easily expressed by a weighted convolution structure in Fourier space. We show that this property hold for a large family of singular angular scattering cross sections, whose parameters ε will control the approximation rate of such ε-grazing collision limit.

More specifically, in Theorem 1 we prove that if the probability density function $f_\varepsilon(v)$ satisfies the condition $\mathcal{F}(f_\varepsilon \, \tau_{\mathbf{u}} f_\varepsilon)(\zeta) < \mathcal{A}(\zeta)/(1+|u|^3)$ for $\mathcal{A}(\zeta) \leq k(1+|\zeta|)^{-5}$ uniformly in $\mathbb{R}^d$, where $f_\varepsilon(v) = f_\varepsilon(v,t)$ is the solution of the Boltzmann equation for the ε-grazing collision family associated with an angular cross section $b_\varepsilon(\cos\theta)$ given in within a class of singular functions satisfying suitable properties for such limit to be realized. Our analysis shows this approximation ε-rate of convergence explicitly depends on the rate of the non-integral singularity rate associated to ε-grazing collision angular cross section.

In particular the Rutherford angular scattering [28] cross section family depending on an ε-logarithmic parameter belongs to these admissible family of scattering mechanisms is shown to be the smallest singular behavior the family of ε-grazing collision angular cross section may have in order to obtain the Landau limit. From this point of view, Rutherford angular scattering [28] is *the critical case of grazing collision limit to Landau operator* in the sense that any other angular singularity that is admissible for this grazing collision limit to the Landau operator in Fourier space is stronger than the one for the Rutherford one, and so its ε-decay of approximation will be faster.

More specifically, our result shows that the L^∞-difference of the Fourier transforms of Landau operator Q_L and the Boltzmann for grazing collisions operator Q_{b_ε} acting on $f_\varepsilon(v)$ converges to zero with an ε-logarithmic rate as $\varepsilon \to 0$. In particular, we show by numerical means that the convergence of the computed solution of the Boltzmann equation to the corresponding one the Landau equation is ε-logarithmic slow when using the physically relevant Rutherford angular cross section, while is much faster with ε-linear decay when using an ε-grazing collision angular cross section with a stronger singularity at the vanishing scattering angle. This example benchmarks the nature of the approximation of the grazing collision limit of the Boltzmann solutions to the ones of the Landau equation, depending on the singularity and corresponding rates of decay of grazing limits associated to the angular functions. These analytical facts are carefully discussed in Section 3 of this manuscript, while numerical aspects are in Sections 4 and 5.

This article is organized as follows. In Section 2, we present the derivation of the spectral formulation of the collision operator for an arbitrary anisotropic scattering cross section. In Section 3 we present the Landau equation and apply a class of cross sections formulated by Villani [31] and Bobylev [7] within our spectral formulation to study the grazing collisions limit of the Boltzmann equation. In particular, we proved Theorem 1 in order to obtain the rate of asymptotic convergence from the Boltzmann collision operator to the Landau collision operator with a large family of angular singularities that includes the classical screened Rutherford potential for Coulombic interactions and more. In Section 4, we present the details of the numerical method based on this formulation and provide some practical observations on its implementation. In Section 5, we numerically investigate the method's performance for small but finite values of the grazing collision parameter. We conclude with a discussion of future work in this area.

2 The space homogeneous Boltzmann equation

The space homogeneous Boltzmann equation is given by the initial value problem

$$\frac{\partial}{\partial t} f(\mathbf{v}, t) = \frac{1}{Kn} Q(f, f), \tag{1}$$

with

$$\mathbf{v} \in \mathbb{R}^d, \qquad f(v, 0) = f_0(\mathbf{v})$$

where $f(\mathbf{v}, t)$ is a probability density distribution in $\mathbf{v}$-space and f_0 is assumed to be locally integrable with respect to $\mathbf{v}$. The dimensionless parameter $Kn > 0$ is the scaled Knudsen number, which is proportional to the ratio between the mean free path between collisions and a reference macroscopic length scale.

The collision operator $Q(f, f)$ is a bilinear integral form in $(\mathbf{v}, t)$ given by

$$Q(f, f)(\mathbf{v}, t) = \int_{\mathbf{v}_* \in \mathbb{R}^d} \int_{\sigma \in S^{d-1}} B(|\mathbf{v} - \mathbf{v}_*|, \cos\theta)(f(\mathbf{v}'_*) f(\mathbf{v}') - f(\mathbf{v}_*) f(\mathbf{v})) d\sigma d\mathbf{v}_*, \tag{2}$$

where the velocities $\mathbf{v}', \mathbf{v}'_*$ are determined through a given collision rule depending on $\mathbf{v}, \mathbf{v}_*$. The positive term of the integral in (2) evaluates f in the pre-collisional velocities that can result in a post-collisional velocity the direction $\mathbf{v}$. The collision kernel $B(|\mathbf{v} - \mathbf{v}_*|, \cos\theta)$ is a given non-negative function depending on the size of the relative velocity $\mathbf{u} := \mathbf{v} - \mathbf{v}_*$ and $\cos\theta = \frac{\mathbf{u} \cdot \sigma}{|\mathbf{u}|}$, where σ in the $n-1$ dimensional sphere S^{n-1} is referred to as the scattering direction, which coincides with the direction of the post-collisional elastic relative velocity.

For the following we will use the elastic (or reversible) interaction law

$$\mathbf{v}' = \mathbf{v} + \frac{1}{2}(|u|\sigma - \mathbf{u}), \qquad \mathbf{v}'_* = \mathbf{v}_* - \frac{1}{2}(|u|\sigma - \mathbf{u}) \tag{3}$$
$$B(|u|, \cos\theta) = |u|^\lambda b(\cos\theta) \; .$$

The angular cross section function $b(\cos\theta)$ may or may not be integrable with respect to σ on S^{d-1}. The case when integrability holds is referred to as the Grad cut-off assumption on the angular cross section.

The parameter λ regulates the collision frequency as a function of the relative velocity $|\mathbf{u}|$. This parameter corresponds to the inter particle potentials used in the derivation of the collisional kernel and choices of λ are denoted as variable hard potentials (VHP) for $0 < \lambda < 1$, hard spheres (HS) for $\lambda = 1$, Maxwell molecules (MM) for $\lambda = 0$, and variable soft potentials (VSP) for $-3 < \lambda < 0$. The $\lambda = -3$ case corresponds to a Coulombic interaction potential between particles. If $b(\cos\theta)$ is independent of σ we call the interactions isotropic, e.g., in the case of hard spheres in three dimensions.

2.1 Spectral formulation for anisotropic angular cross section

The key step our formulation of the spectral numerical method is the use of the weak form of the Boltzmann collision operator [17]. For a suitably smooth test function $\phi(\mathbf{v})$ the weak form of the collision integral is given by

$$\int_{\mathbb{R}^d} Q(f,f)\phi(\mathbf{v})d\mathbf{v} = \int_{\mathbb{R}^d\times\mathbb{R}^d\times S^{d-1}} f(\mathbf{v})f(\mathbf{v}_*)B(|u|,\cos\theta)(\phi(\mathbf{v}')-\phi(\mathbf{v}))d\sigma d\mathbf{v}_* d\mathbf{v} \tag{4}$$

If one chooses

$$\phi(\mathbf{v}) = e^{-i\zeta\cdot\mathbf{v}}/(\sqrt{2\pi})^d,$$

then (4) is the Fourier transform of the collision integral with Fourier variable ζ:

$$\begin{aligned}
\widehat{Q}(\zeta) &= \frac{1}{(\sqrt{2\pi})^d}\int_{\mathbb{R}^d} Q(f,f)e^{-i\zeta\cdot\mathbf{v}}d\mathbf{v} \\
&= \int_{\mathbb{R}^d\times\mathbb{R}^d\times S^{d-1}} f(\mathbf{v})f(\mathbf{v}_*)\frac{B(|\mathbf{u}|,\cos\theta)}{(\sqrt{2\pi})^d}(e^{-i\zeta\cdot\mathbf{v}'}-e^{-i\zeta\cdot\mathbf{v}})d\sigma d\mathbf{v}_* d\mathbf{v} \\
&= \int_{\mathbb{R}^d} G_b(\mathbf{u},\zeta)\mathcal{F}[f(\mathbf{v})f(\mathbf{v}-\mathbf{u})](\zeta)d\mathbf{u},
\end{aligned} \tag{5}$$

where $\widehat{[\cdot]} = \mathcal{F}(\cdot)$ denotes the Fourier transform and

$$G_b(\mathbf{u},\zeta) = |u|^\lambda \int_{S^{d-1}} b(\cos\theta)\left(e^{-i\frac{1}{2}\zeta\cdot|u|\sigma}e^{i\frac{1}{2}\zeta\cdot\mathbf{u}}-1\right)d\sigma \tag{6}$$

Further simplification can be made by writing the Fourier transform inside the integral as a convolution of Fourier transforms:

$$\widehat{Q}(\zeta) = \int_{\mathbb{R}^d}\widehat{G_b}(\xi,\zeta)\hat{f}(\zeta-\xi)\hat{f}(\xi)d\xi, \tag{7}$$

where the convolution weights $\widehat{G}(\xi,\zeta)$ are given by

$$\begin{aligned}
\widehat{G_b}(\xi,\zeta) &= \frac{1}{(\sqrt{2\pi})^d}\int_{\mathbb{R}^d} G_b(\mathbf{u},\zeta)e^{-i\xi\cdot u}d\mathbf{u} \qquad (8)\\
&= \frac{1}{(\sqrt{2\pi})^d}\int_{\mathbb{R}^d}|u|^\lambda e^{-i\xi\cdot\mathbf{u}}\int_{S^{d-1}} b(\cos\theta)\left(e^{-i\frac{1}{2}\zeta\cdot|u|\sigma}e^{i\frac{1}{2}\zeta\cdot\mathbf{u}}-1\right)d\sigma d\mathbf{u}
\end{aligned}$$

These convolution weights can be precomputed once to high accuracy and stored for future use. For many collisional models, such as isotropic collisions, the complexity of the integrals in the weight functions can be reduced dramatically through analytical techniques [17, 18]. However in this paper we make no assumption on the isotropy of b and derive a more general formula. We remark that this formulation does not separate the gain and loss terms of the collision operator, which is important for obtaining the correct cancellation in the grazing collision limit below.

We begin with $G_b(\mathbf{u},\zeta)$ and define a spherical coordinate system for σ with a pole in the direction of $\mathbf{u}$, i.e. let $\sigma = \cos\theta \frac{\mathbf{u}}{|u|} + \sin\theta\omega$, $\omega \in S^{d-2}$. We obtain

$$G_b(\mathbf{u},\zeta) = |u|^\lambda \int_0^\pi \int_{S^{d-2}} b(\cos\theta)\sin\theta \left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot\mathbf{u}} e^{-i\frac{1}{2}|u|\sin\theta(\zeta\cdot\omega)} - 1 \right) d\theta d\omega. \tag{9}$$

In three dimensions, the unit vector $\sigma = \cos\theta \frac{\mathbf{u}}{|u|} + \sin\theta(\mathbf{j}\sin\phi + \mathbf{k}\cos\phi)$, where $\mathbf{j},\mathbf{k}$ are mutually orthogonal vectors with $\mathbf{u}$. Thus the right hand side of (9) becomes

$$|u|^\lambda \int_0^\pi \int_{\alpha-\pi}^{\alpha+\pi} b(\cos\theta)\sin\theta \left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot\mathbf{u}} e^{-i\frac{1}{2}|u|\sin\theta(\zeta\cdot\mathbf{j}\sin\phi + \zeta\cdot\mathbf{k}\cos\phi)} - 1 \right) d\theta d\phi,$$

for α to be justified below.

Using the trigonometric identity

$$(\zeta\cdot\mathbf{j})\sin\phi + (\zeta\cdot\mathbf{k})\cos\phi = \sqrt{(\zeta\cdot\mathbf{j})^2 + (\zeta\cdot\mathbf{k})^2}\sin(\phi+\gamma),$$

for a unique $\gamma \in [-\pi,\pi]$, the integration with respect to the azimuthal angle ϕ is equivalent to

$$\begin{aligned} G_b(\mathbf{u},\zeta) &= |u|^\lambda \int_0^\pi b(\cos\theta)\sin\theta \left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot\mathbf{u}} \int_{\alpha-\gamma-\pi}^{\alpha-\gamma+\pi} e^{-i\frac{1}{2}|u|\sin\theta|\zeta^\perp|\sin\phi} d\phi - 2\pi \right) d\theta, \\ &= |u|^\lambda \int_0^\pi b(\cos\theta)\sin\theta \left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot\mathbf{u}} \int_{\alpha-\gamma-3\pi/2}^{\alpha-\gamma+\pi/2} e^{i\frac{1}{2}|u|\sin\theta|\zeta^\perp|\cos\phi} d\phi - 2\pi \right) d\theta, \end{aligned}$$

where $\zeta^\perp = \zeta - (\zeta\cdot\mathbf{u}/|u|)\mathbf{u}/|u|$. Finally, let $\alpha = \gamma + \pi/2$, then by symmetry we obtain

$$\begin{aligned} G_b(\mathbf{u},\zeta) &= |u|^\lambda \int_0^\pi b(\cos\theta)\sin\theta \left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot\mathbf{u}} 2 \int_0^\pi e^{i\frac{1}{2}|u|\sin\theta|\zeta^\perp|\cos\phi} d\phi - 2\pi \right) d\theta \\ &= 2\pi|u|^\lambda \int_0^\pi b(\cos\theta)\sin\theta \left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot\mathbf{u}} J_0\left(\frac{|u|\sin\theta|\zeta^\perp|}{2} \right) - 1 \right) d\theta, \end{aligned} \tag{10}$$

where J_0 is the Bessel function of the first kind (see [1] 9.2.21). Note that for the isotropic case the angular function $b(\cos\theta)$ is constant and thus ζ can be used instead of $\mathbf{u}$ as the polar direction for σ, resulting in an explicit expression involving a sinc function [17].

Next, we take $\widehat{G_b}$ to be the Fourier transform of G_b, where this transform is taken on a *ball centered at 0* in order to ensure that the weights are real-valued when computing them numerically.

Then, the convolution weights $\widehat{G}_b(\zeta,\xi)$ from (8), written in 3 dimensions, are computed as follows

$$
\begin{aligned}
\widehat{G}(\zeta,\xi) &= 2\pi \int_{B_L(0)} |u|^\lambda e^{-i\xi\cdot\mathbf{u}} \int_0^\pi b(\cos\theta)\sin\theta \\
&\quad\times \left[e^{\frac{i\zeta}{2}\cdot\mathbf{u}(1-\cos\theta)} J_0\left(\frac{1}{2}|u||\zeta^\perp|\sin\theta\right) - 1\right] d\theta d\mathbf{u} \\
&= 2\pi \int_0^\infty \int_{S^2} r^{\lambda+2} \int_0^\pi b(\cos\theta)\sin\theta \\
&\quad\times \left[e^{-ir(\xi-\frac{\zeta}{2}(1-\cos\theta))\cdot\eta} J_0\left(\frac{1}{2}r|\zeta^\perp|\sin\theta\right) - e^{-ir\xi\cdot\eta}\right] d\theta d\eta dr.
\end{aligned}
$$

We now take ζ to be the polar direction for the spherical integration of η and use that $\widehat{G}_b$ is real-valued to obtain

$$
\begin{aligned}
\widehat{G}_b(\zeta,\xi) &= 4\pi^2 \int_0^L r^{\lambda+2} \int_0^\pi \int_0^\pi b(\cos\theta)\sin\theta\sin\gamma J_0\left(r\left|\xi - \frac{\xi\cdot\zeta}{|\zeta|^2}\zeta\right|\sin\gamma\right) \\
&\quad\times \left[\cos\left(r(\xi-\frac{\zeta}{2}(1-\cos\theta))\cdot\frac{\zeta}{|\zeta|}\cos\gamma\right) J_0\left(\frac{1}{2}r|\zeta|\sin\gamma\sin\theta\right)\right. \\
&\quad\left. - \cos\left(r\xi\cdot\frac{\zeta}{|\zeta|}\cos\gamma\right)\right] d\theta d\gamma dr,
\end{aligned}
\tag{11}
$$

where γ is the polar angle for the η integration.

This requires a three dimensional integral for the N^6 pairs (ζ,ξ), which is two dimensions more than the isotropic case, but just as in the isotropic case these weights are precomputed only once and re-used in any subsequent computations with the collisional model.

3 The grazing collisions limit and convergence to the Landau collision operator

3.1 The Landau collision operator

The Landau collision operator describes binary collisions that only result in very small deflections of particle trajectories, as is the case for Coulomb potentials and Rutherford scattering [28] between charged particles. This can be shown to be an approximation of the Boltzmann collision operator in the case where the dominant collision mechanism is that of grazing collisions. The operator is given by

$$
Q_L(f,f) = \nabla_{\mathbf{v}}\cdot\left(\int_{\mathbb{R}^3} |u|^{\lambda+2}(I - \frac{\mathbf{u}\otimes\mathbf{u}}{|u|^2})(f(\mathbf{v}_*)\nabla_v f(\mathbf{v}) - f(\mathbf{v})(\nabla_{\mathbf{v}} f)(\mathbf{v}_*))d\mathbf{v}_*\right), \tag{12}
$$

and the weak form of this operator is given by [26]

$$\int_{\mathbb{R}^3} Q_L(f,f)\phi(\mathbf{v})dv = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f(\mathbf{v})f(\mathbf{v}_*) \times \left(-4|u|^\lambda \mathbf{u}\cdot\nabla\phi + |u|^{\lambda+2}\left(I - \frac{\mathbf{u}\otimes\mathbf{u}}{|u|^2} : \nabla^2\phi\right)\right) d\mathbf{v}d\mathbf{v}_*\,,$$

where $\nabla^2\phi$ denotes the Hessian of ϕ and ':' is the matrix double dot product.

As done in the Boltzmann case above, we choose ϕ to be the Fourier basis functions and obtain after some calculation

$$\widehat{Q_L}(\zeta) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3} \mathcal{F}\{f(\mathbf{v})f(\mathbf{v}-\mathbf{u})\}(\zeta)\left(4i|u|^\lambda(\mathbf{u}\cdot\zeta) - |u|^{\lambda+2}|\zeta^\perp|^2\right)d\mathbf{u}, \tag{13}$$

where $\zeta^\perp = \zeta - (\zeta\cdot\mathbf{u})/|u|^2\ \mathbf{u}$, the orthogonal component of ζ to $\mathbf{u}$. Thus the weight function $G_L(\mathbf{u},\zeta)$ in terms of (6) is now given by

$$G_L(\mathbf{u},\zeta) = |u|^\lambda(4i(\mathbf{u}\cdot\zeta) - |u|^2|\zeta^\perp|^2)\,. \tag{14}$$

The $\widehat{G_L}$ used in the final computation is the Fourier transform of G_L with respect to $\mathbf{u}$, but we will work with this representation to make the convergence analysis below more clear.

3.2 The grazing collisions limit

To show that the spectral method for Boltzmann operator is consistent with this form of the Landau operator, we must take the grazing collisions limit, which requires that the angular scattering function is consistent with the singular rates of Rutherford-like scattering. Indeed, it is enough to assume that the collision kernel satisfies the following.

Let $\varepsilon > 0$ be the small parameter associated with the grazing collisions limit. A family of kernels $b_\varepsilon(\theta)$ represents grazing collisions if [2, 7]:

- $$\lim_{\varepsilon\to 0} 2\pi\int_0^\pi b_\varepsilon(\cos\theta)\sin^2(\theta/2)\,\sin\theta d\theta = \Lambda_0 < \infty$$

- $$2\pi\int_0^\pi b_\varepsilon(\cos\theta)(\sin(\theta/2))^{2+k}\,\sin\theta d\theta \to_{\varepsilon\to 0} 0 \qquad \text{for}\ \ k\geq 0\,. \tag{15}$$

- $\forall\theta_0 > 0,\ b_\varepsilon(\theta)\to_{\varepsilon\to 0} 0$ uniformly on $\theta > \theta_0$.

These conditions as sufficient show that the collisional integral operator converges to the Landau operator at a rate that depends on the choice of the angular function $b_\varepsilon(\cos\theta)$ as it will be shown in Theorem 3.1.

In fact, there are several angular functions that have been widely used in the calculation of collisional theory with Coulombic potentials (see [7].) The more significant and perhaps physically meaningful is the one of the classical Rutherford scattering corresponding to a family $b_\varepsilon(\cos\theta)$ given by

$$b_\varepsilon(\cos\theta)\sin\theta = \frac{\sin\theta}{-\pi\log\sin(\varepsilon/2)\sin^4(\theta/2)} 1_{\theta\geq\varepsilon}. \tag{16}$$

This ε-parameter family satisfies conditions (15). We note that the logarithmic term that appears here is the *Coulomb logarithm* originally derived by Landau [21], where ε is proportional to the ratio between the mean kinetic energy of the gas and the Debye length.

Another angular cross section that satisfies conditions (15) is given by

$$b_\varepsilon(\cos\theta)\sin\theta = \frac{8\varepsilon}{\pi\theta^4} 1_{\theta\geq\varepsilon}, \tag{17}$$

which we will refer to as the ε-linear cross section. While this cross section is not physically motivated, it is useful for numerical convergence studies. Other angular cross sections that satisfy conditions (15) have been used in DSMC methods for computing the Landau equation; for an overview see [7].

In fact it is possible to identify a large family of possible angular function choices corresponding to long range two body interaction potentials that includes both the one for the Rutherford-Coulombic one (16) and the ε-linear one (17), the former being the critical case for the grazing collision limits.

3.3 A family of angular cross sections for long range interactions

We next introduce a family of long range interaction potentials with a classical small angle cut-off parameter of order ε that will satisfy conditions (15). For this oppose we first introduce two functions $H(x)$ and $C(x)$ related to the angular cross section function b_ε.

The first one is defined such that its derivative satisfies $H'(x) = b(1-2x^2)x^3$. The motivation for this choice of function is due to the representation of the angular cross section function $b(\hat{u}\cdot\sigma)$ written in terms of $\sin(\theta/2)$, taking into account the Jacobian to the spherical transformation and the needed singularity cancellation from the first bullet condition in (15).

Indeed, setting $x = \sin(\theta/2)$ yields

$$\begin{aligned} H'(x)dx = b(1-2x^2)x^3dx &= \frac{1}{2}b(\cos\theta)\sin^3(\theta/2)\cos(\theta/2)d\theta \\ &= \frac{1}{4}b(\cos\theta)\sin^2(\theta/2)\sin(\theta)d\theta = \frac{1}{8}b(\cos\theta)(1-\cos\theta)\sin(\theta)d\theta \end{aligned} \tag{18}$$

By the first bullet condition (15), $H'(x)$ is integrable in $[0,1]$

Similarly, we define a function $C(x)$ such that $C'(x) = b(1-2x^2)x^5$. Then, as computed in (18), this function evaluated at $x = \sin(\theta/2)$ yields

$$\begin{aligned} C'(x)dx = b(1-2x^2)x^5dx &= \frac{1}{2}b(\cos\theta)\sin^5(\theta/2)\cos(\theta/2)d\theta \\ &= \frac{1}{4}b(\cos\theta)\sin^4(\theta/2)\sin(\theta)d\theta = \frac{1}{16}b(\cos\theta)\sin(\theta)(1-\cos\theta)^2d\theta \end{aligned} \tag{19}$$

By the second bullet condition (15), $C'(x)$ is also integrable in $[0,1]$.

In addition, in order to satisfy the third bullet condition (15), it is sufficient that the angular function $b(\cos\theta)$ is singular enough such that

$$\begin{aligned} &\lim_{\varepsilon\to 0}(-H(\sin(\varepsilon/2)))^{-1} = 0 \qquad \text{and} \\ &\max\{|H(1)|, |C(1)|, \sup_{\varepsilon\geq 0}|C(\sin(\varepsilon/2))|\} < \Gamma \end{aligned} \tag{20}$$

for some constant Γ depending only on the functions H and C.

In this way the ε-dependent angular cross section can be written in terms of the H function as follows

$$\begin{aligned} b_\varepsilon(\hat{u}\cdot\sigma)d\sigma &= \frac{1}{-\pi H(\sin(\varepsilon/2))}b(\cos\theta)\sin(\theta)1_{\theta\geq\varepsilon}\,d\phi d\theta \\ &= \frac{1}{-\pi H(\sin(\varepsilon/2))}\frac{H'(x)}{x^2}1_{x\geq\sin(\varepsilon/2)}\,dxd\phi \end{aligned} \tag{21}$$

and, by the condition (20), also satisfies the third bullet condition (15).

One can easily inspect that when the angular function $b(\cos\theta)$ is taken of the form

$$b(\hat{u}\cdot\sigma) = \frac{1}{\sin^{4+\delta}(\theta/2)} \tag{22}$$

then the function $H(x)$ can be explicitly computed from (21)

$$\begin{aligned} b_\varepsilon(\hat{u}\cdot\sigma)d\sigma &= \frac{1}{-\pi H(\sin(\varepsilon/2))}\frac{1}{\sin^{4+\delta}(\theta/2)}\sin(\theta)1_{\theta\geq\varepsilon}\,d\phi d\theta \\ &= \frac{1}{-\pi H(\sin(\varepsilon/2))}\frac{2}{\sin^{3+\delta}(\theta/2)}d(\sin(\theta/2))1_{\theta\geq\varepsilon}d\theta d\phi \\ &= \frac{1}{-\pi H(\sin(\varepsilon/2))}\frac{1}{x^{1+\delta}}\frac{1}{x^2}\,1_{x\geq\sin(\varepsilon/2)}dxd\phi. \end{aligned} \tag{23}$$

Thus, $H(x)$ is the antiderivative of $x^{-(1+\delta)}$ and has the form

$$H(x) = -\frac{x^{-\delta}}{\delta}, \quad \text{for } \delta > 0 \qquad \text{and} \qquad H(x) = \log x\,, \quad \text{for } \delta = 0\,. \tag{24}$$

In addition, the corresponding function C as defined in (19) satisfies

$$\begin{aligned} C'(x)dx &= \frac{1}{\sin^{4+\delta}(\theta/2)}\sin^5(\theta/2)\cos(\theta/2)d\theta \\ &= \sin^{1+\delta}(\theta/2)d\sin(\theta/2) = x^{1-\delta}dx \end{aligned} \tag{25}$$

The choice of the exponent δ must be done in order to satisfy the third bullet condition (15), i.e. conditions (20) for both $H(x)$ and $C(x)$ functions.

In fact, a sufficient condition is that $0 \leq \delta < 2$.

The case $\delta = 0$ yields the classical Rutherford-Coulombic potential where

$$H(x) = \log x \quad \text{and} \quad C(x) = x^2/2 \tag{26}$$

These two functions satisfy conditions (20), as $H(\sin(\pi/2)) = 0$, $C(\sin(\pi/2)) = 1/2$, $C(\sin(\varepsilon/2)) = \sin^2(\varepsilon/2)/2$ are uniformly bounded for $\varepsilon > 0$ and

$$\lim_{\varepsilon \to 0} \frac{1}{-H(\sin(\varepsilon/2))} = \lim_{\varepsilon \to 0} \frac{1}{-\log(\sin(\varepsilon/2))} = 0.$$

For $\delta > 0$, the $H(x)$ and $C(x)$ functions become

$$H(x) = -\frac{x^{-\delta}}{\delta} \quad \text{and} \quad C(x) = \frac{x^{2-\delta}}{2-\delta}. \tag{27}$$

These two functions also satisfy conditions (20), as $H(\sin(\pi/2)) = -1, C(\sin(\pi/2)) \leq (2-\delta)^{-1}, C(\sin(\varepsilon/2)) \leq (2-\delta)^{-1}$ is bounded and

$$\lim_{\varepsilon \to 0} \frac{1}{-H(\sin(\varepsilon/2))} = \lim_{\varepsilon \to 0} \frac{1}{\sin^{-\delta}(\varepsilon/2)} = \lim_{\varepsilon \to 0} \frac{1}{2^\delta} \varepsilon^\delta = 0.$$

Finally, notice that the case $\delta = 1$ corresponds to the the ε-linear cross section (17), as $\sin(\theta/2) \approx \theta/2$ as $\theta \to 0$.

The critical case of $\delta = 0$ corresponds to the Rutherford-Coulombic potential (16), for which the Landau limit would be possible. Clearly, this case is the smallest value of the exponent in the singularity of the cross section written in negative powers of $\sin(\theta/2)$ such that the bullet conditions (15) for the grazing collision limit are satisfied. In this sense *the Rutherford-Coulombic potential* (16) *is the critical case for which for which the Boltzmann operator can converge to the Landau operator.*

In addition, this family breaks down when $\delta > 2$ as condition (20) would not be satisfied on $C(\sin(\varepsilon/2))$. We will actually show in Theorem 3.1 that this value of δ is the critical one at which more terms in the Taylor expansion for the angular cross-section contain singularities, and the second term would need a similar treatment for $C(x)$ as was done for $H(x)$ (see the first terms of the expansions in equations (34) and (35).)

3.4 The grazing collision approximation Theorem

In the following theorem we estimate the difference of the grazing collision limit for the Boltzmann solutions evaluated at the collisional integral and Landau operators for a class of cross sections given by the general form of angular cross sections satisfying (21).

In addition, we will show in Section 5 the numerically computed logarithm of the entropy decay associated to the solution of the initia value problem for the boltzmann equation for the Rutherford-Colombic potential cross section (16) and observe that, as expected from the result of Theorem 3.1, the decay rate for the Rutherford ε-logarithmic cross section (16) is much faster than the one for the ε-linear decaying cross section (17), and the latter one actually mimics the entropy decay rate of the Landau equation. This is in fact an expected observation, as we explain in the forthcoming pages.

We begin by taking a look at the grazing collisions limit for angular cross sections satisfying conditions (21), and all related conditions for the functions H and C as defined in the previous section.

Theorem 3.1 *Assume that f_ε satisfies*

$$|\mathcal{F}\{f_\varepsilon(\boldsymbol{v})f_\varepsilon(\boldsymbol{v}-\boldsymbol{u})\}(\zeta)| \leq \frac{A(\zeta)}{1+|u|^3}, \tag{28}$$

with A uniformly bounded by $k(1+|\zeta|)^{-5}$, with k constant, the angular scattering cross section $b(\cos\theta)$ satisfies conditions in (21) related to the H function in (18) satisfying conditions (20), and $\lambda = -3$, corresponding to Coulombic interactions between particles.

Then the rate of convergence of the Boltzmann collision operator with grazing collisions to the Landau collision operator is given by

$$\|\widehat{Q_L}[f_\varepsilon] - \widehat{Q_{b_\varepsilon}}[f_\varepsilon]\|_{L^\infty(\mathbb{R}^d)} \;\leq\; O\left(\frac{1}{|H(\sin(\varepsilon/2))|}\right) \;\to 0 \quad \text{as } \varepsilon \to 0. \tag{29}$$

Proof : With this angular cross section and $\lambda = -3$, the calculation for the weight function $G_{b_\varepsilon}(\zeta, \mathbf{u})$ can be computed by Taylor expanding the exponential term in (6) to obtain, in terms of the polar and azimuthal angles θ and ϕ, respectively, and ssociated to the change of coordinates $\sigma = \cos\theta\frac{\mathbf{u}}{|u|} + \sin\theta\omega$, $\omega \in S^{d-2}$ used in Section 2.1:

$$\begin{aligned} G_{b_\varepsilon}(\zeta, \mathbf{u}) &= |u|^{-3}\int_{S^2} b_\varepsilon(\hat{u}\cdot\sigma)(e^{-i\frac{\zeta}{2}\cdot(|u|\sigma-\mathbf{u})} - 1)d\sigma \qquad (30)\\ &= |u|^{-3}\int_{S^2} b_\varepsilon(\hat{u}\cdot\sigma)\sum_{n=1}^{\infty}\frac{i^n}{n!}\left(\frac{\mathbf{u}\cdot\zeta}{2} - |u|\frac{\zeta\cdot\sigma}{2}\right)^n d\sigma\,. \end{aligned}$$

As a consequence, the following representation for the weight function $G_{b_\varepsilon}(\zeta, \mathbf{u})$

holds

$$
\begin{aligned}
G_{b_\varepsilon}(\zeta, \mathbf{u}) = & \frac{|u|^{-3}}{-h(\varepsilon)} \int_\varepsilon^\pi \int_0^{2\pi} b(\cos\theta)\sin\theta \\
& \times \sum_{n=1}^{\infty} \frac{i^n}{n!} \left(\frac{\mathbf{u}\cdot\zeta(1-\cos\theta)}{2} - \frac{|u|\sin\theta}{2}(\zeta\cdot\mathbf{j}\sin\phi + \zeta\cdot\mathbf{k}\cos\phi) \right)^n d\phi d\theta \\
& = \frac{|u|^{-3}}{-h(\varepsilon)} \int_\varepsilon^\pi \int_0^{2\pi} b(\cos\theta)\sin\theta \qquad (31) \\
\times & \sum_{n=1}^{\infty} \frac{i^n \sin^n(\theta/2)}{n!} \left(\mathbf{u}\cdot\zeta\sin(\theta/2) - |u|\cos(\theta/2)(\zeta\cdot\mathbf{j}\sin\phi + \zeta\cdot\mathbf{k}\cos\phi) \right)^n d\phi d\theta,
\end{aligned}
$$

where $\mathbf{j}, \mathbf{k}$ are unit vectors mutually orthogonal with $\mathbf{u}$ arising from the choice of spherical coordinates. We stress that this expansion occurs in the convolution weights in this formulation rather than the distribution function as is done in other derivations of the grazing collisions limit.

Next we calculate the terms in this expansion in order to explicitly determine its leading order in terms in ε and to estimate the remainder. Expanding the binomial terms in G_{b_ε} and using the identity $\sin\theta = 2\cos(\theta/2)\sin(\theta/2)$ yields

$$
\begin{aligned}
G_{b_\varepsilon}(\zeta, \mathbf{u}) = & \frac{|u|^{-3}}{-\pi h(\varepsilon)} \sum_{n=1}^{\infty}\sum_{j=0}^{n}\sum_{k=0}^{j} \left(\frac{i^n (\mathbf{u}\cdot\zeta)^{n-j} |u|^j (-1)^j (\zeta\cdot\mathbf{j})^k (\zeta\cdot\mathbf{k})^{j-k}}{n!} \binom{n}{j}\binom{j}{k} \right) \\
& \times \left(\int_\varepsilon^\pi \cos^{j+1}(\theta/2)\sin^{2n-j+1}(\theta/2) b(\cos\theta)\, d\theta \right) \left(\int_0^{2\pi} \sin^k\phi \cos^{j-k}\phi\, d\phi \right) \qquad (32) \\
& := \frac{|u|^{-3}}{-h(\varepsilon)} \sum_{n=1}^{\infty} G_{b_\varepsilon, n}(\zeta, \mathbf{u})
\end{aligned}
$$

At this point we separate the $n = 1, 2$ cases from the rest, as the θ integrand for $n \geq 3$ is bounded independently of ε.

First we observe that for $n = 1, 2$, $G_{b_\varepsilon, n}(\zeta, \mathbf{u})$ is explicitly calculated from (31), yielding

$$
\begin{aligned}
& \frac{|u|^{-3}}{-\pi h(\varepsilon)} (G_{b_\varepsilon,1} + G_{b_\varepsilon,2})(\zeta, \mathbf{u})) = \\
& \frac{2|u|^{-3}}{-\pi h(\varepsilon)} \int_\varepsilon^\pi \int_0^{2\pi} b(\cos\theta)\sin(\theta/2)\cos(\theta/2) \Bigg(i\sin^2(\theta/2)(\mathbf{u}\cdot\zeta) - \frac{\sin^2(\theta/2)}{2} \\
& \qquad \times \Big((\mathbf{u}\cdot\zeta)^2 \sin^2(\theta/2) - (2-i)|u|(\mathbf{u}\cdot\zeta)\sin(\theta/2)\cos(\theta/2)((\zeta\cdot\mathbf{j}\sin\phi + \zeta\cdot\mathbf{k}\cos\phi) \\
& \qquad + |u|^2\cos^2(\theta/2)((\zeta\cdot\mathbf{j})\sin\phi + (\zeta\cdot\mathbf{k})\cos\phi)^2) \Big) \Bigg) d\phi d\theta \qquad (33)
\end{aligned}
$$

We note that $\int_0^{2\pi}(\sin^m\phi, \cos^m\phi)d\phi = 0$ for odd m and further obtain

$$
\begin{aligned}
&\frac{|u|^{-3}}{-\pi h(\varepsilon)}(G_{b_\varepsilon,1}+G_{b_\varepsilon,2})(\zeta,\mathbf{u}) \\
&= \frac{2|u|^{-3}}{-h(\varepsilon)}\int_\varepsilon^\pi b(\cos\theta)\sin(\theta/2)\cos(\theta/2)\Bigg(2\pi i\sin^2(\theta/2)(\mathbf{u}\cdot\zeta) - \frac{\sin^2(\theta/2)}{2} \\
&\quad\times\Big(2\pi(\mathbf{u}\cdot\zeta)^2\sin^2(\theta/2) + \pi|u|^2\cos^2(\theta/2)((\zeta\cdot\mathbf{j})^2+(\zeta\cdot\mathbf{k})^2)\Big)\Bigg)d\theta \\
&= \frac{2|u|^{-3}}{-h(\varepsilon)}\int_\varepsilon^\pi b(\cos\theta)\sin^3(\theta/2)\cos(\theta/2)i(\mathbf{u}\cdot\zeta) - \frac{1}{2}b(\cos\theta)\sin^5(\theta/2)\cos(\theta/2)(\mathbf{u}\cdot\zeta)^2 \\
&\quad - \frac{|u|^2}{4}b(\cos\theta)\sin^3(\theta/2)\cos^3(\theta/2)|\zeta^\perp|^2 d\theta \qquad (34) \\
&= \frac{2|u|^{-3}}{-h(\varepsilon)}\int_{\sin(\varepsilon/2)}^1 \left[\Big(i(\mathbf{u}\cdot\zeta)2H'(x) - (\mathbf{u}\cdot\zeta)^2\,C'(x)\Big) - \frac{|u|^2}{2}|\zeta^\perp|^2\Big(H'(x)-C'(x)\Big)\right]dx \\
&= \frac{2|u|^{-3}}{-h(\varepsilon)}\Big[2i(\mathbf{u}\cdot\zeta)\Big(H(1)-H(\sin(\varepsilon/2))\Big) - (u\cdot\zeta)^2\Big(C(1)-C(\sin(\varepsilon/2))\Big) \\
&\quad - \frac{|\zeta^\perp|^2|u|^2}{2}(H(1)-C(1)-H(\sin(\varepsilon/2))+C(\sin(\varepsilon/2))\,)\Big]
\end{aligned}
$$

We now invoke the properties of functions $H(x)$ and $C(x)$ defined in (18) and (19), respectively, satisfying conditions (20) as well as the identities $h(\varepsilon) = H(\sin(\varepsilon/2))$ and $c(\varepsilon) = C(\sin(\varepsilon/2))$. Thus, replacing in the last terms of the previous identity in (34), yields

$$
\begin{aligned}
&\frac{|u|^{-3}}{-h(\varepsilon)}(G_{b_\varepsilon,1}+G_{b_\varepsilon,2})(\zeta,\mathbf{u})) = |u|^{-3}\left(4i(\mathbf{u}\cdot\zeta) - |u|^2|\zeta^\perp|^2\right) \qquad (35) \\
&\quad - \frac{|u|^{-3}}{h(\varepsilon)}\ \left(2i(\mathbf{u}\cdot\zeta)H(1) - (\mathbf{u}\cdot\zeta)^2(C(1)-c(\varepsilon)) - |\zeta^\perp|^2|u|^2(H(1)-C(1)+c(\varepsilon))\right)
\end{aligned}
$$

Note that the first term is exactly the weight derived for the Landau operator above (14). The second term, having the coefficients $C(1), H(1)$ and $c(\varepsilon)$ bounded, will vanish as $\varepsilon \to 0$ as long as they are incorporated back into the weighted integral convolution associated to the Fourier transform of the collision operator. Indeed, defining

$$\tilde{G}(\zeta,\mathbf{u}) := G_{b_\varepsilon}(\zeta,\mathbf{u}) - G_L(\zeta,\mathbf{u}). \qquad (36)$$

one obtains

$$\widehat{Q_{b_\varepsilon}}[f_\varepsilon](\zeta) = \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v) f_\varepsilon(v-u)\}(\zeta)\tilde{G}(\zeta, \mathbf{u}) du \tag{37}$$

$$= \widehat{Q_L}[f_\varepsilon](\zeta) + \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v) f_\varepsilon(v-u)\}(\zeta)$$

$$\times \Bigg[\frac{|u|^{-3}}{h(\varepsilon)} \left(2i(\mathbf{u}\cdot\zeta)H(1) - (\mathbf{u}\cdot\zeta)^2(C(1)-c(\varepsilon)) - |\zeta^\perp|^2|u|^2(H(1)-C(1)+c(\varepsilon))\right)$$

$$+ \frac{|u|^{-3}}{h(\varepsilon)} \sum_{n=3}^{\infty} G_{b_\varepsilon,n}(\zeta,\mathbf{u}) \Bigg] du.$$

Thus, we need to control the two terms in $\tilde{G}(\zeta, \mathbf{u})$ in order to estimate the convergence rate in (37). We notice that the first term is controlled by

$$\Big| \frac{|u|^{-3}}{h(\varepsilon)} \Big(2i(\mathbf{u}\cdot\zeta)H(1) - (\mathbf{u}\cdot\zeta)^2(C(1)-c(\varepsilon)) - \frac{1}{2}|\zeta^\perp|^2|u|^2(H(1)-C(1)+c(\varepsilon))\Big) \Big| \leq$$

$$\frac{12}{|h(\varepsilon)|} \left(\frac{|\zeta|}{|u|^2} + \frac{|\zeta|^2}{|u|} \right) \Gamma \,. \tag{38}$$

with the constant Γ, defined in (20), is finite. In order to control the second term, we first control the behavior of the $n \geq 3$ terms. We estimate:

$$\left| |u|^{-3} \sum_{n=3}^{\infty} G_{b_\varepsilon,n}(\zeta,\mathbf{u}) \right|$$

$$= \left| \pi^{-1}|u|^{-3} \sum_{n=3}^{\infty}\sum_{j=0}^{n}\sum_{k=0}^{j} \left(\frac{i^n(\mathbf{u}\cdot\zeta)^{n-j}|u|^j(-1)^j(\zeta\cdot\mathbf{j})^k(\zeta\cdot\mathbf{k})^{j-k}}{n!} \binom{n}{j}\binom{j}{k} \right) \right.$$

$$\left. \times \left(\int_\varepsilon^\pi b(cos(\theta)\ \cos^{j+1}(\theta/2)\sin^{2n-j+1}(\theta/2)\ d\theta \right) \left(\int_0^{2\pi} \sin^k\phi \cos^{j-k}\phi\ d\phi \right) \right| \tag{39}$$

One can check that second bullet condition (15) grants the boundedness of the polar angular integral involving $b(\theta)$, and that clearly that azimuthal integration integral in ϕ is also bounded. Then, the right hand side of inequality (39) is controlled by

$$
\begin{aligned}
&\leq 2\pi|\zeta|^3 \left| \sum_{n=3}^{\infty} \frac{i^n |\mathbf{u}|^{n-3} |\zeta|^{n-3}}{n!} \sum_{j=0}^{n} (-1)^j \binom{n}{j} \sum_{k=0}^{j} \binom{j}{k} \right| \\
&= 2\pi|\zeta|^3 \left| \sum_{n=3}^{\infty} \frac{i^{n-3} |\mathbf{u}|^{n-3} |\zeta|^{n-3}}{n!} \sum_{j=0}^{n} (-2)^j \binom{n}{j} \right| \\
&= 2\pi|\zeta|^3 \left| \sum_{n=3}^{\infty} \frac{i^{n-3} |\mathbf{u}|^{n-3} |\zeta|^{n-3}}{n!} (-1)^n \right| \\
&= 2\pi|\zeta|^3 \left| \sum_{n=0}^{\infty} \frac{(-i|\mathbf{u}||\zeta|)^n}{(n+3)!} \right| \\
&= 2\pi|\zeta|^3 \left| -\frac{|\zeta|^2}{|u|} - \frac{2i|\zeta|}{|u|^2} - 2\frac{e^{-i|u||\zeta|} - 1}{|u|^3} \right| \\
&\leq 2\pi|\zeta|^3 \left(\frac{|\zeta|^2}{|u|} + \frac{2|\zeta|}{|u|^2} + \frac{2\sqrt{2}\sin(2|u||\zeta|)}{|u|^3} \right). \qquad (40)
\end{aligned}
$$

Thus we have that the second term in (37) is controlled by

$$
\frac{2\pi|\zeta|^3}{|h(\varepsilon)|} \left(\frac{|\zeta|^2}{|u|} + \frac{2|\zeta|}{|u|^2} + \frac{2\sqrt{2}\sin(2|u||\zeta|)}{|u|^3} \right) \qquad (41)
$$

Gathering the estimates from (38) and (41), we have

$$
\begin{aligned}
|\tilde{G}(\zeta, \mathbf{u})| \leq \; & \frac{12}{|h(\varepsilon)|} \Big(\frac{|\zeta|}{|u|^2} + \frac{|\zeta|^2}{|u|} \Big) \Gamma \\
& + \frac{2\pi|\zeta|^3}{|h(\varepsilon)|} \left(\frac{|\zeta|^2}{|u|} + \frac{2|\zeta|}{|u|^2} + \frac{2\sqrt{2}\sin(2|u||\zeta|)}{|u|^3} \right). \qquad (42)
\end{aligned}
$$

Thus,

$$
\begin{aligned}
& |\widehat{Q_{b_\varepsilon}}[f_\varepsilon](\zeta) - \widehat{Q_L}[f_\varepsilon](\zeta)| \\
&= \Bigg| \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v) f_\varepsilon(v-u)\}(\zeta) \\
&\times \left(\frac{|u|^{-3}}{|h(\varepsilon)|} \; (12\Big(|\zeta||u| + \frac{|\zeta|^2}{|u|}\Big) \Gamma + \frac{|u|^{-3}}{|h(\varepsilon)|} \sum_{n=3}^{\infty} G_{b_\varepsilon, n}(\zeta, \mathbf{u}) \right) du \Bigg|, \\
&\leq \frac{2}{|h(\varepsilon)|} \left| \int_{\mathbb{R}^n} \mathcal{F}\{f_\varepsilon(v) f_\varepsilon(v-u)\}(\zeta) \right| \\
&\times \left| \left(\frac{6\Gamma|\zeta|^2 + \pi|\zeta|^5}{|u|} + \frac{2\pi|\zeta|^4 + 6\Gamma|\zeta|}{|u|^2} + \frac{2\pi\sqrt{2}|\zeta|^3 \sin(2|u||\zeta|)}{|u|^3} \right) \right|. \qquad (43)
\end{aligned}
$$

Note that $\sin(2|u||\zeta|)/|u|^3 \approx 2|\zeta|/|u|^2$ for $|u| << 1$, thus all of the terms have integrable singularities in $|u|$ at zero.

Using the assumption (28) on the Fourier transform of $f_\varepsilon(\mathbf{v})f_\varepsilon(\mathbf{v}-\mathbf{u})$, we

$$\left|\widehat{Q_L}[f_\varepsilon](\zeta) - \widehat{Q_{b_\varepsilon}}[f_\varepsilon](\zeta)\right| \;\leq\; O\left(\frac{1}{|H(\sin(\varepsilon/2))|}\right) \to 0 \quad \text{as } \varepsilon \to 0 \qquad (44)$$

uniformly in $\zeta \in \mathbb{R}^d$, and therefore (29) follows immediately. ∎

Remark 1 The result from this theorem illustrates that *the convergence to the Landau collision operator is highly dependent on the model chosen for* $b_\varepsilon(\cos\theta)$.

The classical case of the Rutherford-Coulombic potential corresponds to the choice of H from (26), and so the limiting behavior in (29) is logarithmically slow, implying that the time scale for grazing collision effects with the Rutherford potential is much longer than the mean free time between collisions used in nondimensionalizing the Boltzmann equation. When solving a space inhomogeneous problem, this presents a time scale separation between the grazing collisional terms and the Vlasov terms on the left hand side of a space inhomogenous problem. Solving Coulombic interaction problems with finite ε should therefore capture more of the correct physics at the usual time scales for these types of problems. Furthermore, this potential gives a faster decay rate to equilibrium than the Landau equation alone owing to the keeping the error term controlled by $\log\sin(\varepsilon/2)$ (as shown in Figure 3).

For other choices of $b_\varepsilon(\cos\theta)$ that satisfy (15), the rate of convergence depends on the strength of the singularity at $\theta = 0$ trough the parameter $\delta > 0$ as shown in (27). The choice $\delta = 1$ corresponds to the ε-linear angular scattering cross section similar to those used recently in [7]

Thus, as it should be expected, we observe that the choice (16) for the scattering cross-section gives an ε-logarithmic rate of convergence to the solution of the Landau equation of the order $O\left(|\log\sin(\varepsilon/2)|^{-1}\right)$, which is known to be slow in the parameter ε to be studied numerically.

Instead, when choosing the ε-linear angular scattering kernel (17), the corresponding convergence ε-rate of the Boltzmann grazing collision limit to the solution of the Landau equation yields the limit (29), but with an linear convergence in ε instead of ε-logarithmic. This faster decay can be observed in our simulations of the logarithm of the entropy of the corresponding Boltzmann and Landau solutions in Figure 3. Thus we have $\|\widehat{Q_L}(\zeta) - \widehat{Q_{b_\varepsilon}}(\zeta)\|_{L^\infty(\mathbb{R}^d)} = O(\varepsilon)$ for this choice of cross section.

Remark 2 If $f(t,\mathbf{v})$ is a Maxwellian distribution in $\mathbf{v}$ space, the assumption (28) holds. Indeed, take for ease of presentation that $f = e^{-|\mathbf{v}|^2/2}$. Then we have that

$$
\begin{aligned}
\mathcal{F}\{f(\mathbf{v})f(\mathbf{v}-\mathbf{u})\}(\zeta) &= \int_{R^3} e^{-|\mathbf{v}|^2/2} e^{-|\mathbf{v}-\mathbf{u}|^2/2} e^{-i\zeta\cdot\mathbf{v}} d\mathbf{v} \\
&= e^{-|\mathbf{u}|^2/2} \int_{R^3} e^{-(\mathbf{v}\cdot\mathbf{v}-\mathbf{v}\cdot\mathbf{u})} e^{-i\zeta\cdot\mathbf{v}} d\mathbf{v} \\
&= e^{-|\mathbf{u}|^2/4} \int_{R^3} e^{-|\mathbf{v}-\mathbf{u}/2|^2} e^{-i\zeta\cdot\mathbf{v}} d\mathbf{v} \\
&= e^{-3|\mathbf{u}|^2/4} \int_{R^3} e^{-|\mathbf{w}|^2} e^{-i\zeta\cdot\mathbf{w}} d\mathbf{w} \\
&= \frac{1}{\sqrt{2}} e^{-3|\mathbf{u}|^2/4} e^{-|\zeta|^2/4} \le \frac{(1+|\zeta|)^{-5}}{\sqrt{2}(1+|u|^3)}
\end{aligned} \tag{45}
$$

4 The Conservative Numerical Method

4.1 Velocity space discretization

In order to compute the Boltzmann equation we must work on a bounded velocity space, rather than all of $\mathbb{R}^d$. However typical distributions are supported on the entire domain, for example the Maxwellian equilibrium distribution. Even if one begins with a compactly supported initial distribution, each evaluation of the collision operator spreads the support by a factor of $\sqrt{2}$, thus we must use a working definition of an *effective support* of size R for the distribution function. Bobylev and Rjasanow [9] suggested using the temperature of the distribution function, which typically decreases as $\exp(-|v|^2/2T)$ for large $|v|$, and used a rough estimate of $R \approx 2\sqrt{2T}$ to determine the cutoff. Thus, we assume that the distribution function is negligible outside of a ball

$$
B_{R_x}(\mathbf{V}(\mathbf{x})) = \{\mathbf{v} \in \mathbb{R}^d : |\mathbf{v} - \mathbf{V}(\mathbf{x})| \le R_x\}, \tag{46}
$$

where $\mathbf{V}(\mathbf{x})$ is the local flow velocity which depends in the spatial variable $\mathbf{x}$. For ease of notation in the following we will work with a ball centered at 0 and choose a length R large enough that $B_{R_x}(\mathbf{V}(\mathbf{x})) \subset B_R(0)$ for all $\mathbf{x}$.

With this assumed support for the distribution f, the integrals in (7) will only be nonzero for $\mathbf{u} \in B_{2R}(0)$. Therefore, we set $L = 2R$ and define the cube

$$
C_L = \{\mathbf{v} \in \mathbb{R}^d : |v_j| \le L,\ j = 1, \dots, d\} \tag{47}
$$

to be the domain of computation. With this domain the comptuation of the weight function integral (11) is cut off at $r = L$.

Let $N \in \mathbb{N}$ be the number of points in velocity space in each dimension. Then we establish a uniform velocity mesh with $\Delta v = \frac{2L}{N-1}$ and due to the formulation of the discrete Fourier transform the corresponding uniform Fourier space mesh size is given by $\Delta\zeta = \frac{(N-1)\pi}{NL}$.

4.2 Collision step discretization

To simplify notation we will use one index to denote multidimensional sums with respect to an index vector $\mathbf{m}$

$$\sum_{\mathbf{m}=0}^{N-1} = \sum_{m_1,\ldots,m_d=0}^{N-1}.$$

To compute $\widehat{Q}(\zeta_{\mathbf{k}})$, we first compute the Fourier transform integral giving $\hat{f}(\zeta_k)$ via the FFT. The weighted convolution integral is approximated using the trapezoidal rule

$$\widehat{Q}(\zeta_{\mathbf{k}}) = \sum_{\mathbf{m}=0}^{N-1} \widehat{G}(\xi_{\mathbf{m}}, \zeta_{\mathbf{k}}) \hat{f}(\xi_{\mathbf{m}}) \hat{f}(\zeta_{\mathbf{k}} - \xi_{\mathbf{m}}) \omega_{\mathbf{m}}, \tag{48}$$

where $\omega_{\mathbf{m}}$ is the quadrature weight and we set $\hat{f}(\zeta_{\mathbf{k}} - \xi_{\mathbf{m}}) = 0$ if $(\zeta_{\mathbf{k}} - \xi_{\mathbf{m}})$ is outside of the domain of integration. We then use the inverse FFT on $\widehat{Q}$ to calculate the integral returning the result to velocity space.

Note that in this formulation the distribution function is not periodized, as is done in the collocation approach of Pareschi and Russo [24]. This is reflected in the omission of Fourier terms outside of the Fourier domain. All integrals are computed directly only using the FFT as a tool for faster computation and the convolution integral is accurate to at least the order of the quadrature. The calculations below use the trapezoid rule, but in principle Simpson's rule or some other uniform grid quadrature can be used. However, it is known that the trapezoid rule is spectrally accurate for periodic functions on periodic domains (which is the basis of spectral accuracy for the FFT), and the same arguments can apply to functions with sufficient decay at the integration boundaries [4]. These accuracy considerations will be investigated in future work. The overall cost of this step is $O(N^{2d})$.

4.3 Discrete conservation enforcement

This implementation of the collision mechanism does not conserve all of the quantities of the collision operator. To correct this, we formulate these conservation properties as a Lagrange multiplier problem. Depending on the type of collisions we can change this constraint set (for example, inelastic collisions do not preserve energy), but we will focus on the case of elastic collisions, which preserve mass, momentum, and energy.

Let $M = N^d$ be the total number of grid points, let $\tilde{\mathbf{Q}} = (\tilde{Q}_1, \ldots, \tilde{Q}_M)^T$ be the result of the spectral formulation from the previous section, written in vector form, and let ω_j be the quadrature weights over the domain in this ordering. Define the integration matrix

$$\mathbf{C}_{5\times M} = \begin{pmatrix} \omega_j \\ v_j^i \omega_j \\ |\mathbf{v}_j|^2 \omega_j \end{pmatrix},$$

where v^i, $i = 1, 2, 3$ refers to the ith component of the velocity vector. Using this notation, the conservation method can be written as a constrained optimization problem.

$$\text{Find } \mathbf{Q} = (Q_1, \ldots, Q_M)^T \text{ that minimizes } \frac{1}{2}\|\tilde{\mathbf{Q}} - \mathbf{Q}\|_2^2 \text{ such that } \mathbf{CQ} = \mathbf{0} \quad (49)$$

Formulating this as a Lagrange multiplier problem, we define

$$L(\mathbf{Q}, \gamma) = \sum_{j=1}^{M} (\tilde{Q}_j - Q_j)^2 - \gamma^T \mathbf{CQ} \quad (50)$$

The solution is given by

$$\begin{aligned} \mathbf{Q} &= \tilde{\mathbf{Q}} + \mathbf{C}(\mathbf{CC}^T)^{-1}\mathbf{C}\tilde{\mathbf{Q}} \\ &:= \mathbf{P}_N \tilde{\mathbf{Q}} \end{aligned} \quad (51)$$

Overall the collision step in semi-discrete form is given by

$$\frac{\partial \mathbf{f}}{\partial t} = \mathbf{P}_N \tilde{\mathbf{Q}} \quad (52)$$

The overall cost of the conservation portion of the algorithm is a $O(N^d)$ matrix-vector multiply, significantly less than the computation of the weighted convolution.

4.4 Computing $\widehat{G}$ for singular scattering kernels

Numerically calculating the weights $\hat{G}$ to high accuracy can be difficult for singular scattering kernels, due to the precise nature of the cancellation at the left endpoint of the integral. The θ integral in (11) can be simplified as

$$\int_{\varepsilon}^{\pi} b_\varepsilon(\cos\theta)\sin\theta(\cos(c_1(1-\cos\theta) - c_3)J_0(c_2\sin\theta) - \cos(c_3))d\theta, \quad (53)$$

where c_1, c_2, c_3 depend on the current values of ϕ, r, ζ, ξ following from the full formulation of $\widehat{G}$. When $\varepsilon << 1$ the bulk of the integration mass occurs near the left endpoint of the θ interval, however this presents a challenge for a numerical quadrature package to compute. For $\theta << 1$ there is a subtraction of two nearly equal numbers (the two cosine terms), which causes floating point errors. To alleviate this, we split the integration interval into two pieces, and use the first term of the Taylor expansion of the troublesome part of the integrand for $\theta << 1$ and obtain

$$\begin{aligned} &\left(-\frac{c_2^2}{4}\cos(c_3) + \frac{c_1}{2}\sin(c_3)\right)\int_{\varepsilon}^{\sqrt{\varepsilon}} \theta^2 b_\varepsilon(\cos\theta)d\theta \\ &+ \int_{\sqrt{\varepsilon}}^{\pi} b_\varepsilon(\cos\theta)\sin\theta(\cos(c_1(1-\cos\theta) - c_3)J_0(c_2\sin\theta) - \cos(c_3))d\theta. \end{aligned}$$

These integrals are computed using the GNU Scientific Laboratory integration routines [14]. We use `cquad` to compute the first θ integral, which appears to be most stable choice for this near-singular integrand. The adaptive Gauss-Konrod quadrature `qag` is used for all other integrals used in computing the weights $\widehat{G}$. Speedup of this high-dimensional calculation is done using OpenMP and MPI on a cluster, as each weight can be calculated independently [16, 19].

5 Numerical results

To illustrate that this method captures the correct behavior for grazing collisions, we take a Coulombic potential ($\lambda = -3$) and set $\varepsilon = 10^{-4}$. Similar to what was done in [10, 25] based on the original work of Rosenbluth et al. [27] for the Landau equation, we set the axially symmetric initial condition

$$f(\mathbf{v}, 0) = 0.01\exp\left(-10\left(\frac{|\mathbf{v}| - 0.3}{0.3}\right)^2\right).$$

Using the ε-linear cross section (17), we take a domain size of $L = 1$, glancing parameter $\varepsilon = 10^{-4}$, $N = 16$, and compute to time $t = 900$ with a timestep of 0.01. The results are shown in Figure 1. Note that our symmetric grid is not aligned with $v_1 = 0$, so it is slighly offset from the figures from the earlier works.

To verify the linear convergence rate for the artificial cross section, we take a single timestep of the example above for $\varepsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$ with the artificial cross section (17). We compare these values with the result of a single step of the Landau equation (14). We represent the error by examining the difference in the values in the central slice of the solution, which are the same values plotted in Figures 1 and 2. In Table 1 we present the average error between the Landau and Boltzmann solution in this subset. As expected, the convergence is linear.

ε	average $\lvert Q_L - Q_\varepsilon \rvert$	ratio
10^{-1}	1.35×10^{-4}	
10^{-2}	1.47×10^{-5}	8.98
10^{-3}	1.51×10^{-6}	9.68
10^{-4}	1.52×10^{-7}	9.89

Table 1: Error between Boltzmann collision operator with grazing collisions and Landau collision operator

In Figure 2 we plot the evolution of the Boltzmann equation using the Rutherford cross section (16) and compare it to the numerical solution of the Landau equation. We again take $L = 1$, $\varepsilon = 10^{-4}$, and $N = 16$. This figure illustrates the large error between the two models for this cross section, as well as the different convergence rates to equlibrium. Indeed, we can see this more explicitly in Figure 3, where we can see the solution of the Boltzmann equation converges to equilibrium at a faster rate than the Landau equation.

Here we remark that the recent work of Bobylev and Potapenko [7] proves that the order of approximation between the Boltzmann and Landau operators is no worse than $\sqrt{\varepsilon}$, which would seem to contradict our logarithmic convergence result. However, the Rutherford potential does not satisfy the assumptions on the scattering kernel in their work, so there is no contradiction.

Due to the spectral formulation some of the grid values may be negative. Recent work by Alonso, Gamba, and Tharkabhushanam [3] has shown that the scheme maintains its spectral properties provided that the 'energy' of the negative grid points remains small compared to the energy of the rest of the computed distribuition. In Figure 4 we plot the percentage

$$\frac{\int_D |f_-||v|^2 dv}{\int_D f_+|v|^2 dv},$$

where f_- is the grid cells where the discrete distribution function is negative and vice versa for f_+.

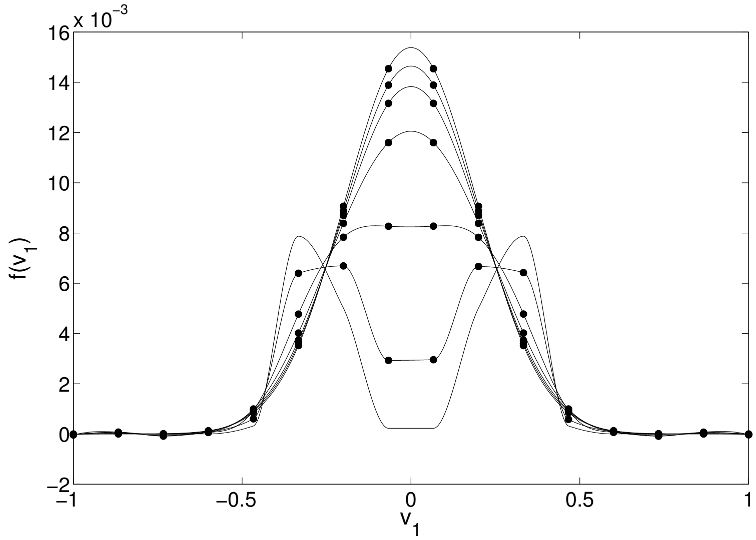

Figure 1: Slice of the distribution marginal function at times $t = 0, 9, 36, 81, 144, 225, 900$. Solid lines: Hermite spline reconstruction of Landau equation solution. Solid circles: Boltzmann solution with artificial cross section (17) . $\varepsilon = 10^{-4}, N = 16$.

6 Conclusions and future work

We have derived the spectral formulation for the more general case of anisotropic collisional models for the Boltzmann equation. We also showed that the spectral method for the Boltzmann equation is consistent with the limiting Landau equation under suitable assumptions on the scattering kernel, and that using the grazing collision Boltzmann equation may capture more of the correct physics in the case of Coulombic interactions. One other important thing to note is that this method could be a good candidate for collisional models where the collision mechanism is unknown and only experimentally determined, and future work will attempt to simulate the Boltzmann equations with these cross sections. In addition, as the Landau equation is used to model collisions of charged particles in plasma we will seek to add field effects to the space inhomogeneous Boltzmann equation, resulting in the Boltzmann-Poisson or Boltzmann-Maxwell systems. The inhomogeneous method uses operator splitting between the collision and the transport terms, so in principle one can use an already developed Vlasov solver for the spatial terms in the equation.

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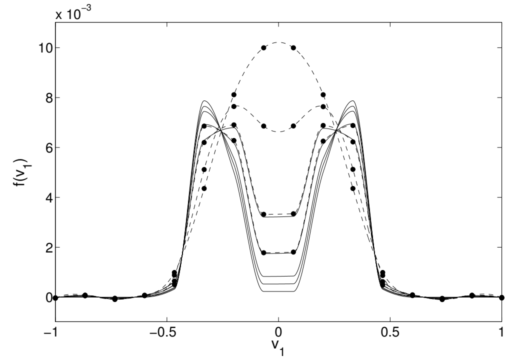
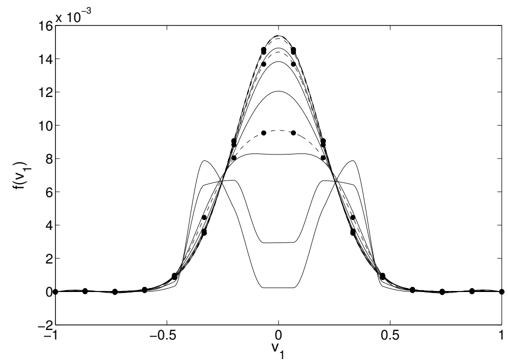


(a) Early times



(b) Long times

Figure 2: Comparisons of solutions to Boltzmann using Rutherford cross section (16) and to Landau equations. *(a)* Slice of the distribution marginal function at early times $t = 0, 1, 2, 5, 10$. *(b)* Slice of the distribution marginal function at times $t = 0, 9, 36, 81, 144, 225, 900$. Solid lines: spline reconstruction of Landau equation solution. Dashed lines with solid circles: spline reconstruction of Boltzmann equation. Spline reconstruction uses Hermite polynomials for times below $t = 10$ to avoid a reconstruction the generate negative values in the marginal tails $\varepsilon = 10^{-4}, N = 16$.

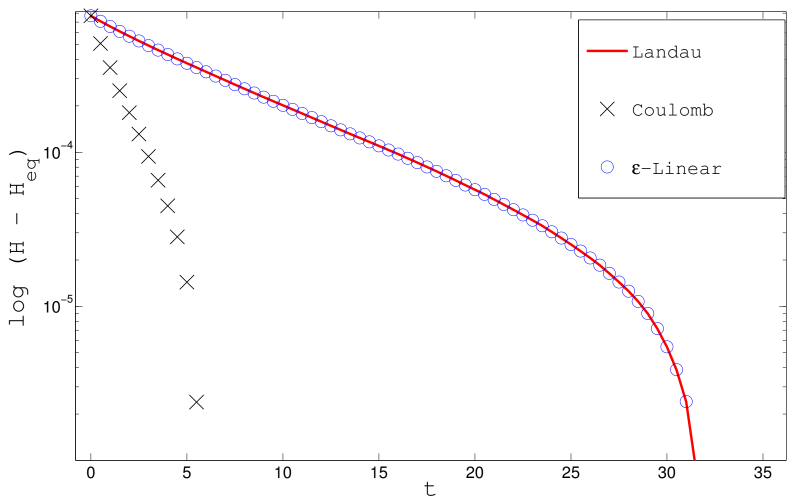


Figure 3: Convergence of entropy to equilibrium: Log of entropy decay for Boltzmann solution with the Rutherford cross section (16) with crosses, Boltzmann solution with the ε-linear cross section (17) with circles, and Landau solution with solid curve. $N = 16$, $\varepsilon = 10^{-4}$.

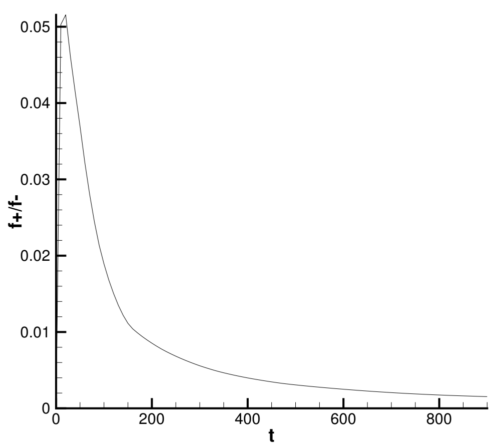


Figure 4: Ratio of energy in negative grid points to energy in positive grid points.