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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 method for the Boltzmann collision operator with anisotropic scattering cross-sections. The method is an extension of the conservative spectral method of Gamba and Tharkabhushanam [17,18], which uses the weak form of the collision operator to represent the collisional term as a weighted convolution in Fourier space. The method is tested by computing the collision operator with a suitably cut-off angular cross section and comparing the results with the solution of the Landau equation. We analytically study the convergence rate of the Fourier transformed Boltzmann collision operator in the grazing collisions limit to the Fourier transformed Landau collision operator under the assumption of some regularity and decay conditions of the solution to the Boltzmann equation. Our results show that the angular singularity which corresponds to the Rutherford scattering cross section is the critical singularity for which a grazing collision limit exists for the Boltzmann operator. Additionally, we numerically study the differences between homogeneous solutions of the Boltzmann equation with the Rutherford scattering cross section and an artificial cross section, which give convergence to solutions of the Landau equation at different asymptotic rates. We numerically show the rate of the approximation as well as the consequences for the rate of entropy decay for homogeneous solutions of the Boltzmann equation and Landau equation.

1. Introduction

The initial focus of this manuscript was the study of simulating the Boltzmann equation with anisotropic, singular angular scattering cross sections by spectral methods. However, while attempting to verify numerical results based on this method by examining the grazing collision limit of the Boltzmann operator, we found an analytical argument that gives not only an explicit representation of the effect of angular averaging for a family of singular grazing collision angular cross sections, but also the rate of convergence of the grazing collision limit of the Boltzmann operator to the Landau operator. The bulk of this manuscript will address both the numerical and analytical aspects of this grazing collision limit of the Boltzmann equation in physically relevant regimes, which includes the case of Coulombic intermolecular potential scattering mechanisms.

While numerical methods for solving the Boltzmann equation generally use the assumption of spherical particles with 'billiard ball' like collisions, a more physical model is to assume that particles interact via two-body potentials. Under this assumption the Boltzmann equation can be formulated in a very similar manner [11], but in this case the scattering cross section is highly anisotropic in the angular variable. In many cases, such as the physically relevant case of Coulombic interactions between charged particles, the derivation of the Boltzmann equation breaks down completely due to the singular nature of this scattering cross section. Physical arguments by Landau [21] as well as a later derivation by Rosenbluth et al.

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[27] showed that the dynamics of the Boltzmann equation can be 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 the Boltzmann equation near this grazing collision limit. 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 with 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 neither estimates nor computations were done for the Boltzmann equation near the grazing collisions limit. 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 non-linear 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) which can be done with $O(N^{\frac{5}{3}} \log N)$ in 3D. Spectral methods have 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 L^2 in the computational domain to the output of the collision term that conserves the macroscopic quantities. This optimization problem is the approximation of the projection of the Boltzmann solution to the space of collision invariants associated to the corresponding collision operator [3]. In addition 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. They are also shown in the space homogeneous, hard potential case, to converge to the Maxwellian distribution with the conserved moments corresponding to the endowed collision invariants. Such convergence and error estimates results heavily rely on the discrete constrained optimization problem (see [3] for a complete proof and details).

The proposed computational approach is complemented by the analysis of the approximation from the Boltzmann operator with grazing collisions to the Landau operator 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 holds for a family of singular angular scattering cross sections with a suitably cut-off Coulomb potential. The parameter $0 \leqslant \delta < 2$ corresponds to the strength of the singularity in the angular cross section and the parameter ε corresponds to the angular cutoff, which gives the *grazing collision limit* as $\varepsilon \to 0$.

The case when the parameter $\delta = 0$ corresponds to the classical Rutherford scattering cross section [28], and includes an inverse logarithmic term in ε that ensures the limit. This value of δ is critical to obtain the grazing collision limit in the following sense: if $\delta < 0$ then the error between the Boltzmann and the Landau operators will not necessarily converge to zero in ε. In addition, for any other value $0 < \delta < 2$, the rate of convergence of the Boltzmann to the Landau operator is faster in ε. In these sense we can assert that the Rutherford scattering cross section [28] is the one that contains the weakest possible singularity in the angular cross section for which one can achieve a grazing collision limit to the Landau equation.

These results are shown in Theorem 3.1 and are written for the three dimensional case. There we prove that the L^∞-difference of the Fourier transforms between the Landau operator Q_L and the Boltzmann operator for this family of cross