Adaptive polynomial expansion method for the numerical solution of the Lenard-Balescu equation

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1 Introduction

Plasma [1] is a state of matter in which electrons are no longer bound to their atomic nuclei. This ionization can be partial, in which atoms may retain some of their electrons, or total, in which all electrons are stripped. The mathematical description of plasmas is a very important area of research, which has impact across a broad range of physical applications, such as stellar astrophysics, giant planets, and fusion research [2]. However, an accurate description is very difficult to obtain in general due to the long-range nature of the Coulomb interaction, the huge number of particles involved (densities can vary from 10^{14} to 10^{28} particles per cubic centimeter) and the range of temperature that must be covered (from about 1000 to 10^8 Kelvin). Various techniques may be applied in some areas of this large range, but for many important conditions of temperature and density, the only way to extract information is to perform large-scale and costly computer simulations. However, this project deals with the regime in which we may apply a technique called kinetic theory.

We will assume that the temperature and density are such that the energy in the system is dominated by the kinetic energy (KE) of the particles with the interaction or potential energy (PE) playing only a small role, i.e., $\Gamma \equiv$ PE/KE $<<$ 1. This is referred to as the weak coupling regime and is governed by the Lenard-Balescu equation. Before getting to this equation, we will give a brief description of kinetic theory, but additional reading is highly recommended (see [3], chapter 13).

2 Kinetic theory

Usually, one is not interested in positions and velocities of individual electrons or ions, and much of the relevant information about the plasma is encapsulated in the particle distribution function

$$f(x, y, z, v_x, v_y, v_z)dxdydzdv_xdv_ydv_z = f(\boldsymbol{r}, \boldsymbol{v})d^3\boldsymbol{r}d^3\boldsymbol{v}, \tag{1}$$

which is defined as the average number of particles between x and $x + dx$, v_x and $v_x + dv_x$, etc. The average can be defined as an ensemble average, a spatial average, a time average, or some combination of these. The particle distribution function satisfies a kinetic equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \frac{1}{m}\boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = C(f), \tag{2}$$

where $\boldsymbol{F}$ is the external force on the particles and $C(f)$ is called the collision operator. It is in the function $C(f)$ that all the physics related to particle collisions resides, and different approximations lead to different forms for C. In general $C(f)$ is a complicated integral over the distribution function, with our chosen form, the Lenard-Balescu operator, being a notorious example. Before getting to those details, a few more simplifications will be made.

In general, we will consider only homogeneous plasmas, in which the distribution has no spatial dependence. We will also assume there are no external forces, so all that remains on the left hand side of (2) is the time derivative. Generally speaking, if inter-particle collisions are the only interaction in the system (i.e., there is no external force or coupling to some other process), then the system will evolve from its initial state and ultimately end up in its equilibrium distribution. Depending on the kind of particles we have, and whether we are accounting for certain quantum mechanical effects, the equilibrium distribution can take a variety of forms. In our case, we will assume that at equilibrium we have the Maxwell distribution (see [3], chapter 7), meaning,

$$f^{\mathrm{eq}}(\boldsymbol{v}) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right), \tag{3}$$

where T is the temperature, k_B is Boltzmann's constant, m is the particle mass, n is the number density (number of particles per unit volume), and

$$v \equiv \sqrt{v_x^2 + v_y^2 + v_z^2} \tag{4}$$

is the speed. This is the classical equilibrium distribution; that is, it takes no account of the fact that electrons and protons are fermions that obey the exclusion principle. Although our collision operator will be quantum mechanical, it too does not take account of exclusion and thus the Maxwell distribution is the correct equilibrium distribution. This is an approximation of course, but at the conditions of interest to us, it should be reasonable (and simplifies the problem immensely).

In the situation we are considering, where we have two species of particles, namely electrons and ions, each species has its own distribution, f_e and f_i, which satisfy separate kinetic equations. We also need two collision terms on the left-hand side of equation (2). For example, in the equation for the electron distribution, we would need to account for the fact that electrons interact not only with the ions, but also with each other. This means that our system of equations is of the form

$$\frac{\partial f_e}{\partial t} = C_{ee}(f_e) + C_{ep}(f_e, f_p) \tag{5}$$

$$\frac{\partial f_p}{\partial t} = C_{pp}(f_p) + C_{pe}(f_p, f_e) \ . \tag{6}$$

We now just need the collision operators.

3 Lenard-Balescu collision operator

The Lenard-Balescu collision operator [4, 5], also called the Lenard-Balescu-Guernsey operator, is the focus of our work. Many physical assumptions and approximations are built into this formula. It describes charged particles interacting via the Coulomb potential:

$$v_{\sigma\sigma'}(r) = \frac{Z_\sigma Z'_\sigma e^2}{r} \tag{7}$$

where e is the magnitude of the electron charge and Z_σ is the charge number of the species σ (for example, for electrons $Z_e = -1$ and for protons $Z_p = 1$). A major approximation is that all interactions between particles result in only small deflections. Loosely speaking, this "small-angle scattering" approximation holds only if the particles are distant, or they approach each other with high velocity (one can make these notions more precise by examining the Rutherford cross section). Once again, at our weak-coupling

conditions, where kinetic energy dominates over potential, this approximation should be fine. Even though the interaction between two particles is Coulomb, in practice this can be significantly modified due to the presence of the other particles. This leads to a phenomenon called screening, which is also accounted for in the Lenard-Balescu operator.

The quantum Lenard-Balescu collision operator is given by the expression

$$\begin{aligned} C_{ij}(f_i, f_j) &= -\frac{1}{4\pi^2\hbar^2}\int d^3\mathbf{v}' \int d^3\mathbf{k} \frac{|\phi(k)|^2}{\left|\epsilon\left(k, \mathbf{k}\cdot\mathbf{v} + \frac{\hbar k^2}{2m_i}\right)\right|^2} \delta[\mathbf{k}\cdot(\mathbf{v}-\mathbf{v}') + \hbar k^2/2\mu] \\ &\times \left[f_i(\mathbf{v}) f_j(\mathbf{v}') - f_i(\mathbf{v}+\hbar\mathbf{k}/m_i) f_j(\mathbf{v}'-\hbar\mathbf{k}/m_j)\right] , \end{aligned} \tag{8}$$

where $\hbar$ is Planck's constant, m_i is the first species mass, m_p the second, $\mu = m_i m_j/(m_i+m_j)$ is called the reduced mass, $\phi(k)$ is the Fourier transform of the Coulomb potential, i.e.,

$$\phi(k) = \frac{4\pi e^2}{k^2}, \tag{9}$$

and $\epsilon(k,\omega)$ is the dielectric function, which accounts for screening by reducing the bare Coulomb interaction in Fourier space. The latter is a somewhat complicated function of the distribution, f, but, luckily, for the purposes of this project we will set $\epsilon(k,\omega) = 1$. To get, say, C_{ep} simply substitute $i = e$ and $j = p$.

With this collision operator, the system defined by (5) and (6) is the non-degenerate quantum Lenard-Balescu equation for a two-component (i.e., electrons and protons), spatially homogeneous plasma with no external force. Although equation (8) is a quantum mechanical equation (it contains Planck's constant), in this project we will be testing a numerical solution scheme on its classical limit, $\hbar \to 0$. However, as is sometimes the case, the quantum system is easier to work with and we will thus retain $\hbar$ throughout our calculations and take the limit only at the end. Note that if we set $\epsilon(k,\omega) = 1$ and take $\hbar \to 0$, the resulting equation is called the Landau equation.

4 Solution method

The numerical solution of the Lenard-Balescu equation is a difficult subject which has scarcely been studied. The 2014 RIPS team explored a solution method based on an expansion in Laguerre polynomials. This ultimately proved to be successful and we will build on this success in this project.

The key point to understand here is that when we expand the distributions in orthogonal polynomials, our partial integro-differential equations become an infinite set of *ordinary* differential equations. Truncating this system at some order then gives us our approximation to the solution. In practice, we have used a maximum of 40 polynomials because the amount of work required goes as $\mathrm{O}(N^3)$ where N is the number of polynomials. This places a limitation on the range of distributions we can resolve, and we will try to remedy this problem by considering an adaptive expansion scheme. Before describing this, we review some properties of Laguerre polynomials and their use in this problem.

4.1 Laguerre polynomials

First, we assume that, like the equilibrium situation, the distribution is isotropic in velocity space, meaning there is no preferred direction in the system. This symmetry reduces the number of velocity variables to one:

$$f(\boldsymbol{v}) = f(v) \tag{10}$$

where

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2}. \tag{11}$$

We then expand the distribution of species i in the form

$$f_i(v) = f_i^{\mathrm{eq}}(v) \sum_{n=0}^{\infty} A_n^i(t) L_n^{(\alpha)} \left(\frac{\beta m_i v^2}{2} \right), \tag{12}$$

where $f_i^{\mathrm{eq}}(v)$ is the equilibrium distribution given in equation (3), $\beta \equiv 1/(k_B T)$ and $L_n^{(\alpha)}(x)$ are the associated Laguerre polynomials (often called Sonin polynomials). It will be necessary to become well-acquainted with these functions and many good references exist, but probably the most useful resource is the Wikipedia page. The reason for including the Maxwell distribution out front is that in the absence of any effects beyond particle collisions, the action of the kinetic equation is to drive the system to equilibrium, and in our chosen expansion equilibrium is just given by $A_n = \delta_{n0}$. Therefore the coefficients with $n > 1$ measure how far we are out of equilibrium, and they have a natural tendency to vanish as the calculation proceeds. The reason for choosing the Laguerre polynomials is that they have the convenient orthogonality property

$$\int_0^{\infty} x^{\alpha} e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) dx = \frac{\Gamma(n + \alpha + 1)}{n!} \delta_{nm}. \tag{13}$$

When we perform the integrals in equation (2), we will often find ourselves integrating against the Maxwell distribution, and after making the substitution $x \equiv \beta m v^2/2$, equation (13) will prove useful.

Another great advantage of our expansion is that it automatically handles conservation laws, provided we make some appropriate choices. During the calculation, we require the system to conserve both energy and particle number. Conservation of particle number implies

$$\int f(\boldsymbol{v}) d^3\boldsymbol{v} = n. \tag{14}$$

Using the isotropy of the distribution, this expression becomes

$$\int_0^\infty f(v) v^2 dv = \frac{n}{4\pi}. \tag{15}$$

Similarly, conservation of energy is given by

$$\int_0^\infty f(v) v^4 dv = \frac{3}{4\pi}\frac{n}{m\beta}. \tag{16}$$

With an appropriate choice of α, conservation of particles can be guaranteed by fixing $A_0 = 1$. Fixing another of the coefficients similarly imposes energy conservation. It will be a good starting exercise to determine the optimal choice of α and the coefficient to be fixed to conserve energy.

Once these choices are made, the problem becomes a numerical solution of the ordinary differential equations for the coefficients $\{A_n^e(t)\}$ and $\{A_n^p(t)\}$ for $n > 1$. These ordinary differential equations are found by plugging the expansion (12) into the kinetic equations (5) and (6), multiplying both sides by $L_k^{(\alpha)}\left(\frac{\beta m_i v^2}{2}\right)$ and integrating over v.

5 Adaptive method

We have listed the advantages of our method above. What about its disadvantages? The main one is that we sometimes have trouble resolving physically interesting distribution functions. We could try to add more polynomials, but the expense of this grows rapidly. So instead, we will try to make more efficient use of our current number. The starting point is to use the modified Laguerre expansions

$$f_e(v) = f_e^{\mathrm{eq}}(v) \sum_{n=0}^{\infty} A_n^e(t) L_n^{(\alpha)}\left(\frac{\beta_e m_e v^2}{2}\right), \tag{17}$$

$$f_p(v) = f_p^{\text{eq}}(v) \sum_{n=0}^{\infty} A_n^p(t) L_n^{(\alpha)} \left(\frac{\beta_p m_p v^2}{2} \right). \tag{18}$$

That is, for the temperature parameter in the expansion we no longer use the final equilibrium temperature, but each species has its own value. Of course, these temperatures must also be used in the equilibrium distributions $f_e^{\text{eq}}(v)$ and $f_p^{\text{eq}}(v)$. Periodically throughout the calculation, we will vary these temperatures and compute a new set of coefficients based on the new temperatures. This we refer to as reprojection, which, if done in the correct way, may allow us to represent a much wider variety of functions without having to add more polynomials. We will go into more detail on this later. The first task will be to use the above expansions in the equations (5) and (6) to find the resulting ordinary differential equations. The 2014 RIPS team did this calculation for a single-species plasma and you should use their calculation as a guide.

6 Project goals

Our goal is to verify that the adaptive scheme for solving the Lenard-Balescu equation will be feasible and we will test this on the much simpler Landau equation. The steps of the project can be broken down as follows:

1. The first part will be devoted to deriving the ordinary differential equations governing the coeffients, $A_n^e(t)$ and $A_n^p(t)$, which is a conceptually straightforward but tedious and time-consuming procedure. It will involve inserting the expansions into the kinetic equations and performing the various integrals analytically. We do this by setting $\epsilon = 1$ but leaving $\hbar \neq 0$. Note however, that without the dielectric function, the k-integral is divergent as $k \to 0$, and this will have to be addressed by using a cutoff. When we later take $\hbar = 0$, the integral also diverges as $k \to \infty$ and we need a cutoff there too, resulting in an object called the Coulomb logarithm. We will have more to say on this later.

2. Once we have the differential equations in hand, we will turn to their numerical solution. We will focus on equilibration calculations, in which we start with an arbitrary distribution and let the system evolve to equilibrium. A particular problem to study here is one in which each species starts off in the Maxwell distribution at different temperatures.

The initial coefficients are then trivial. We then want to solve the differential equations for the coefficients and, if we separate the initial temperatures enough, we should run out of resolution and the solver will crash.

3. The final step will be to remedy this crashing by periodically reprojecting the functions onto expansions with adjusted temperatures. By judiciously choosing these new temperatures, we should be able to retain enough resolution throughout the whole calculation. Many things need to be explored here, such as how to determine when reprojection is needed, how to choose the new temperatures, and how to efficiently carry out the reprojection.

Perhaps a third of the time will be spent on each point above. On the other hand, if you complete these tasks before the end of the project, we would be able to add more complications into the mix, such as reinstating the dielectric function. Although we eventually want a C or C++ code to solve these equations, for this project you may use any numerical methods with which you are comfortable, e.g., Mathematica or Matlab. For background reading, we strongly recommend reading the 2014 RIPS report to see how the non-adaptive solver works.

References

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