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., $\Gamma \equiv \text{PE/KE} << 1$. 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 interesting physics 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 we should have the sum $C(f_e) = C_{ee}(f_e) + C_{ei}(f_e, f_i)$, and similarly for the ion equation. However, we will assume there is only a single species, say the electrons, to develop our solution method. This is referred to as a one-component plasma (to maintain charge neutrality in the system, we assume a uniform positive charge background but this will not come up in our calculations). Once we have done this, the generalization to the two-component plasma, our real interest, is completely straightforward.

3 Lenard-Balescu equation

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:

$$v_{\sigma\sigma'}(r) = \frac{Z_\sigma Z'_\sigma e^2}{r} \tag{5}$$

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

$$\begin{aligned} C_{QLB}(\boldsymbol{v}) &= -\frac{1}{4\pi^2\hbar^2}\int d^3\boldsymbol{v}'\int d^3\boldsymbol{q}\frac{|\phi(q)|^2}{\left|\epsilon\left(q,\boldsymbol{q}\cdot\boldsymbol{v}+\frac{\hbar q^2}{2m}\right)\right|^2}\delta[\boldsymbol{q}\cdot(\boldsymbol{v}-\boldsymbol{v}')+\hbar q^2/m] \\ &\times \left[f(\boldsymbol{v})f(\boldsymbol{v}')-f(\boldsymbol{v}+\hbar\boldsymbol{q}/m)f(\boldsymbol{v}'-\hbar\boldsymbol{q}/m)\right], \end{aligned} \tag{6}$$

where $\hbar$ is Planck's constant, m is the particle mass, $\phi(q)$ is the Fourier transform of the Coulomb potential, i.e.,

$$\phi(q) = 4\pi\frac{Z_\sigma Z'_\sigma e^2}{q^2}, \tag{7}$$

and $\epsilon(q,\omega)$ 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, and to start the project we will simplify the problem by setting $\epsilon(q,\omega)=1$. It is worth noting that equation (6) is a quantum mechanical equation (it contains Planck's constant) whereas the actual equation derived independently by Lenard and Balescu was purely classical. The equation we are using here was first derived by Wyld and Pines [6]. Nevertheless, equation (6) is often referred to as the quantum Lenard-Balescu equation, with the original classical operator appearing when we take the limit $\hbar\to 0$. Taking this limit is quite non-trivial and the resulting classical equation is more complicated than even equation (6). Therefore, in practice, even if we want to do a classical calculation it is much easier to solve the quantum equation, and then take the $\hbar\to 0$ limit at the end rather than starting with the classical equation.

The equation we wish to solve is

$$\frac{\partial f(\boldsymbol{v})}{\partial t} = C_{QLB}(\boldsymbol{v}). \tag{8}$$

This is an integro-differential equation which is furthermore non-linear due to the product of distribution functions inside the integral, and the dependence on f of the dielectric function.

4 Proposed solution method

The numerical solution of the Lenard-Balescu equation is a difficult subject which has scarcely been studied [7]. A simplified version of this system arises when we set $\epsilon(k,\omega) = 1$ and take the limit $\hbar \to 0$. This is called the Landau collision operator, and it can be shown that the resulting kinetic equation may be mapped onto an equivalent Fokker-Planck equation. Actually, when one makes these simplifications, the q-integral in equation (6) becomes divergent in both the $q \to 0$ and $q \to \infty$ limits, so cutoffs must be introduced. This procedure is well-motivated physically but it results in predictions that are accurate in order of magnitude only (i.e., one has to accept being off by factors like 3 or 4). However, the Landau/Fokker-Planck system has been studied extensively [8], and a widely-used discretization method exists for its solution. It may be possible to adapt this method to solve the Lenard-Balescu equation, but that is not the approach we will take. Instead, we will investigate the possibility of solving equation (6) with an expansion in orthogonal polynomials.

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:

$$f(\boldsymbol{v}) = f(v) \tag{9}$$

where

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2}. \tag{10}$$

We then expand the distribution in the form

$$f(v) = f^{\text{eq}}(v) \sum_{n=0}^{\infty} A_n(t) L_n^{(\alpha)} \left(\frac{\beta m v^2}{2} \right), \tag{11}$$

where $f^{\text{eq}}(v)$ 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

$$\int_0^\infty x^\alpha e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) dx = \frac{\Gamma(n+\alpha+1)}{n!} \delta_{nm}. \tag{12}$$

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 (12) will prove useful.

Another great advantage of our proposed 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

$$\int f(\boldsymbol{v}) d^3\boldsymbol{v} = n. \tag{13}$$

Using the isotropy of the distribution, this expression becomes

$$\int_0^\infty f(v) v^2 dv = \frac{n}{4\pi}. \tag{14}$$

Similarly, conservation of energy is given by

$$\int_0^\infty f(v) v^4 dv = \frac{3}{4\pi} \frac{n}{m\beta}. \tag{15}$$

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 $\{A_n\}$ for $n > 1$. These ordinary differential equations are found by plugging the expansion (11) into the kinetic equation (8), multiplying both sides by $L_m^{(\alpha)}\left(\frac{\beta m v^2}{2}\right)$ and an appropriate factor and integrating over v.

5 Project goals

Our eventual goal is to have a numerical method for solving the Lenard-Balescu equation given in equation (8). We hope that the polynomial expansion method given above will do this. However, this is an area of current research, meaning we do not know in advance how well it will work! On the other hand, a similar approach has been tried for the Landau/Fokker-Planck system ($\epsilon = 1, \hbar = 0$), with success [9, 10]. To begin this project we will therefore consider a simplified system with $\epsilon(q, \omega) = 1$ while retaining the physical value of $\hbar$, a sort of "quantum Landau" equation. The project will have two main pieces:

1. The first part will be devoted to deriving the ordinary differential equations governing the coeffients, A_n, which is a conceptually straightforward but tedious and time-consuming procedure. It will involve inserting the expansion into the kinetic equation and performing the various integrals analytically. For the case $\epsilon = 1$, we believe this can be done completely analytically by the use of various identities (i.e., no numerical integrations will be needed in the end – we think!). Note however, that without the dielectric function, the q-integral is divergent as $q \to 0$, and this will have to be addressed by using a cutoff.

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. We wish to learn exactly what kinds of initial distributions we can resolve with the method, and how well the method performs compared with standard techniques for this system. What features of the distribution trip up the method? How many polynomials do we need to solve interesting problems, and how difficult are the equations to solve numerically? These are all questions we would like to address, and we are not sure of the answers to any of them.

Perhaps half 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, and studying two-component plasmas. 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.

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