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A LORENTZ FORMULATION FOR AN ELECTRON GAS USING THE GAS KINETIC METHOD

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Abstract. *This work outlines efforts in the theoretical development of the connection between electron gas equations and the Boltzmann equation using the Gas Kinetic Method - GKM. The relationship between the Boltzmann equation and electron gas equation is reviewed and the corresponding relationship between the Boltzmann equation with the Lorentz force is explored. The Boltzmann equation is discussed with respect to the nature of the body force term (the Lorentz force). The consequences of this choice regarding the accuracy of the physical phenomena captured is discussed. The importance of introducing the Lorentz force in the GKM formulation is highlighted.*

Keywords: *gas kinetic method, Lorentz force, electron gas, Boltzmann equation*

1. INTRODUCTION

Plasmas can be found in a great variety of problems in science from the study of coronal mass ejections of the sun to fusion reactors. Additionally, many engineering problems rely on the correct understanding of the plasma dynamics, such as the arc interruption in circuit breakers and mass ejection in electric thrusters. This work is a part of a larger effort to develop a plasma simulation tool that is capable of capturing the correct physics for low to moderate Knudsen number flows. Here we develop a kinetic model of an electron gas that will be implemented in a numerical scheme known as the Gas Kinetic Method (GKM).

In §2.we present the simplified macroscopic equations that our kinetic model intends to recover. In §3. we introduce a kinetic model for an electron gas and perform a multi-scale analysis in order to obtain the macroscopic equations outlined in §2. In §4. the effect of the electromagnetic field on the macroscopic transport coefficients is analyzed. Finally, we give a brief overview of GKM in §5.

2. GOVERNING EQUATIONS FOR AN ELECTRON GAS

Plasma may be approximated with a two fluid model of electrons and ions. In practice, plasma is comprised by a large range of particles that may include electrons and various types of ions and neutral particle species. First, we will begin with conservation equations for an electron gas, and next we will consider the effects that we would like to recover in the transport coefficients by introduction of the Lorentz force (Samuel, 1967). The mass conservation, momentum conservation or Navier-Stokes equation - NS - and energy conservation are given by,

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0\,, \tag{1}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \boldsymbol{\nabla} \cdot \left[\rho \mathbf{u}\mathbf{u} + \underline{\underline{\boldsymbol{\Phi}}} + \underline{\underline{\mathbf{I}}} p\right] = \mathbf{J} \times \mathbf{B}\,, \tag{2}$$

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(E + p) + \boldsymbol{\nabla} \cdot \mathbf{q} + \mathbf{u} \cdot \underline{\underline{\boldsymbol{\Phi}}}\right] = \mathbf{J} \cdot \mathbf{E}\,. \tag{3}$$

In the equations above, $\mathbf{u}$ is the fluid velocity, $\mathbf{q}$ is heat flux vector, ρ is density, p is the thermodynamic pressure, $\mathbf{J}$ is current density, E is total energy, $\underline{\underline{\boldsymbol{\Phi}}}$ is the viscous stress tensor and $\mathbf{B}$ is the magnetic field. The current density is given by,

$$\mathbf{J} = q_e n_e \mathbf{u}\,, \tag{4}$$

where q_e is the electron charge and n_e is the particle density. The evolution of magnetic and electric fields are give by the Maxwell equations. In this work we are considering a formulation for a single species, which can be electrons or ions. Hence, this is an electron or ion gas formulation. This formulation will be useful for building a two fluid model in future work. We are considering that the external electrical field is null $\mathbf{E} = 0$. Together with Equation 4, this consideration gives us the following set of conservation equations:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0 \tag{5}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \left[\rho \mathbf{u}\mathbf{u} + \underline{\underline{\boldsymbol{\Phi}}} + \underline{\underline{\mathbf{I}}} p\right] = q_e n_e \mathbf{u} \times \mathbf{B} \tag{6}$$

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(E+p) + \boldsymbol{\nabla} \cdot \mathbf{q} + \mathbf{u} \cdot \underline{\underline{\boldsymbol{\Phi}}}\right] = 0 \tag{7}$$

We are interested in the effect of the magnetic field on the transport coefficient. The next section will outline how to recover the above set of equations from the Boltzmann equation.

3. CONSIDERATIONS IN KINETIC MODELS

Consider the full Boltzmann equation below,

$$\partial_t f + \xi_i \partial_i f + F_i \partial_{\xi_i} f = \frac{1}{\tau}\left(f^{(0)} - f\right)\,, \tag{8}$$

where f is the distribution function, $f^{(0)}$ is the equilibrium distribution function, ξ_i are the components of microscopic velocity, τ is the relaxation time, ∂_i and ∂_{ξ_i} are the spatial and velocity gradients, respectively, and F_i is a component of the body force. Integrating Equation 8 over the velocity space $\boldsymbol{\xi}$ for the generic moment Q, an evolution equation for the moments of Q is obtained,

$$\partial_t \langle Q\rangle - \langle \partial_t Q\rangle + \partial_i \langle \xi_i Q\rangle - \langle \xi_i \partial_i Q\rangle - \langle F_i \partial_{\xi_i} Q\rangle = I\,[Q]\,, \tag{9}$$

where $\langle\cdot\rangle = \int f \cdot d^3\xi$, and $[Q] = \int Q\,(1/\tau)\left(f^0 - f\right) d^3\xi$. The body force in the Boltzmann equation will be the Lorentz force,

$$F_k = (\mathbf{J} \times \mathbf{B})_k = \left(\frac{e}{m_e}\boldsymbol{\xi} \times \mathbf{B}\right)_k\,, \tag{10}$$

where we employ the constitutive relationship $\mathbf{J} = \frac{e}{m_e}\boldsymbol{\xi}$. Following this with the Chapman-Enskog expansion, with ϵ as the Knudsen number,

$$f = f^{(0)} + \epsilon^1 f^{(1)} + \epsilon^2 f^{(2)} + \cdots\,,$$
$$\partial_t = \partial_{t_0} + \epsilon^1 \partial_{t_1} + \epsilon^2 \partial_{t_2} + \cdots\,,$$

we arrive at the macroscopic equations,

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0 \tag{11}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \boldsymbol{\nabla} \cdot \left[\rho \mathbf{u}\mathbf{u} + \underline{\underline{\boldsymbol{\Phi}}} + \underline{\underline{\mathbf{I}}} p\right] = \langle \mathbf{F}\rangle^0 = q_e n_e\, \mathbf{u} \times \mathbf{B} \tag{12}$$

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla} \cdot \left[\mathbf{U}(E+p) + \boldsymbol{\nabla} \cdot \mathbf{q} + \mathbf{u} \cdot \underline{\underline{\boldsymbol{\Phi}}}\right] = 0 \tag{13}$$

Where $\langle \mathbf{F}\rangle^0 = \int f^{(0)} \mathbf{F} d^3\xi$. Writing the body force term in the Boltzmann equation as $\mathbf{F} \cdot \boldsymbol{\nabla}_\xi f = \mathbf{F} \cdot \boldsymbol{\nabla}_\xi f^{(0)}$ recovers the macroscopic body force term. It is clear from this that the body force in the Boltzmann equation has first order influence in the NS equation. We can investigate the effect on the transport coefficients analyzing the $f^{(1)}$ term explicitly,

$$\begin{aligned} -\nu \frac{f^{(1)}}{f^{(0)}} = \frac{1}{\rho}\left(-\rho \boldsymbol{\nabla} \cdot \mathbf{u} + c_j \frac{\partial \rho}{\partial x_j}\right) + \frac{\beta}{T}\left(\frac{3}{2}\beta^{-1} - c^2\right)\left(\frac{2}{3} T \boldsymbol{\nabla} \cdot \mathbf{u} - c_j \frac{\partial T}{\partial x_j}\right) \\ -2\beta c_n \left[\frac{1}{\rho}\frac{\partial p}{\partial x_n} + \left(F_n - \frac{1}{\rho}\langle F_n\rangle\right) - c_k \frac{\partial u_n}{\partial x_k}\right]\,, \end{aligned} \tag{14}$$

where $\mathbf{c} = \boldsymbol{\xi} - \mathbf{u}$ is the peculiar velocity. The term that depends on the body force will cancel,

$$c_n \left(F_n - \frac{1}{\rho} \langle F_n \rangle \right) = 0\,. \tag{15}$$

With this, $f^{(1)}$ does not depend on the body force,

$$f^{(1)} = -\tau \left[\frac{1}{kT} \left(c_j c_k - \frac{c^2}{3} \delta_{jk} \right) \frac{\partial u_j}{\partial x_k} - \left(\frac{1}{2kT} c^2 - \frac{5}{2} \right) \frac{c_j}{T} \frac{\partial T}{\partial x_j} \right] f^{(0)}\,, \tag{16}$$

and the transport coefficients do not depend on the magnetic field,

$$\Phi^{(1)}_{jk} = \int f^{(1)} c_j c_k d^{\xi} = \tau p\,, \tag{17}$$

$$q^{(1)}_k = \frac{1}{2} \int f^{(1)} c^2 c_k d^3\xi = \lambda_0 \partial_k T\,, \tag{18}$$

where $\lambda_0 = \tau \frac{5}{2} kp$, where k is the Boltzmann constant.

The Boltzmann equation is a flux equation in phase space where the physical information spreads through collisions. The transport coefficients that are obtained with the Chapman-Enskog expansion give us information about how the viscosity and termal conductivity are affected through collisions in the fluid. The influence of the magnetic field on the fluid is not spread by collisions.

4. INFLUENCE OF MAGNETIC FIELD ON THE TRANSPORT COEFFICIENTS

In the last section it was shown that the transport coefficients obtained via Chapman-Enskog expansion do not depend on the magnetic field. When a magnetic field is applied to the fluid, all particles are subjected to it at the same time. As a result, the particle undergoes a circular motion with the cyclotron frequency $\omega_c \sim |\mathbf{B}|$. If the cyclotron frequency is the same order of magnitude as the collision frequency, the particle experiments a diffusion motion in the direction given by $\boldsymbol{\xi} \times \mathbf{B}$. This is known as the Hall effect and breaks the symmetry of the transport coefficients. We analyze this effect on the thermal conductivity. For this, we make $Q = c^2 c_k$ in Equation 9, which gives us a transport equation for q_k,

$$\begin{aligned}\partial_t q_k - (p\,\delta_{jk} + P_{jk} + \frac{3}{2} p\,\delta_{jk}) \frac{1}{\rho} \partial_n (p\,\delta_{nj} + P_{nj}) + \partial_j (\frac{5}{2} kTp\delta_{jk} + \frac{7}{2} kTP_{jk} + u_j q_k) \\ + \frac{2}{5}(q_n \delta_{jk} + q_j \delta_{nk} + q_k \delta_{nj}) \partial_n u_j + q_j \partial_j u_k + (\mathbf{q} \times \mathbf{B})_k = -\nu q_k\,,\end{aligned} \tag{19}$$

where,

$$P_{ij} = \int f c_i c_j d^3\xi - p\delta_{ij}\,. \tag{20}$$

Performing an asymptotic expansion of P_{jk} and q_k in terms of the collision frequency ν, we obtain,

$$P_{jk} = Z^0_{jk} + \frac{Z^1_{jk}}{\nu} + \frac{Z^2_{jk}}{\nu^2} + \cdots\,, \tag{21}$$

$$q_k = D^0_k + \frac{D^1_k}{\nu} + \frac{D^2_k}{\nu^2} + \cdots\,. \tag{22}$$

Under a cartesian coordinate system, we consider the flow of a fluid in the x-direction with an external magnetic field applied in the z-drection. If $\omega_c \sim \nu$, it is possible to show that,

$$q_k = \frac{\omega_c}{\nu} (\mathbf{q} \times \hat{\mathbf{e}}_{\mathbf{z}})_k - \lambda_0 \frac{\partial T}{\partial x_k}\,, \tag{23}$$

where $\lambda_0 = \frac{5pk}{2\nu}$. The heat flux vector can be written as,

$$\mathbf{q} = \underline{\underline{\boldsymbol{\lambda}}} \cdot \boldsymbol{\nabla} T\,, \tag{24}$$

where,

$$\underline{\underline{\boldsymbol{\lambda}}} = \begin{bmatrix} \lambda_\perp & \lambda_{||} & 0 \\ -\lambda_{||} & \lambda_\perp & 0 \\ 0 & 0 & -\lambda_0 \end{bmatrix}\,, \tag{25}$$

$$\lambda_\perp \equiv \frac{\lambda_0 \nu^2}{\nu^2 + \omega_c}\,, \tag{26}$$

$$\lambda_{||} \equiv \frac{\lambda_0 \nu \omega_c}{\nu^2 + \omega_c}\,. \tag{27}$$

This highlights the thermal Hall effect. For $\omega_c/\nu \ll 1$, Fourier's heat conduction law is recovered,

$$q_k = \lambda_{kj} \left(\boldsymbol{\nabla} T\right)_j \approx -\lambda_0 \left(\boldsymbol{\nabla} T\right)_k \,. \tag{28}$$

5. OVERVIEW OF GKM AND THE CONTRIBUTION OF BODY FORCE IN THE BOLTZMANN EQUATION

At its core, GKM (Xu *et al.*, 1995; Xu, 2001) is a finite-volume numerical scheme for solving the Navier-Stokes equations. It is a hybridization of fluid and kinetic methods originally developed for shock capturing in high Mach number flows, but has since been shown to be effective even at weakly compressible limits (Kerimo and Girimaji, 2007). The "fluid" aspect of the method involves the macroscopic properties as cell volume-averaged quantities that are evolved in time by computing fluxes at cell interfaces. The "kinetic" feature of the method is related to how these fluxes are calculated, which is by explicitly taking moments of a particle distribution function. The full derivation of the numerical scheme for solving the Navier-Stokes equations by the gas-kinetic method is given by Xu (2001). In general, there are three stages to the method, which include reconstruction, gas evolution, and projection. The governing equation for GKM can be written as the following:

$$\frac{\partial}{\partial t} \int \begin{pmatrix} \rho \\ \rho \mathbf{U} \\ E \end{pmatrix} d\Omega + \oint \begin{pmatrix} \mathbf{F}_\rho \\ \mathbf{F}_{\rho \mathbf{U}} \\ \mathbf{F}_E \end{pmatrix} \cdot d\mathbf{A} = 0 \tag{29}$$

Equation 29 is simply the finite-volume formulation of the general conservation laws, where a macroscopic property (i.e. density ρ, momentum $\rho\mathbf{U}$, and energy E) in a control volume (Ω) changes in time due to a given flux ($\mathbf{F} = \int f\xi(1, \xi, \xi^2/2)^T d\xi$) through the control volume surface (A). During the reconstruction stage, the values of the cell-center macroscopic variables are used to create piecewise-continuous functions of these variables for all of the cells in a given computational domain. In other words, the cell-centered values are extrapolated and connected to other cell centers in a piecewise-continuous manner using limiters. For this step, the MGKM code utilizes the weighted essentially non-oscillatory (WENO) limiter, which is commonly used in shock capturing schemes (Kumar *et al.*, 2013).

The gas evolution stage, wherein the inter-cell fluxes are calculated, represents the true kinetic aspect of GKM. For simplicity, only the one-dimensional formulation is presented here, i.e. in the U_1-direction, however in three-dimensions the fluxes are calculated in a similar manner (see e.g. Kumar *et al.* (2013)). The flux in density F_ρ, momentum $F_{\rho U_1}$, and energy F_E across the $i + 1/2$ cell interface is given by:

$$\begin{pmatrix} F_\rho \\ F_{\rho U_1} \\ F_E \end{pmatrix} = \int_{-\infty}^{\infty} u_1 \begin{pmatrix} 1 \\ u_1 \\ \frac{1}{2}(u_1^2 + \xi^2) \end{pmatrix} f(x_{i+\frac{1}{2}}, t, u_1, \xi)\, d\Xi, \tag{30}$$

where $d\Xi = du_1 d\xi$ is the volume element in phase space, U_1 is the macroscopic fluid velocity, and u_1 is the microscopic particle velocity. The variable ξ represents the molecular internal degrees of freedom and is specific to a particular gas depending on the ratio of specific heats. The non-equilibrium particle distribution function, f, is explicitly evaluated at the cell interface by approximating the integral solution to the Boltzmann Bhatnagar-Gross-Krook (BGK) equation, which at the $i + 1/2$ cell interface is given as the following:

$$f(x_{i+\frac{1}{2}}, t, u_1, \xi) = \frac{1}{\tau} \int_0^t f^{(0)}(x_1', t', u_1, \xi) e^{-(t-t')/\tau}\, dt' + e^{-t/\tau} f_0(x_{i+\frac{1}{2}} - u_1 t). \tag{31}$$

In equation 31, τ is the collisional relaxation time, and the only unknowns are $f^{(0)}$, which is the equilibrium distribution function, and f_0, which is the initial gas distribution function at the beginning of each time step. It can be shown that both $f^{(0)}$ and f_0 can be uniquely approximated from the macroscopic variables on both the left and right sides of the cell interface. Once f has been updated fluxes are calculated and the projection stage is performed in order to update the cell center macroscopic values. For the one-dimensional case, the macroscopic variables at time step $n + 1$ are updated according to,

$$\begin{pmatrix} \rho \\ \rho U_1 \\ E \end{pmatrix}^{n+1} = \begin{pmatrix} \rho \\ \rho U_1 \\ E \end{pmatrix}^{n} - \frac{1}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} \int_t^{t+\triangle t} \left[\begin{pmatrix} F_\rho \\ F_{\rho U_1} \\ F_E \end{pmatrix}_{i+\frac{1}{2}} - \begin{pmatrix} F_\rho \\ F_{\rho U_1} \\ F_E \end{pmatrix}_{i-\frac{1}{2}} \right] dt. \tag{32}$$

6. CONCLUSIONS AND FUTURE WORK

In the current implementation of GKM, the non-equilibrium particle distribution function, f, is calculated from Boltzmann equation without the external force term $\mathbf{F} \cdot \boldsymbol{\nabla}_\xi f$. However, this term is relevant to the MHD equations. The

Lorentz force $\mathbf{J} \times \mathbf{B}$ is implemented in GKM only in the volume integral of Equation 29. For a more accurate GKM implementation, it is necessary consider the influence of the Lorentz force on the flux terms that are calculated by Equation 31 at the volume interface. Current work is directed in inserting the Lorentz force as an external body force in the Boltzmann equation in order to get the flux contribution at the cell volume interface. With this we will recover the effect of the magnetic field in the breaking of symmetry of the transport coefficients, as was demonstrated in §3.

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