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Uniformization of the density in reacting magnetohydrodynamic flows

Manuel Núñez

Departamento de Análisis Matemático, Universidad de Valladolid, 47005 Valladolid, Spain

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ABSTRACT

Ionization and recombination provide a transfer between species in a partially ionized plasma. These phenomena modify the continuity equation for each species by linking them together in a common system. The consequences are specially clear when the velocities of ions and neutrals coincide and the flow is weakly compressible: the densities along each trajectory tend to a definite limit depending only on the initial total density and not on the ion/neutral rate. For the general case a weaker global estimate on the final rate between species may be proved.

1. Introduction

Multifluid MHD plasmas are ubiquitous in several astrophysical settings, such as interstellar and protogalactic clouds; their importance in astrophysics has been known for a long time [1]. Their evolution is described by separate kinetic equations for each species, linked together by collisional terms and appropriate forcings, such as the Lorentz force for charged species. In addition the magnetic field is governed by the induction equation. The whole system is so complex that several simplifications have been introduced in the many models studied so far: in the absence of neutrals a two-fluid flow is appropriate for magnetic reconnection [2–4]; usually electron inertia and advective terms are also neglected. When neutrals are present, the following assumptions are often made: quasineutrality of the whole plasma; state equation of ideal gases; comparable ion and electron temperatures. Thus, making zero the quotient between the electron and ion masses, and neglecting heat conduction, a working model is obtained [5–7]. A more extreme simplification is the strong coupling approximation [8–12]. When the effects of pressure may be ignored, an existence theorem may be proved [13]. The total energy evolution equation shows the presence of dissipative collisional terms of the forms $-\nu_{ij}|\mathbf{v}_i-\mathbf{v}_j|^2$, where $\mathbf{v}_i$ is the velocity of the ith species and ν_{ij} is a collisional coefficient [14]. Therefore energy losses are minimized when the velocities of species are similar, and this is the limit state in the absence of separate forcings: in certain instances this coupling of flows is very fast [8]. This justifies our later hypothesis that the velocities of ions and neutrals coincide.

An effect not often included in simulations concerns the possibility of chemical reactions within the plasma. Specifically we consider ionization, which converts neutrals into ions, and ion–electron recombination, which converts ions into neutrals. Since the first reaction depends on an external effect (e.g. photoionization), it involves separate particles, so the rate of creation of ions is proportional to the density of neutrals. Recombination, by contrast, needs pairs ion–electron, assumed to have the same number density. Hence the rate of creation of neutrals should be proportional to the square of the density of ions [15,16]. Therefore, if we denote by ρ_i the density of ions, by ρ_n the one of neutrals, the mass balance equation becomes

$$\frac{\partial\rho_i}{\partial t}+\nabla\cdot(\rho_i\mathbf{v}_i)=\zeta\rho_n-\alpha\rho_i^2, \tag{1}$$

$$\frac{\partial\rho_n}{\partial t}+\nabla\cdot(\rho_n\mathbf{v}_n)=-\zeta\rho_n+\alpha\rho_i^2. \tag{2}$$

ζ is the ionization coefficient and α the recombination one; both will be assumed constant (see [5,17]; notice that there is a typographical error in Eqs. (37) and (38) of [5], where $\zeta\rho_i$ is written instead of $\zeta\rho_n$). We intend to study the limit of both densities under these continuity equations. In the classical case, when there is no interchange of species and the right-hand side of both (1) and (2) is zero, each separate density evolves along the corresponding streamline according to the ordinary differential equation

$$\frac{D\rho_\alpha}{Dt}=-\rho_\alpha\nabla\cdot\mathbf{v}_\alpha, \tag{3}$$

E-mail address: mnjmhd@am.uva.es.

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where D/Dt represents the Lagrangian derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}_\alpha \cdot \nabla.$$

The meaning of (3) is simply that the mass along an evolving volume must be kept constant. Obviously there is no connection between the final densities for both species.

Some instances where recombination and ionization effects cannot be ignored include the formation of current sheets in the interstellar medium [9], interstellar shock waves [16,18], and the ionosphere–thermosphere system on Earth [5]. In [8] it is asserted that for dense molecular clouds the balance occurs when $\rho_i \propto \rho_n^{1/2}$, but we will see that this is not the general case.

2. The static case

Assume that both the ions and the neutrals are at rest. This would imply in the classical case of non-reacting plasmas that the density is stationary as well, but now the reactions within the fluid change this situation. We will see that the densities at every point converge exponentially to a definite limit, depending only on the total (sum of ion and neutral) density at the instant zero. The original ratio of ion and neutral densities is irrelevant: the equilibrium will not depend on it. Thus, if e.g. the total density is constant at every point of the fluid, the ionic and neutral densities will also tend to be constant and original irregularities in the distribution will disappear at an exponential rate. By contrast, in the absence of reactive terms, the original distribution would not change and there could exist stratifications of density.

Eqs. (1) and (2) are now

$$\frac{\partial \rho_i}{\partial t} = \zeta\rho_n - \alpha\rho_i^2, \tag{4}$$

$$\frac{\partial \rho_n}{\partial t} = -\zeta\rho_n + \alpha\rho_i^2, \tag{5}$$

from which immediately follow that the total density $\rho_i + \rho_n$ remains constant through time and therefore is a function of the point. Let us fix a point $\mathbf{x}$ in the domain Ω and denote $C := \rho_i(0,\mathbf{x}) + \rho_n(0,\mathbf{x})$. We will omit henceforth the reference to $\mathbf{x}$, and denote for simplicity ρ_i by ρ. We may write (4) as

$$\frac{\partial \rho}{\partial t} = \zeta C - \zeta\rho - \alpha\rho^2. \tag{6}$$

This is a Riccati equation, and a very simple one: since C, ζ, and α are all constant for the fixed point $\mathbf{x}$, it has two obvious solutions: the stationary ones. Those are given by

$$\rho = -\frac{\zeta}{2\alpha} \pm \sqrt{\frac{\zeta^2}{4\alpha^2} + \frac{\zeta C}{\alpha}}. \tag{7}$$

Since a density must be positive, the only relevant solution is

$$\rho_* = -\frac{\zeta}{2\alpha} + \sqrt{\frac{\zeta^2}{4\alpha^2} + \frac{\zeta C}{\alpha}}, \tag{8}$$

which indeed satisfies $0 < \rho_* < C$ for $C > 0$, as it should be. For $C = 0$ always $\rho_* = 0$, and in fact $\rho_i = \rho_n = 0$; this vacuum case is obviously uninteresting. It is well known that the change of variables $\rho = \rho_* + 1/z$ will change the equation into a linear one for z. This turns out to be

$$\dot{z} = (2\alpha\rho_* + \zeta)z + \alpha, \tag{9}$$

whose solution, after denoting $\mu = 2\alpha\rho_* + \zeta$, is

$$z(t) = e^{\mu t}z(0) + \frac{\alpha}{\mu}\left(e^{\mu t} - 1\right), \tag{10}$$

which shows $|\rho(t) - \rho_*| \leqslant e^{-\mu t}|\rho(0) - \rho_*|$. Since $\mu > \zeta$, this proves the exponential convergence of ρ to ρ_*, uniform for all points of the domain. Moreover,

$$z(t) - z(0) = \left(e^{\mu t} - 1\right)\left(z(0) + \frac{\alpha}{\mu}\right). \tag{11}$$

Thus, if $\rho(0) > \rho_*$, $z(0) > 0$ and *a fortiori* $z(0) + \alpha/\mu > 0$; hence $z(t) - z(0)$ increases to ∞, so that $\rho(t)$ decreases to ρ_*.

If $\rho(0) < \rho_*$, $2\rho_* > \rho_* - \rho(0)$, which implies

$$z(0) + \frac{\alpha}{\mu} < \frac{1}{\rho(0) - \rho_*} + \frac{1}{2\rho_*} < 0.$$

Therefore $z(t) - z(0)$ decreases to $-\infty$, which means that $\rho(t)$ increases to ρ_*. Thus the density converges exponentially and monotonically to the equilibrium state ρ_*. Needless to say, $\rho_n = C - \rho$ behaves exactly in the same way, converging to $C - \rho_*$.

3. Incompressible flows

When $\mathbf{v}_i = \mathbf{v}_n$ and both represent an incompressible flow, $\nabla \cdot \mathbf{v}_i = 0$, the equations of continuity may be written as

$$\frac{D\rho_i}{Dt} = \zeta\rho_n - \alpha\rho_i^2, \tag{12}$$

$$\frac{D\rho_n}{Dt} = -\zeta\rho_n + \alpha\rho_i^2, \tag{13}$$

where, if $\boldsymbol{\xi}(t,\mathbf{a})$ represents the fluid trajectory such that $\boldsymbol{\xi}(0,\mathbf{a}) = \mathbf{a}$, the Lagrangian derivative D/Dt satisfies

$$\left(\frac{D\rho}{Dt}\right)\big(t,\boldsymbol{\xi}(t,\mathbf{a})\big) = \frac{d}{dt}\rho\big(t,\boldsymbol{\xi}(t,\mathbf{a})\big).$$

The same arguments of the previous section may be applied to the function $t \to \rho_i(t,\boldsymbol{\xi}(t,\mathbf{a}))$, and we find

$$\lim_{t\to\infty}\rho_i\big(t,\boldsymbol{\xi}(t,\mathbf{a})\big) = \rho_*(\mathbf{a}), \tag{14}$$

where

$$\rho_*(\mathbf{a}) = -\frac{\zeta}{2\alpha} + \sqrt{\frac{\zeta^2}{4\alpha^2} + \frac{\zeta}{\alpha}\big(\rho_i(0,\mathbf{a}) + \rho_n(0,\mathbf{a})\big)}. \tag{15}$$

The ion density increases if $\rho_i(0,\mathbf{a}) < \rho_*(\mathbf{a})$, decreases otherwise. Notice that $\boldsymbol{\xi}(t,\mathbf{a})$ does not need to have any limit when $t \to \infty$, so we cannot predict $\lim_{t\to\infty}\rho_i(t,\mathbf{b})$ for fixed $\mathbf{b}$. However, if e.g. the total density is constant in the whole domain, the final rate ion/neutral is constant everywhere, and the convergence is exponential.

4. Weakly compressible flows

The presence of the viscosity complicates the analysis. Instead of (12) and (13), we have now

$$\frac{D\rho_i}{Dt} = \zeta\rho_n - \alpha\rho_i^2 + f\rho_i, \tag{16}$$

$$\frac{D\rho_n}{Dt} = -\zeta\rho_n + \alpha\rho_i^2 + f\rho_n, \tag{17}$$

where $f = -\nabla \cdot \mathbf{v}_i$. By adding both equations we obtain

$$\frac{D}{Dt}(\rho_i + \rho_n) = f(\rho_i + \rho_n). \tag{18}$$

This is a linear scalar differential equation along the trajectory. As such its classical solution is

$$(\rho_i + \rho_n)\big(t,\boldsymbol{\xi}(t,\mathbf{a})\big) = (\rho_i + \rho_n)(0,\mathbf{a})\exp\left(\int_0^t f\big(s,\boldsymbol{\xi}(s,\mathbf{a})\big)\,ds\right). \tag{19}$$

Let us fix the initial point $\mathbf{a}$, and consider $\rho(t) = \rho_i(t, \boldsymbol{\xi}(t, \mathbf{a}))$. Let $C = (\rho_i + \rho_n)(0, \mathbf{a})$,

$$F(t) = \exp\left(\int_0^t f\left(s, \boldsymbol{\xi}(s, \mathbf{a})\right) ds\right).$$

Then $\rho_n = CF - \rho$, and ρ satisfies

$$\dot{\rho} = -\alpha\rho^2 + (f - \zeta)\rho + \zeta CF. \tag{20}$$

This is again a Riccati equation, but without constant coefficients. Since we cannot find a particular solution, we will convert it into a standard type and use comparison theorems. Let us define x by

$$\rho = \frac{x}{\alpha} + \frac{f - \zeta}{2\alpha}. \tag{21}$$

A simple calculation shows that x satisfies

$$\dot{x} + x^2 = -\frac{\dot{x}}{2} + \frac{1}{4}(f - \zeta)^2 + \alpha\zeta CF. \tag{22}$$

Notice that for $f = 0$, $F = 1$ and (22) reduces to

$$\dot{x} + x^2 = \frac{1}{4}\zeta^2 + \alpha\zeta C. \tag{23}$$

We need a comparison theorem to estimate the difference between the solutions to (22) and (23); the last one is equivalent to the one studied in the previous section. These theorems are classical and may be found e.g. in [19]. However, since the proof is so simple, we will recall the result to make the paper reasonably self-contained.

Lemma 1. *Let $a \in (0, 1)$, $0 < ak_1(t) < k_2(t) < (1/a)k_1(t)$. Let x_i be one solution of $\dot{x}_i + x^2 = k_i(t)$. If $ax_1(0) < x_2(0) < (1/a)x_1(0)$, then $ax_1(t) < x_2(t) < (1/a)x_1(t)$ for all $t \in (0, \infty)$.*

Proof. Let us show first that for $k_i > 0$ and $x_i(0) > 0$, the solution is always positive. Otherwise, at the first point t_0 where $x_i(t_0) = 0$, the solution should be decreasing, but the equation yields $\dot{x}_i(t_0) = k_i(t_0) > 0$. Moreover, since the solution cannot grow faster than the primitive of k_i, if this function is e.g. continuous the solution exists for all time. To prove the lemma, we need to show that $x_2(t)/x_1(t) > a$ for all time. Since this occurs at $t = 0$, let t_1 be the first point where $x_2(t_1)/x_1(t_1) = a$. There the quotient should be decreasing, but

$$\frac{d}{dt}\left(\frac{x_2}{x_1}\right) = \frac{1}{x_1^2}(\dot{x}_2 x_1 - \dot{x}_1 x_2),$$

and

$$\begin{aligned}
\dot{x}_2 x_1 - \dot{x}_1 x_2 &= \left(k_2 - x_2^2\right)x_1 - \left(k_1 - x_1^2\right)x_2 \\
&= k_2 x_1 - k_1 x_2 + x_1 x_2 (x_1 - x_2) \\
&> ak_1 x_1 - k_1 x_2 + x_1 x_2 (x_1 - x_2) \\
&= k_1(ax_1 - x_2) + x_1 x_2 (x_1 - x_2).
\end{aligned}$$

At the point t_1, we have $(ax_1 - x_2)(t_1) = 0$, so that

$$\frac{d}{dt}\left(\frac{x_2}{x_1}\right)(t_1) > a(1 - a)x_1(t_1) > 0,$$

so that the quotient is increasing, which contradicts the hypothesis. The second inequality follows by considering $\bar{k}_1 = k_2$, $\bar{k}_2 = (1/a)k_1$.

In our case, we take

$$k_1 = \frac{1}{4}\zeta^2 + \alpha\zeta C, \tag{24}$$

$$k_2 = -\frac{\dot{x}}{2} + \frac{1}{4}(f - \zeta)^2 + \alpha\zeta CF \tag{25}$$

and

$$x_1(0) = x_2(0) = \alpha\rho(0) + \frac{1}{2}\left(\zeta - f(0)\right).$$

If f, $\dot{f}$ are small enough (or ζ large enough) so that there exist $a \in (0, 1)$ satisfying $x_1(0) > 0$, $ak_1 < k_2 < (1/a)k_1$, by the previous lemma $ax_1(t) < x_2(t) < (1/a)x_1(t)$ for all time. Now, x_1 corresponds to the solution found in the previous section: it tends exponentially and monotonically to $\alpha\rho_*(\mathbf{a}) + \zeta/2$. Therefore $\rho(t, \boldsymbol{\xi}(t, \mathbf{a}))$ also tends exponentially to the limit $\rho_*(\mathbf{a})$ of Eq. (15),

$$\rho_*(\mathbf{a}) = -\frac{\zeta}{2\alpha} + \sqrt{\frac{\zeta^2}{4\alpha^2} + \frac{\zeta}{\alpha}\left(\rho_i(0, \mathbf{a}) + \rho_n(0, \mathbf{a})\right)},$$

although we cannot guarantee monotonous convergence.

5. The general case

When the velocities of ions and neutrals are different, or the divergence of the flow is uncontrollable, we cannot find pointwise estimates: the continuity equations represent differentials along different trajectories. Nonetheless, some bounds on the mean densities may be established. Assume that the domain is closed by both flows, so that $\mathbf{v}_i \cdot \mathbf{n}|_{\partial\Omega} = \mathbf{v}_n \cdot \mathbf{n}|_{\partial\Omega} = 0$. Then integration of $\nabla \cdot \mathbf{v}_j$ in Ω yields the value zero. Hence

$$\frac{d}{dt}\int_\Omega \rho_i \, dV = \zeta \int_\Omega \rho_n \, dV - \alpha \int_\Omega \rho_i^2 \, dV, \tag{26}$$

$$\frac{d}{dt}\int_\Omega \rho_i \, dV = -\zeta \int_\Omega \rho_n \, dV + \alpha \int_\Omega \rho_i^2 \, dV. \tag{27}$$

This naturally implies that the total mass M is a constant. M is the sum of the ion M_i and neutral M_n masses, which are not constant: the definition is obviously

$$M_j = \int_\Omega \rho_j \, dV.$$

(26) and (27) reduce to

$$\frac{dM_i}{dt} = \zeta M - \zeta M_i - \alpha \int_\Omega \rho_i^2 \, dV. \tag{28}$$

Let V denote the volume of Ω. By the inequality of Cauchy–Schwarz,

$$M_i \leqslant V^{1/2}\left(\int_\Omega \rho_i^2 \, dV\right)^{1/2}. \tag{29}$$

Therefore

$$\frac{dM_i}{dt} \leqslant \zeta M - \zeta M_i - \alpha V^{-1} M_i^2. \tag{30}$$

We know that the equation

$$\dot{x} = \zeta M - \zeta x - \alpha V^{-1} x^2, \tag{31}$$

has a unique positive stationary solution

$$M_{i*} = -\frac{\zeta V}{2\alpha} + \sqrt{\frac{\zeta^2 V^2}{4\alpha^2} + \frac{\zeta M V}{\alpha}}. \tag{32}$$

Notice that $M_{i*} < M$, as expected. Any other solution of (31) tends to M_{i*} exponentially for any positive initial condition $x(0) = M_i(0)$. Since $M_i(t)$ satisfies inequality (30), $M_i(t) \leqslant x(t)$ for all time, and therefore

$$\limsup_{t\to\infty} M_i(t) \leqslant M_{i*}. \tag{33}$$

To obtain a lower estimate, we need an upper bound on the ion density, $\rho_i \leqslant P$. Then

$$\int_\Omega \rho_i^2\,dV \leqslant P\int_\Omega \rho_i\,dV = PM_i. \tag{34}$$

Therefore (28) implies

$$\frac{dM_i}{dt} \geqslant \zeta M - (\zeta + \alpha P)M_i. \tag{35}$$

Any solution of the linear equation

$$\dot y = \zeta M - (\zeta + \alpha P)y, \tag{36}$$

tends exponentially to $m_{i*} = \zeta M/(\zeta + \alpha P)$ when $t \to \infty$. Therefore

$$m_{i*} \leqslant \liminf_{t\to\infty} M_i(t). \tag{37}$$

Notice that these estimates cannot be improved in general, since for ρ_i constant in Ω (although depending on time) the inequalities (30) and (35) become equalities. We conclude

$$\frac{\zeta M}{\zeta + \alpha P} \leqslant \liminf_{t\to\infty} M_i(t) \leqslant \limsup_{t\to\infty} M_i(t) \leqslant -\frac{\zeta V}{2\alpha} + \sqrt{\frac{\zeta^2 V^2}{4\alpha^2} + \frac{\zeta M V}{\alpha}}. \tag{38}$$

Hence the final ion (and therefore neutral) mass is bounded *a priori* by certain quantities depending on the coefficients of ionization and recombination. Obviously, an analogous bound holds for the neutral mass.

6. Summary

The dual effects of ionization and recombination in a plasma composed of neutral particles, ions and electrons provide an interchange between species which modifies the continuity equations satisfied by the density of each species. It has been often assumed that these densities reach an equilibrium state, but this is not clear in general. In the static case, the equilibrium is in principle different for each point, since it depends on the initial total density there, plus the ionization and recombination coefficients; it is reached exponentially fast. This may be extended to the situation where ions and electrons share the same velocity, which is the limit state when collisions act for a long time in the plasma. In this case we need the fluid to be incompressible, or weakly compressible by comparison to the ionization coefficient: results analogous to the static ones may be proved for each trajectory, although the trajectory itself does not need to tend to any point. Since incompressibility, even approximate, is highly unusual in astrophysical plasmas, a study of the general case is necessary; this also includes the case where the trajectories of ions and neutrals are different. The study is performed by means of certain integral inequalities: the results are obviously less precise than those previously obtained, but upper and lower bounds on the asymptotic limits of the masses of each species may be found. These bounds depend only on a priori quantities and the ionization and recombination coefficients.

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