ACT I. Scene 5: Energy Conservation & Thermodynamics

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1. Introduction

The internal energy density of an aggregate of particles in the continuum fluid limit is a very delicate thing. Like the coefficient of viscosity, the dielectric properties of the fluid, the opacity and emissivity, one might anticipate that it requires some definite working knowledge of the microphysics. That fact that it can be handled, and in fact even computed, without such detailed knowledge is a somewhat curious and quite remarkable fact. And it underscores the power and generality of the subject of thermodynamics—a topic which contains only three laws (one of which is more of a calibration of a scale than an actual law) and which has none-the-less managed to fill volumes and volumes of books and treatises and journals for almost two centuries.

2. Perhaps Way Too Much Thermodynamics

The first law of thermodynamics, and the only one we will have much need for, is simply a statement of the conservation of energy for a system. It is usually framed in the context of vessels or boxes of some largely unspecified material which have a volume V [dimensions: cm³] and contain a certain amount of energy E [dimensions: gm cm² sec⁻² — or ergs]. One is allowed to add or extract some heat Q [dimensions: ergs] from the box by various means, and to apply forces to change the volume of the box which exerts an outward pressure p [dimensions: gm cm⁻¹ sec⁻²]. Then the first law says

$$\delta Q = dE + pdV$$

the heat added to the material in the box ($\delta Q \ge 0$) can go into increasing the energy contained in the box and/or supplying energy for the box to do work on its surroundings if it expands $dV \ge 0$. Thats it.

I've put a δ in front of the Q because we recognize this as a Pfaffian and we don't actually know if it is the total differential of some scalar function. For this to be so, recall that we would need

$$\frac{\partial p}{\partial E} = \frac{\partial 1}{\partial V} = 0 \; .$$

The chances that the pressure of the unspecified contents of the box might be independent of the energy contained in the box seems pretty remote. So, we know from Pfaff's Theorem that there is an integrating factor that will convert δQ to a dS, say, and we call that integrating factor the absolute temperature T [dimensions: deg K — degrees Kelvin]:

$$dS = \frac{1}{T}\delta Q = \frac{1}{T}dE + \frac{p}{T}dV$$

We call S [dimensions: erg K^{-1}] the entropy. And by design, we also know that

$$\frac{\partial}{\partial V}\frac{1}{T} = \frac{\partial}{\partial E}\frac{p}{T}$$

because, S = S(E, V).

The box contains a certain mass of material, say M [dimensions: gm], and so we can divide Q, S, E and V by the constant M to get q, s, e and v, respectively. And the equivalent first law

$$de = Tds - pdv$$

now reckoned on a *per unit mass* basis. This completely equivalent way of looking at this system turns out to be more portable for our purposes. And since v is the volume per unit mass, it's reciprocal is ρ the mass per unit volume, and ρe is the energy per unit volume, or, what looks like a very reasonable approximation to the internal energy density of the material in the box. Which is what, after all, we are incrested in!

Notice that the pressure and the temperature do not end up being replaced by small letters (of course, the pressure already is a small letter, but you get the point) but remain the same. While we are thinking of all these quantities as thermodynamic variables or state parameters, p and T are extensible in the sense that they just don't care how much mass is actually in the box, or how big the box happens to be, in this sense they characterize the total system viewed as a whole, not merely as the sum of some parts. This makes them quite special as we shall see. As we noted earlier in the discussion of Euler's Equation, the fact that p is a constant for an entire box means that it is in mechanical equilibrium, there are no large scale flow fields present because there are no pressure gradients. The fact that T is a constant means that the box is also in *thermal equilibrium*, there are no temperature gradients and conduction of heat within the box. Indeed part of the reason thermodynamics will turn out to be so effective is this implicit assumption that the system in question, no matter what it happens to be, has settled down into mechanical and thermal equilibrium.

Of course de is a total differential, so Pfaff tells us that

$$T(s,v) = \left(\frac{\partial e}{\partial s}\right)_v$$
, and $p(s,v) = -\left(\frac{\partial e}{\partial v}\right)_s = \rho^2 \left(\frac{\partial e}{\partial \rho}\right)_s$,

where, since e = e(s, v), the first partial derivative is taken at constant specific volume v or density ρ , while the second is taken at constant entropy. So these two extensive quantities that represent some wholistic description of the system inside the box are the first partial derivatives of the energy per unit mass with respect to the specific entropy and the specific volume. And in principle, they too obviously can depend upon s and v. Therefore:

$$dT = Zds - Ydi$$

$$dp = Yds - Xdv$$

where

$$X(s,v) \equiv \frac{\partial^2 e}{\partial v^2}$$
, $Y(s,v) \equiv -\frac{\partial^2 e}{\partial s \partial v}$, $Z(s,v) \equiv \frac{\partial^2 e}{\partial s^2}$

The fact that Y appears twice in these equations is because

$$\left(\frac{\partial p}{\partial s}\right)_v + \left(\frac{\partial T}{\partial v}\right)_s = 0$$

i.e., de is a total differential.

While the state of a system in thermal and mechanical equilibrium is completely specified by (s, v), the behavior of the system as one (slowly) pushes on the walls to change the volume, or (gradually) adds or extracts heat, is specified by the three functions X, Y, Z. So they describe how the system gets from one state to another *if it maintains mechanical and thermal equilibrium* as it passes through intermediate states. If this is not the case, that is to say, a nuclear bomb is set off next to the box, then the system accesses states that are not in mechanical and thermal equilibrium and all bets are off.

As we demonstrate in the Appendix to this Scene, the functions X, Y and Z can be related to more familiar quantities like the specific heats at constant density c_V and constant pressure c_p and the adiabatic sound speed

$$a^2 \equiv \left(\frac{\partial p}{\partial \rho}\right)_s$$

taken at constant entropy (which we denote by a to avoid confusion with the speed of light c). We prefer to leave them in this generic form because it simplifies notation considerably.

Now here is why all of this matters. If we assume that our radiating magnetofluid is locally, on very small spatial scales well below the scales we are treating, in both mechanical and thermal equilibrium, then we may take the first law

$$de + pdv = Tds = \delta q$$

and apply it to each tiny parcel of fluid which is assumed to locally, at least, be in thermal and mechanical equilibrium (e.g., LTE). Since

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0 ,$$

and $v = 1/\rho$ it follows that

$$\frac{\partial v}{\partial t} + \mathbf{u} \cdot \nabla v - v \nabla \cdot \mathbf{u} = 0 \; .$$

So regarding the first two terms of this equation as the Lagrangean time derivative following a parcel of fluid that remains in LTE as it is (slowly) influenced by its surroundings (passing always through a sequence of LTE states) we have, from the first law of thermodynamics,

$$\frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = \frac{\delta q}{\delta t} = T \left(\frac{\partial s}{\partial t} + \mathbf{u} \cdot \nabla s \right) \,,$$

where $\delta q/\delta t$ is the heat added to a parcel of fluid by thermal conduction say, or viscous dissipation, or radiative heating, or perhaps ohmic dissipation, as it moves along its trajectory!

Voilà!

So we have to determine this local heating function $\delta q/\delta t$. But in terms of this function, we now have an equation for the internal energy per unit mass:

$$\frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = \frac{\delta q}{\delta t} ,$$

or the specific entropy

$$\frac{\partial s}{\partial t} + \mathbf{u} \cdot \nabla s = \frac{1}{T} \frac{\delta q}{\delta t} \;,$$

or the temperature

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T + \frac{Y}{\rho} \nabla \cdot \mathbf{u} = \frac{Z}{T} \frac{\delta q}{\delta t} ,$$

or the pressure

$$\frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p + \frac{X}{\rho} \nabla \cdot \mathbf{u} = \frac{Y}{T} \frac{\delta q}{\delta t} \ .$$

Of course there is only one independent equation amongst these four, since we only require two thermodynamic variables to describe our LTE parcel of fluid, and we already have one in

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0 \ .$$

So, you are free to take your pick of which one you would actually like to solve. Notice in particular that because δq is not an exact differential, we do not solve an equation for this quantity, but instead use it as a source term that leads to a change in the specific entropy of the fluid. And also observe that the three functions X, Y, Z make their presence felt if we choose not to work with the energy per unit mass as our second thermodynamic variable. Finally, in keeping with the no free lunch theorem, if we choose to solve the equation for the pressure, which is after all what we are after to have as many equations as unknowns, we require knowledge of both the X and Y functions.

In case this is not enough thermodynamics for you, there is an Appendix waiting with even more remarkable things that can be deduced for a perfect and not-so-perfect gas.

3. Conservation of Energy

At any rate, we take

$$\frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = \frac{\delta q}{\delta t} ,$$

from our sojourn into thermodynamics and develop here an expression for $\delta q/\delta t$. Multiplying this equation by ρ and the continuity equation by e and adding, we obtain $\delta q = \delta q$

or

$$\begin{split} & \frac{\partial}{\partial t}\rho e + \nabla \cdot \rho e \mathbf{u} + p \nabla \cdot \mathbf{u} = \rho \frac{\partial q}{\delta t} \ , \\ & \frac{\partial}{\partial t}\rho e + \nabla \cdot (\rho e + p) \mathbf{u} - \mathbf{u} \cdot \nabla p = \rho \frac{\delta q}{\delta t} \end{split}$$

which is the desired equation for the internal energy of the fluid. As expected we can increase or decrease this internal energy by adding or removing heat, or compressing or rarefacting it. So far so good.

The work done compressing or rarefacting the material comes at the expense of the kinetic energy density, so we must next set about obtaining an expression for

$$\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{u}|^2 = \frac{1}{2}\Big(\rho\mathbf{u}\cdot\frac{\partial\mathbf{u}}{\partial t} + \mathbf{u}\cdot\frac{\partial}{\partial t}\rho\mathbf{u}\Big) \ ,$$

which we can obtain from Scene 2. The algebra is straightforward but somewhat tedious, so we'll just quote the result

$$\frac{\partial}{\partial t}\frac{1}{2}\rho|\mathbf{u}|^2 + \nabla \cdot \frac{1}{2}\rho|\mathbf{u}|^2\mathbf{u} = -\mathbf{u}\cdot\nabla p + \mathbf{u}\cdot[\nabla\sigma + \rho(\mathbf{g} + \mathbf{a}^{EM} + \mathbf{a}^R)]$$

Adding this equation to the equation for the internal energy density above, gives an equation for the *total* energy density of the material:

$$\begin{split} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho e \right) + \nabla \cdot \left[\mathbf{u} \cdot \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho e + p - \sigma \right) \right] &= \rho \frac{\delta q}{\delta t} - \sigma : \nabla \mathbf{u} + \\ \rho \mathbf{u} \cdot \left(\mathbf{g} + \mathbf{a}^{EM} + \mathbf{a}^R \right) \,. \end{split}$$

Recall, from Scenes 1, 3, and 4 that we have previously identified

$$\begin{split} \mathbf{a}^G &= \mathbf{g} = -\nabla \Phi \ , \\ \mathbf{a}^{EM} &= \frac{1}{\rho} \left(\delta \mathbf{E} + \frac{1}{c} \mathbf{J} \times \mathbf{B} \right) \ , \end{split}$$

and

$$\mathbf{a}^{R} = -\frac{1}{\rho c} \int_{0}^{\infty} d\nu \oint d\mathbf{n} \, \mathbf{n} [\eta_{\nu} - \chi_{\nu} I_{\nu}] \; ,$$

by conservation of total momentum. So these terms are in some sense "known" in terms of the gravitational, electromagnetic, and radiation fields.

Notice that we took part of the viscous contribution to the kinetic energy equation and moved it into a energy flux, and left the remainder on the left side of the total energy equation. We can write term on the left as

$$\sigma_{ij}\frac{\partial u_i}{\partial x_j} = \frac{1}{2}\sigma_{ij}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

because σ is a symmetric tensor. But, recall that

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \delta_{ij} \left(\zeta - \frac{2}{3} \mu \right) \nabla \cdot \mathbf{u} ,$$

therefore

$$\boldsymbol{\sigma} \colon \nabla \mathbf{u} = \frac{\mu}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left(\zeta - \frac{2}{3} \mu \right) (\nabla \cdot \mathbf{u})^2 ,$$

is a nonnegative quantity often referred to as the viscous dissipation function. Obviously, $\rho \delta q / \delta t$ must include this term as it accounts for the transfer of kinetic energy density to the internal (heat) energy density through viscous dissipation.

As usual, it is the term $\rho \mathbf{u} \cdot \mathbf{g}$, and the gravitational field, which continues to be our bête noire. It is no wonder that the replacement of Newton-Poisson by General Relativity was such a heralded event. Again, we find two different expressions for this contribution depending upon whether the gravitational potential Φ is supplied by material *outside* of the domain of interest, or generated through Poisson's Equation by the density ρ *inside* the system. In either case, we can simply multiply the continuity equation by Φ to get

$$-\rho \mathbf{u} \cdot \mathbf{g} = \frac{\partial}{\partial t} \rho \Phi + \nabla \cdot \rho \Phi \mathbf{u} - \rho \frac{\partial \Phi}{\partial t}$$

The first term on the right is the potential energy of the material in the gravitational field. The second term is the divergence of the energy flux associated with the movement of the material in the gravitational potential.

If we neglect the self-gravitation of the matter in our system, then the last term on the right side of the equation accounts for the fact that the universe outside of our system can do work on, or have work done to it by, the material in our system. We have to leave this term as it is, and accept the fact that our system is not *closed*, but can transfer energy with the universe external to it by this term, which, in the end, we must find some way to specify. Usually, the way to specify this term is to say that the externally applied gravitational field does not change in time, so $\partial \Phi / \partial t \equiv 0$, and this term vanishes. Now, our system is, in fact, *closed*.

If we include self-gravity, on the other hand, this equation is still correct as it stands, but the last term does not in general, vanish because ρ depends upon t. One of the exercises at the end of this Scene leads you through the derivation of the following result

$$\rho \frac{\partial \Phi}{\partial t} = \frac{1}{2} \frac{\partial}{\partial t} \rho \Phi - \nabla \cdot \frac{1}{8\pi G} \left(\frac{\partial \Phi}{\partial t} \nabla \Phi + \Phi \nabla \frac{\partial \Phi}{\partial t} \right) \ ,$$

which is correct only for a self-gravitating system! The first term on the right side of this equation, cancels half of the contribution back in our original equation, and the second term is an energy flux carried by the gravitational field. Notice that the gravitational field only gets to store energy (the first term) by virtue of there being matter around, although (the second term) it can transport energy without there necessarily being any matter present in the exact location where the transport is taking place. To simplify the notation, we'll designate this energy flux by $\mathbf{G}(\mathbf{x}, t)$, so

$$\rho \frac{\partial \Phi}{\partial t} = \frac{1}{2} \frac{\partial}{\partial t} \rho \Phi - \nabla \cdot \mathbf{G} \; .$$

So, our final result, which encompasses all possibilities, is

$$-\rho \mathbf{u} \cdot \mathbf{g} = \frac{2-\gamma}{2} \frac{\partial}{\partial t} \rho \Phi + \nabla \cdot (\rho \Phi \mathbf{u} + \gamma \mathbf{G}) - \rho \frac{\partial \Phi_{\text{ext}}}{\partial t}$$

Here, $\Phi_{\text{ext}}(\mathbf{x}, t)$ is a solution of Lapace's Equation and is the gravitational potential supplied by all the matter external to our system, and γ is a Boolean variable which is equal to 0 if self-gravity is ignored, and is equal to 1, otherwise. Notice that when $\gamma = 1$ we can have an external gravitational field in addition to our self-gravity if we so choose.

We can now use this result in our total energy equation to eliminate the gravitational term from the right side and replace it by the time derivative of an energy density and the divergence of an energy flux as follows

$$\begin{split} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho e + \frac{2 - \gamma}{2} \rho \Phi \right) + \nabla \cdot \left[\mathbf{u} \cdot \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho [e + \Phi] + p - \sigma \right) + \gamma \mathbf{G} \right] = \\ \rho \frac{\delta q}{\delta t} - \sigma : \nabla \mathbf{u} + \rho \mathbf{u} \cdot (\mathbf{a}^{EM} + \mathbf{a}^R) + \rho \frac{\partial \Phi_{\text{ext}}}{\partial t} \ . \end{split}$$

We are now ready to finish with our identification of $\rho \delta q / \delta t$. First we recall from Scene 3, the energy conservation statement for the electromagnetic fields,

$$\frac{\partial}{\partial t} \left(\frac{|\mathbf{E}|^2 + |\mathbf{B}|^2}{8\pi} \right) + \nabla \cdot \mathbf{S} = -\mathbf{J} \cdot \mathbf{E} \ .$$

Adding this equation to the total energy equation for the material, we have a total energy equation for the *combined* matter and electromagnetic fields:

$$\begin{split} &\frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho e + \frac{2 - \gamma}{2} \rho \Phi + \frac{|\mathbf{E}|^2 + |\mathbf{B}|^2}{8\pi} \right) + \\ &\nabla \cdot \left[\mathbf{u} \cdot \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho [e + \Phi] + p - \sigma \right) + \gamma \mathbf{G} + \mathbf{S} \right] = \\ &\rho \frac{\delta q}{\delta t} - \sigma {:} \nabla \mathbf{u} + \rho \mathbf{u} \cdot (\mathbf{a}^{EM} + \mathbf{a}^R) - \mathbf{J} \cdot \mathbf{E} + \rho \frac{\partial \Phi_{\text{ext}}}{\partial t} \ . \end{split}$$

And finally, from Scene 4, we need the energy conservation equation for the radiation field:

$$\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{F} = \int_0^\infty d\nu \oint d\mathbf{n} \, \left[\eta_\nu - \chi_\nu I_\nu \right] \, .$$

Again, adding this equation to the previous energy equation gives the final equation for the conservation of energy between the combined material, electromagnetic and radiation fields:

$$\begin{split} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho e + \frac{2 - \gamma}{2} \rho \Phi + \frac{|\mathbf{E}|^2 + |\mathbf{B}|^2}{8\pi} + E \right) + \\ \nabla \cdot \left[\mathbf{u} \cdot \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho [e + \Phi] + p - \sigma \right) + \gamma \mathbf{G} + \mathbf{S} + \mathbf{F} \right] = \\ \rho \frac{\delta q}{\delta t} - \sigma : \nabla \mathbf{u} + \rho \mathbf{u} \cdot (\mathbf{a}^{EM} + \mathbf{a}^R) - \mathbf{J} \cdot \mathbf{E} + \int_0^\infty d\nu \oint d\mathbf{n} \ [\eta_\nu - \chi_\nu I_\nu] + \rho \frac{\partial \Phi_{\text{ext}}}{\partial t} \end{split}$$

Now, because energy must be conserved, and the only work that can be done on our system is through the external gravitational potential, it must be the case that

$$0 = \rho \frac{\delta q}{\delta t} - \boldsymbol{\sigma} : \nabla \mathbf{u} + \rho \mathbf{u} \cdot (\mathbf{a}^{EM} + \mathbf{a}^{R}) - \mathbf{J} \cdot \mathbf{E} + \int_{0}^{\infty} d\nu \oint d\mathbf{n} \left[\eta_{\nu} - \chi_{\nu} I_{\nu} \right]$$

This is a very beautiful result! And, it allows us to finally determine all the right sides of the equivalent thermodynamic equations for the matter:

$$\begin{split} \frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} &= \frac{\delta q}{\delta t} \ , \\ \frac{\partial s}{\partial t} + \mathbf{u} \cdot \nabla s &= \frac{1}{T} \frac{\delta q}{\delta t} \ , \\ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T + \frac{Y}{\rho} \nabla \cdot \mathbf{u} &= \frac{Z}{T} \frac{\delta q}{\delta t} \ , \\ \frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p + \frac{X}{\rho} \nabla \cdot \mathbf{u} &= \frac{Y}{T} \frac{\delta q}{\delta t} \ . \end{split}$$

Well, *almost*! There is one additional transport process which astrophysical radiating plasmas possess and that is the capacity to transport energy by means of thermal conduction. And generally speaking, if viscous effects are important in a given situation, thermal conduction effects are likely to be equally important, if not more so. A theory of thermal conduction, like viscous dissipation, again requires a sojourn into the world of microphysics. But the bottom line is that we can incorporate a wide variety of microphysical processes by making the replacement

$$\rho \frac{\delta q}{\delta t} \to \rho \frac{\delta q}{\delta t} + \nabla \cdot \mathbf{k} \cdot \nabla T \ ,$$

where $\kappa(\mathbf{x}, t)$ is the (symmetric) thermal conductivity tensor [dimensions: gm cm sec⁻³ deg K⁻¹].

Therefore, our final expression for heat added or subtracted from the material is

$$\rho \frac{\delta q}{\delta t} = \nabla \cdot \kappa \cdot \nabla T + \sigma : \nabla \mathbf{u} - \rho \mathbf{u} \cdot (\mathbf{a}^{EM} + \mathbf{a}^{R}) + \mathbf{J} \cdot \mathbf{E} - \int_{0}^{\infty} d\nu \oint d\mathbf{n} \left[\eta_{\nu} - \chi_{\nu} I_{\nu} \right] \,,$$

and the *total* energy conservation equation for our entire system reads

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho e + \frac{2-\gamma}{2} \rho \Phi + \frac{|\mathbf{E}|^2 + |\mathbf{B}|^2}{8\pi} + E \right) + \nabla \cdot \left[\mathbf{u} \cdot \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho [e + \Phi] + p - \sigma \right) + \gamma \mathbf{G} + \mathbf{S} + \mathbf{F} - \kappa \cdot \nabla T \right] = \rho \frac{\partial \Phi_{\text{ext}}}{\partial t}$$

An even more beautiful result!!

But not just beautiful...*extremely* useful for sorting things out and getting our priorities straight! There are five terms in the expression for the total energy density of the system: material kinetic, material thermal, gravitational, electromagnetic and radiative. It is cosmically unlikely that all of these terms are the same size everywhere and at all times. The ratios of these terms are dimensionless numbers which help to order the relative importance of the terms. Any one of the terms can be taken as the *standard* and the relative importance of the remainder assessed in terms of that standard. If one can determine that a certain dimensionless ratio is tiny everywhere and at all times (a somewhat more probable proposition than all of these terms being the same size), then it may be permissible to simplify the analysis by dropping the recessive term initially and then checking a posteriori that such an omission is consistent with the outcome.

The choice of standard is arbitrary, but we'll take the internal (thermal) energy of the matter, which for an ideal gas, depends only on the temperature and the number density

$$\rho e = \frac{3}{2} N k_B T = 2.071 \times 10^{-16} \left(\frac{N}{1 \text{ cm}^{-3}}\right) \left(\frac{T}{1 \text{ deg K}}\right) \text{ erg cm}^{-3}$$

where k_B is Boltzmann's constant. Our material may not be an ideal gas, but for the purpose of estimating the size of various terms this proves to be a reasonable starting point.

If it is in thermal equilibrium with the material—again, another assumption that is often (but not always!) not unreasonable for an order of magnitude estimate—the radiation field is isotropic and has a frequency distribution given by the Planck Function,

$$J_{\nu} = B_{\nu}[T] = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/k_B T) - 1} ,$$

where h is Planck's Constant. The energy density in the radiation field, E is $4\pi/c$ times the integral of J_{ν} over all ν :

$$E = \frac{8\pi^5 k_B^4}{15c^3 h^3} T^4 \equiv a_R T^4 = 7.564 \times 10^{-15} \left(\frac{T}{1 \text{ deg K}}\right)^4 \text{ erg cm}^{-3}$$

Hence the ratio

$$\frac{\rho e}{E} = 2.738 \times 10^{-2} \left(\frac{N}{1 \text{ cm}^{-3}}\right) \left(\frac{T}{1 \text{ deg K}}\right)^{-3}$$

tells us that in hot tenuous astrophysical systems, the radiation field can hold more energy than the thermal part of the material. Convesely in cool and dense regimes, the energy density in the radiation field is negligible (which, see below, need not imply that the radiation field itself is negligible!). In the solar atmosphere, this ratio is 10^4 , and it drops to 500 in the core of the Sun. In neither case is the radiation energy density a major factor in solar dynamics. In an O star atmosphere, however, this ratio can be as low as 10^{-1} . Notice that under the same assumptions the ratio of the thermal pressure of the material pto the radiation pressure $P \equiv |\mathbb{P}|$ is

$$\frac{p}{P} = \frac{\frac{2}{3}\rho e}{\frac{1}{3}E} = 5.476 \times 10^{-2} \left(\frac{N}{1 \text{ cm}^{-3}}\right) \left(\frac{T}{1 \text{ deg K}}\right)^{-3}$$

Other energy density ratios can be assessed in a similar fashion, for example,

$$\frac{8\pi\rho e}{|\mathbf{B}|^2 + |\mathbf{E}|^2} = 5.204 \times 10^{-15} \left(\frac{N}{1 \text{ cm}^{-3}}\right) \left(\frac{T}{1 \text{ deg K}}\right) \left(\frac{1 \text{ Gauss}}{\max(|\mathbf{B}|, |\mathbf{E}|)}\right)^2 \ .$$

Finally the ratio of the thermal to the kinetic energy density of the material is $2\rho e/\rho |\mathbf{u}|^2$, which is proportional to the inverse square of the *Mach Number*, since the energy per unit mass is itself proportional to the sound speed.

One can approach the eight terms that contribute to the energy flux in a similar fashion. We can take the material enthalpy flux

$$(\rho e + p)|\mathbf{u}|$$

as our standard. For the radiation field we can estimate

$$|\mathbf{F}| \approx \frac{1}{4} a_R c T^4 \equiv \sigma_R T^4$$

from the emission from a blackbody, to obtain (again for an ideal gas and radiation field in thermal equilibrium at the *same* temperature T),

$$\frac{(\rho e + p)|\mathbf{u}|}{|\mathbf{F}|} = \frac{20|\mathbf{u}|}{3c} \left(\frac{\rho e}{E}\right) = 1.825 \times 10^{-1} \left(\frac{|\mathbf{u}|}{c}\right) \left(\frac{N}{1 \text{ cm}^{-3}}\right) \left(\frac{T}{1 \text{ deg K}}\right)^{-3}$$

Because $|\mathbf{u}|/c$ can be quite small in many situations, this ratio can actually be much less than unity, while the ratio of energy densities is much greater than unity. In orther words, the radiation field can be very effective at transporting energy (relative to the enthalphy flux) even though it has little energy density (relative to the thermal energy reservoir)! This, indeed, is one of the essential reasons that we care about RMHD even in fairly pedestrian astrophysical situations! This dimensionless ratio—modulo the usual overall factor of unity is referred to as the *Boltzmann Number*. Indeed, authors sometimes settle on different order-unity numerical factors in front of this and other dimensionless constants as it suits their needs. This is fine, because we are really interested in identifying situations in which these dimensionless constants are much greater or much less than one. In any event, we can conclude that *small Boltzmann Numbers mean that radiation is important for energy transport in an astrophysical system*.

If you compute the ratio of the material enthalpy flux to the (electromagnetic) Poynting vector $|\mathbf{S}|$, you will see that there is no analogous tiny factor multiplying the rato of the energy densities. The reason is in MHD, for example, $|\mathbf{E}| \sim |\mathbf{u}||\mathbf{B}|/c$, and in the opposite limit of EHD the same result holds with $|\mathbf{E}|$ and $|\mathbf{B}|$ exchanged. This reflects the fact that these quasistatic electric and magnetic fields are intimately tied into the material.

Another interesting dimensionless energy flux ratio

$$\frac{(\rho e + p)|\mathbf{u}|}{|\mathbf{k} \cdot \nabla T|}$$

is the *Peclet Number*. It tells us whether thermal conduction is important (small Peclet Numbers). In the solar corona, which is extremely optically-thin, radiation no longer interacts much with the material, and thermal conduction replaces radiation as the dominant method of energy transfer.

The ratio

$$\frac{|\mathbf{u}|^2}{2|\boldsymbol{\sigma}|}$$
,

is (again to within factors of unity) the *Reynolds Number*. It usually arises in the dimensional analysis of the Navier Stokes Equations, as we saw in Scene 2, but it appears here as well in energy transport. And finally the *Prandtl Number* is the ratio of the Peclet Number to the Reynolds Number.

There are many more dimensionless numbers that can be extracted, obviously, and some of them have names. Nomenclature is not what is critical here. Rather, an astrophysical system with *five* energy reservoirs and *eight* methods of transporting energy is an absolute nightmare to make sense of even—and one might in fact venture to say, *especially*—computationally where round off and significant digits bring their own headaches.

4. Saha, Boltzmann, and Chemical Potentials

Now we take a brief interlude to tarnish this beautiful result. But with more words and less equations. We remarked earlier that p and T are extensible thermodynamic variables and that when they are constants across an entire system that system is in mechanical and thermal equilibirum respectively. There is a third type of extensible variable, called *chemical potentials*, that must come into play when the individual objects that make up the matter have some sort of internal structure, and that allows them to carry, or better find themselves in, a series of states of internal energy, or, perhaps are allowed to adhere to one another and form aggregates. In all such cases, the individual entities in our

fluid can have energy associated with them that is different from their random thermal kinetic energy. The energy e that resides in

$$\frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = \frac{\delta q}{\delta t} \ ,$$

takes account only of the random thermal motions (thermal kinetic energy) of the individual constituents that make up the fluid.

To make matters concrete, in real astrophysical plasmas, atoms and molecules have a series of internal energy levels. Molecules can form or be disassociated, and atoms can be ionized any number of times and recombine. And then the Hydrogen atom can actually bind a second electron very weakly, to form (massive) negatively charged objects, called anions.

One can, and many do, try to continue using the thermodynamic approach by generalizing the first law of thermodynamics to

$$de = Tds - pdv - \mu_i dN^i ,$$

where one includes as many thermodynamic chemical potentials μ_i and number densities of "chemical" constituents N^i required to completely account for the relevant species of molecules, ions and atoms. It is workable but can sometimes be more awkward than simply addressing the kinetics and microphysics directly. What is useful about the thermodynamic description is the sense of *chemical equilibrium*, which is achieved if the potentials μ_i are constant across a system.

As systems are knocked out of equilibrium by some impact or impulse, the return to equilibrium often takes place over several different times scales. In many systems, *mechanical equilibrium* is achieved first—flows develop and reduce pressure gradients to some modest level. Next, *thermal equilibrium* is achieved—energy is transported by various processes to reduce temperature gradients across the system. Finally, *chemical equilibrium* is achieved—the population levels of the various components adjust to come into a balance such that destruction and creation of species through forward and backward reactions is in a detailed balance.

In astrophysical systems we are for the most part interested in tracking the dynamical relaxation towards a mechanical equilibrium. However, often systems are continually forced in such a fashion that pressure equilibration across an astrophysical system is never achieved. RMHD is aimed precisely at describing these situations. Tracking astrophysical systems on longer thermal time scales proves often to be much more difficult because it is necessary to find some way to average over dynamic (mechanical) time scales, or to carry out a numerical simulation for a very very long time. And chemical equilibration is even harder.

All of these concepts are valid at a local level in a fluid. Just as we assume via LTE that a given parcel of fluid has a well definied (more or less) constant pressure and temperature, we must likewise assess whether it has achieved chemical equilibrium as well.

In many astrophysical applications chemical equilibrium is *not* achieved rapidly enough even in small volumes. The lack of detailed balance has dramatic impacts on the radiation field in particular, through the opacity and source function. For this reason, it usually makes sense to eschew the thermodynamic approach and chemical potentials and work directly with the relevant microphysics.

In practice, the microphysics approach, starts with

$$\frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = \frac{\delta q}{\delta t} ,$$

which is correct as far as it goes for the random kinetic (thermal) motions of the different species present in the fluid (assuming, which is generally the case, that their thermal "temperatures" have all equilibrated), and invokes some combination of adding an additional internal energy density that is nonthermal in character and appropriately modifying what is now considered a catch-all term $\delta q/\delta t$.

If, and only if, chemical equilibrium is in force, then the population of bound energy levels in a given entity (be it a molecule, atom, or ion) is given by *Boltzmann's Equation*, and the relative number densities of different species are related by *Saha's Equation* (and its generalizations). Both of these equations require the specification of a temperature, which should be the thermal kinetic temperature shared by all the entities. This implementation continues to be termed LTE—*local thermodynamic equilibrium*, although technically speaking it is local thermal and "chemical" equilibrium.

When this extended LTE cannot be achieved then the situation is dramatically more complicated and it is necessary to track the time-dependence of the number densities of the species and perhaps the internal energy level populations. This is not necessarily difficult to do in principle, but in practice it is terribly complicated and requires a variety of microphysics rate coefficients. In keeping with our program in these lectures, we will be satisfied at this point to simply refer you to the bibliography where you can find some very accessible treatments of these approaches.

5. The Tensor Virial Equations

We've seen how the conservation of mass, momentum and energy has been essential for sorting out how matter, and the three fields gravitation, electromagnetic and radiation interact dynamically in astrophysical systems. It's natural to inquire if there are other conservation laws, or similar constructs, which can provide additional isights and possibly constraints on how systems evolve.

The answer is "yes"—and the *tensor virial equations* are one, but certainly not the only, step in this direction. The idea here is to define a collection of *moments* of the system according to

$$I_{ijk\cdots}^{mno\cdots}(t) \equiv \int d\mathbf{x} \ \rho(\mathbf{x},t) \ x_i x_j x_k \cdots u_m(\mathbf{x},t) u_n(\mathbf{x},t) u_o(\mathbf{x},t) \cdots ,$$

where you can have as many indices on top, and on the bottom, that you like. Notice that the angular momentum resides in one of these objects! This is a little bit like an extended version of thermodynamics, since our moments describe the system as a whole, and, in particular,

$$I(t) \equiv M(t) = \int d\mathbf{x} \ \rho(\mathbf{x}, t) \ ,$$

is just the total mass of the system. The mass conservation equation then tells us that

$$\frac{dM}{dt} = -\oint d\mathbf{S} \cdot \rho \mathbf{u} \; ,$$

where the surface integral is taken over the outer boundary of the system, possibly at infinity. This *surface* term does the honorable thing of accounting for mass loss or gain through the outer boundary of the system due to a wind, or accretion. This is not a very profound result obviously, but its still nice to see it emerges from this program without much effort.

Next come I_i and I^m .

$$I_i(t) \equiv \int d\mathbf{x} \ \rho(\mathbf{x}, t) \ x_i \ \equiv M(t) \mathbf{X}(t)$$

defines the center of mass of the system $\mathbf{X}(t)$. To compute the time derivative of this quantity we again make use of the continuity equation

$$\frac{dI_i}{dt} = I^i(t) - \oint dS_j \ \rho u_j x_i \ .$$

The surface terms makes perfect sense, but what to make of the other term? To compute dI^i/dt we need the momentum conservation equation, which we take from Scene 2:

$$\frac{\partial}{\partial t}\rho \mathbf{u} + \nabla \cdot \left(p\mathbb{1} - \boldsymbol{\sigma} + \rho \mathbf{u} \mathbf{u}\right) = \rho(\mathbf{g} + \mathbf{a}^{EM} + \mathbf{a}^{R}) \ .$$

Which then gives

$$\frac{dI^i}{dt} = \int d\mathbf{x} \ \rho(g_i + a_i^{EM} + a_i^R) - \oint dS_j \ (\rho u_j u_i - \sigma_{ij} + p\delta_{ij}) \ .$$

Now $I^i(t)$ are the three components of the momentum of the material for the entire system. The surface term shows that we can again lose or gain net momentum through the outer boundary of the system, and the second term indicates that the three fields can impart net linear momentum to the material. *However*, remember that for the self-gravitational part of **g** this term is equivalent to the divergence of the \mathbb{G} tensor, and so

$$\frac{dI^i}{dt} = \int d\mathbf{x} \ \rho([g_{\text{ext}}]_i + a_i^{EM} + a_i^R) - \oint dS_j \ (G_{ij} + \rho u_j u_i - \sigma_{ij} + p\delta_{ij}) \ ,$$

so, in fact, only the *externally supplied* gravitational field can affect the net momentum of the matter—a very nice result!

Now we can use this result in our equation for the center of mass to obtain

$$\frac{d^2 I_i}{dt^2} = \int d\mathbf{x} \ \rho([g_{\text{ext}}]_i + a_i^{EM} + a_i^R) - \oint dS_j \ \text{stuff}_{ij} \ ,$$

where I haven't bothered to write out all the terms that appear in the integrand of the surface integral. For *compact* astrophysical systems, the surface terms always vanish, but when there are winds or accretion, they do not. This is just Newton's law of motion for the entire ensemble of matter. Again, nice, but still not profound.

Profundity begins to emerge when we look at the next set of moments with two indices. The easy one is the *moment of inertia*:

$$\frac{dI_{ij}}{dt} = I_i^j + I_j^i - \oint dS_k \ \rho x_i x_j u_k \ ,$$

and the more laborious calculation is the time-derivative of the mixed moment

$$\frac{dI_i^j}{dt} = \int d\mathbf{x} \ \rho x_i([g_{\text{ext}}]_j + a_j^{EM} + a_j^R) - \int d\mathbf{x} \ T_{ij} - \oint dS_l \ x_i T_{lj}$$

where

$$T_{ij} \equiv G_{ij} + \rho u_j u_i - \sigma_{ij} + p \delta_{ij} ,$$

can be loosely called the stress energy tensor. Combining these equations gives

$$\frac{d^2 I_{ij}}{dt^2} - 2 \int d\mathbf{x} \ T_{ij} = -\oint dS_l \ \text{stuff}_{lij} + \int d\mathbf{x} \ \rho \ \left[x_i([g_{\text{ext}}]_j + a_j^{EM} + a_j^R) + x_j([g_{\text{ext}}]_i + a_i^{EM} + a_i^R) \right] \ .$$

Now we do have something profound. Consider for example a compact system, with no external gravity and let's forget about the radiation and electromagnetic fields for the moment. Then, summing the diagonal of the moment of intertia tensor, we obtain (Einstein summation)

$$\frac{d^2 I_{ii}}{dt^2} = 2 \int d\mathbf{x} \left(3p + \rho |\mathbf{u}|^2 + G_{ii} \right) \,.$$

Notice that because the trace of the viscous stress tensor is zero, this term is absent from the sum of the diagonal components of this moment. Now, recall from Scene 2 that for a self-gravitating fluid

$$G_{ij} = \frac{1}{8\pi G} \left(2 \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_j} - \delta_{ij} \frac{\partial \Phi}{\partial x_k} \frac{\partial \Phi}{\partial x_k} \right) \,,$$

hence

$$\frac{d^2 I_{ii}}{dt^2} = 2 \int d\mathbf{x} \left(3p + \rho |\mathbf{u}|^2 - \frac{1}{8\pi G} |\nabla \Phi|^2 \right) \ .$$

This result is called the *virial theorem*. A compact system can remain compact only if the left side of this equation is less than or equal zero! Gravity, of course, does the honorable thing of trying to hold the system together, while the pressure (disordered motions) and flows (ordered motions) are doing the opposite. Systems which cannot keep the right side of this equation from becoming positive, must generally develop winds and expand.

For a compact radiating magentofluid, of course, it is necessary, and particularly fascinating, to figure out what the term

$$\int d\mathbf{x} \ \rho \ \left[x_i (a_j^{EM} + a_j^R) + x_j (a_i^{EM} + a_i^R) \right] \ ,$$

is doing. To help us here, we need to recall the momentum conservation results from Scenes 3 and 4 as follow:

$$\frac{1}{c^2} \frac{\partial \mathbf{S}}{\partial t} + \nabla \cdot \mathbb{M} = -\delta \mathbf{E} - \frac{1}{c} \mathbf{J} \times \mathbf{B} = -\rho \mathbf{a}^{EM} ,$$
$$\frac{1}{c^2} \frac{\partial \mathbf{F}}{\partial t} + \nabla \cdot \mathbb{P} = \frac{1}{c} \int_0^\infty d\nu \oint d\mathbf{n} \, \mathbf{n} [\eta_\nu - \chi_\nu I_\nu] = -\rho \mathbf{a}^R$$

which gives after a little algebra,

$$\frac{d^2 I_{ii}}{dt^2} = 2 \int d\mathbf{x} \left(3p + \rho |\mathbf{u}|^2 - \frac{1}{8\pi G} |\nabla \Phi|^2 + P_{ii} + \frac{1}{8\pi} [|\mathbf{E}|^2 + |\mathbf{B}|^2] \right) + O(c^{-2}) \; .$$

In so far that the contributions of the electromagnetic and radiation fields to the moment of inertia of our system are generally far smaller than the contribution provided by the material, the $O(c^{-2})$ terms can almost always be discarded. Fnally, the trace of the radiation pressure tensor is the energy density of the radiation field, E, so our final result is

$$\frac{d^2 I_{ii}}{dt^2} = 2 \int d\mathbf{x} \left(3p + \rho |\mathbf{u}|^2 - \frac{1}{8\pi G} |\nabla \Phi|^2 + E + \frac{1}{8\pi} [|\mathbf{E}|^2 + |\mathbf{B}|^2] \right) \,.$$

Among the many conclusions you can start to draw from this, one that stands out in particular, is that using magnetic fields to try to confine an astrophysical system against the tendency for kinetic and thermal energy to cause it to expand is not going to work. The only contribution to the integrand with a negative sign is the self-gravity.

6. Summing it all Up

Perhaps it is worth a moment and some space to recapitulate what we have accomplished in these first five Scenes.

By carefully considering the conservation equations for the matter and the gravitational, electromagnetic, and radiation fields, respectively, *and*, demanding that overall mass, (vector) momentum, and energy be conserved for all four systems taken together, we derived explicit expressions for how momentum and energy are exchanged between the material and the three fields.

Specifically, we find the mometum equation for matter is

$$\frac{\partial}{\partial t}\rho \mathbf{u} + \nabla \cdot \left(p\mathbb{1} - \boldsymbol{\sigma} + \rho \mathbf{u}\mathbf{u}\right) = \rho(\mathbf{g} + \mathbf{a}^{EM} + \mathbf{a}^{R}) \ ,$$

where

$$\rho \mathbf{a}^G = \rho \mathbf{g} = -\rho \nabla \Phi ,$$

$$\rho \mathbf{a}^{EM} = \delta \mathbf{E} + \frac{1}{c} \mathbf{J} \times \mathbf{B} ,$$

and

$$\rho \mathbf{a}^{R} = -\frac{1}{c} \int_{0}^{\infty} d\nu \oint d\mathbf{n} \, \mathbf{n} [\eta_{\nu} - \chi_{\nu} I_{\nu}] \; ,$$

describe the exchange of momentum with the gravitational, electromagnetic, and radiation fields, respectively.

Auxiliary equations, Poisson's Equation for Φ , Maxwell's Equations for **E** and **B**, and the equation of radiative transfer I_{ν} complete the specification of the problem once a closure prescription for $\{\delta, \mathbf{J}, \chi_{\nu}, \eta_{\nu}, p, \sigma\}$ in terms of other known quanities is provided.

The (internal) energy equation for the matter is

$$\frac{\partial}{\partial t}\rho e + \nabla \cdot \rho e \mathbf{u} + p \nabla \cdot \mathbf{u} = \rho \frac{\delta q}{\delta t} \; ,$$

where

$$\rho \frac{\delta q}{\delta t} = \nabla \cdot \kappa \cdot \nabla T - \sigma : \nabla \mathbf{u} + \rho \mathbf{u} \cdot (\mathbf{a}^{EM} + \mathbf{a}^R) - \mathbf{J} \cdot \mathbf{E} + \int_0^\infty d\nu \oint d\mathbf{n} \, \left[\eta_\nu - \chi_\nu I_\nu \right] \,.$$

This adds only two additional quantities to our closure list, which finally stands at $\{\delta, \mathbf{J} \mid \chi_{\nu}, \eta_{\nu} \mid p, T, \sigma, \kappa\}$. I've divided the closure issues into three compartments. The first is electromagnetic in nature and depends upon the plasma physical state of the material and its response to imposed electric and magnetic fields. The second is radiative in character and hinges upon precisely how the matter and radiation are able to interact. The third is essentially thermodynamical, and can be resolved in terms of kinetic theory and statistical mechanics.

The most effective and reliable means to attain closure involves understanding these various processes as they operate in the comoving frame of the material. This is in turn complicated by the fact that observers in the laboratory and comoving frames measure different physical quantities because of the Lorentz Transformations, or better, the overall requirement that light travels at the speed c in every inertial frame of reference.

In the next Act, we derive and motivate the Lorentz Transformations, and then we return to the closure problem and put these results to use.

7. Exercises

Exercise 1: GRAVITATIONAL ENERGY FLUX

Fill in the missing steps to derive

$$\mathbf{G} = \frac{1}{8\pi G} \left(\frac{\partial \Phi}{\partial t} \nabla \Phi + \Phi \nabla \frac{\partial \Phi}{\partial t} \right) \ .$$

(Hint: Look at Ogilvie [**O** 1] or Kulsrud [**K** 1], if you get stuck.) *Exercise 2*: <u>THAT VICIOUS DISSIPATION FUNCTION</u> Is the expression,

$$\boldsymbol{\sigma} : \nabla \mathbf{u} = \frac{\mu}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left(\zeta - \frac{2}{3} \mu \right) (\nabla \cdot \mathbf{u})^2 ,$$

really non-negative? The first term certainly is, but what about the second term, particularly when $\zeta > 2\mu/3$?

8. Further Reading

As we have encountered previously, there is no shortage of material out there on thermodynamics in all its guises. I've mostly followed Eckart $[\mathbf{E} \ \mathbf{1}]$ and Shu $[\mathbf{S} \ \mathbf{1}]$ in my treatment presented here. If you *did* want to delve just a little deeper, an essential read is

*[H 3] Kerson Huang, <u>Statistical Mechanics</u>, (New York, NY: John Wiley & Sons; 1965), xiii+470.

The virial equations and their tensor extension have a single monograph devoted to them,

*[C 4] George W. Collins, II, The Virial Theorem in Stellar Astrophysics, (Tucson, AZ: Pachart Publishing House1978), viii+135,

which, unfortunately for me, I find inscrutable. So just in case you are like me, here are two other selections which are much easier to decipher:

[CF 1] S. Chandrasekhar & E. Fermi, "Problems of gravitational stability in the presence of magnetic fields", *Astrophysical Journal*, **118**, 116-41, 1953,

[P 7] Eugene N. Parker, "Tensor virial equations", *Physical Review*, 96(6), 1686-90, 1954.

Ionization is treated in a wholistic, i.e., chemical potential, fashion by Mihalas & Mihalas $[\mathbf{MM 1}]$ and again by Shu $[\mathbf{S 1}]$. Also, any monograph that deals with stellar interiors has to find a way to handle it in this macroscopic sense. However, in stellar photospheres, and abundance determinations the comprehensive approach presented in the second Appendix is required. The MURaM simulation, for example, uses this latter approach. This material I have lifted and modified from a notational perspective from a very beautiful but hard to find early article by Dimitri Mihalas,

*[M 5] Dimitri Mihalas, "The calculation of model stellar atmospheres", in Berni Alder, Sidney Fernbach & Manuel Rotenberg, eds., Methods in Computational Physics. Volume 7: Astrophysics, (New York, NY: Academic Press; 1967), pp. 1-52.

Finally, I need to provide some references for the technical data needed to actually make use of the ideas presented in Appendix B. Mihalas [M 5] provides

the necessay fits to the Υ 's for Hydrogen, which contain the Partition Functions as part of the package. He cites

[V 1] M.S. Vardya, "Physical atmospheric parameters for late-type stars", Astrophysical Journal, 133, 107-29, 1961,

as the source of his fits. You will also find

[I 1] Alan W. Irwin, "Polynomial partition function approximations for 344 atomic and molecular species", Astrophysical Journal Supplement Series, 45, 621-33, 1981,

of use. I am sure in today's data intensive age there are entire software packages or data bases that compute all of these partition functions and statistical equilibrium population levels for an arbitrary admixture of every conceivable element and molecule under the Sun. If you find them, let me know, please.

9. Appendix A: The Perfect Gas (for all occasions)

Although few gases are actually *perfect*, many of them have high aspirations and often manage to fit the bill for the most part. Perfect gases also permit substantial progress in analytic methods, which can be useful for understanding how *real* gases behave. Here we record some essential formulae appropriate for a perfect gas. What makes the perfect gas so perfect, is that we can actually write down exact expressions for all the thermodynamic quantities instead of relying on differential (Pfaffian) relations.

Let m [dimensions: gm] denote the mass of the identical particles which make up the gas (or more generally the mean mass of the different particles which make up the gas). Then the energy per unit mass is

$$e(s,v) = \left(\frac{3\pi\hbar^2}{m^{8/3}}\right)v^{-2/3}\exp\left[\frac{s}{c_V} - \frac{5}{3}\right] ,$$

is simply proportional to the temperature

$$e(s,v) = \frac{3k_B}{2m}T(s,v) \equiv c_V T = \frac{3}{2}\frac{p(s,v)}{v} ,$$

where c_V is the specific heat at constant volume, and k_B is Boltzmann's constant. From this last result we obtain the *equation of state*

$$p(s,v) = \frac{2e}{3v} = \left(\frac{5k_B}{2m} - \frac{3k_B}{2m}\right)\rho T(s,v) \equiv (c_p - c_V)\rho T ,$$

where, $\rho = 1/v$, and c_p is the specific heat at constant pressure, which is also a constant.

With these in hand, it is now straightforward to compute the second partial derivatives of e:

$$\begin{split} X(s,v) &= \frac{5}{3} \frac{p(s,v)}{v} \ , \\ Y(s,v) &= \frac{p(s,v)}{c_V} \ , \end{split}$$

$$Z(s,v) = \frac{T(s,v)}{c_V}$$

A familiar example of an *imperfect gas*, is water, a.k.a., a liquid! In particular, *salt water* makes up a substantial fraction of our home planet. Often oceanographers treat salt water as being *incompressible*. To see why this is the case, a good working equation of state for salty water is

$$v(p, S, T) = v_{\infty}(T) - \kappa_1 S + \frac{\lambda(T)}{p + p_0(T) + \kappa_2 S} ,$$

where S is the salinity.

When the salinity is zero, this expression takes the simpler form

$$p(v,T) = \frac{\lambda(T)}{v - v_{\infty}(T)} - p_0(T) ,$$

where

$$\lambda = 1788.316 + 21.55053 \left(\frac{T}{1^{\circ}C}\right) - 0.4695911 \left(\frac{T}{1^{\circ}C}\right)^2 + \dots \quad \frac{\text{bar cm}^3}{\text{gm}}$$
$$p_0 = 5918.499 + 58.05267 \left(\frac{T}{1^{\circ}C}\right) - 1.1253317 \left(\frac{T}{1^{\circ}C}\right)^2 + \dots \quad \text{bar}$$
$$v_{\infty} = 0.6980547 - 7.435626 \times 10^{-4} \left(\frac{T}{1^{\circ}C}\right) + 3.704258 \times 10^{-5} \left(\frac{T}{1^{\circ}C}\right)^2 + \dots \quad \frac{\text{cm}^3}{\text{gm}}$$

and a bar $= 10^6 \text{ gm cm}^{-1} \text{ sec}^{-2}$.

It is now an interesting exercise to compute the *isothermal compressibility*

$$\varkappa_T \equiv \frac{1}{\rho} \left(\frac{\partial \rho}{\partial p} \right)_T$$

for our atmosphere (more or less an ideal gas although for a variety of reasons we won't go into here the ratio of specific heats c_p/c_V is more like 7/5 than 5/3) and water, at room temperature and one atmosphere of pressure!

10. Appendix B: The Less Perfect Gas-Ionization

For an ideal gas, with a constant ratio of specific heats, $\gamma = c_p/c_V$, the closure relation is simply

$$p(e,\rho) = (\gamma - 1)\rho e$$
,

where we typically have in mind $\gamma = 5/3$. We have the continuity equation to determine ρ and the internal energy equation to determine e, and the pressure follows directly from this relation. For an ideal gas we also know all the second partial derivatives X, Y, and Z, so, if we choose, we can evolve the temperature T instead of the internal energy per unit mass e. and use the closure relation

$$p(\rho,T) = (c_p - c_V)\rho T \; .$$

Variables that are advanced in time via evolution equations, like ρ and e are called *prognostic*, while those that are computed at each time step, like p and T are called *diagnostic*.

There are many slipshod and haphazard ways to treat ionization in astrophysics. These cludges work fairly well if your gas is fully ionized or barely ionized, and if it consists only of Hydrogen and maybe some Helium. But if you are going to bother with partial ionization because it is an important ingredient of your problem then it pays to do it right from the start. Incidentally, the MURaM calculation we have been analyzing in these notes is an example of the latter sort of situation: the ionization is highly variable, most of the free electrons near the base of the photosphere are being supplied by Iron, Sodium and Potassium and neutral Hydrogen is actually picking up some of these free electrons to make a curious anion (a negatively charged ion) that turns out to be the dominant source of opacity for wavelenths greater than 200 - 300 nm. Oh, and did I forget to mention that there is molecular Hydrogen floating about?

So, following Dimitri Mihalas, who did *everything* the correct way, I present here his fairly robust scheme for dealing with ionization. The essential assumption inherent in this method is LTE—local thermodynamic equilibrium. The relative populations of the ionization stages and the excited levels within an atom/ion obey the Boltzmann and Saha Equations, which means that they depend essentially only upon two quantities, the temperature $T(\mathbf{x}, t)$ and the electron number density $N^e(\mathbf{x}, t)$ or equivalently the partial pressure contributed by the free electrons, $p^e(\mathbf{x}, t) \equiv N^e k_B T$. These are diagnostic variables.

This is both good and bad. Good because only two macroscopic quantities are involved. Bad because our RMHD equations are set up to evolve the density $\rho(\mathbf{x}, t)$ and the internal energy per unit mass $e(\mathbf{x}, t)$, and need the entire pressure $p(\mathbf{x}, t)$ not simply the part due to the electrons on their own. Bad, also, because we can't obtain an evolution equation for the temperature $T(\mathbf{x}, t)$ without knowledge of Y and Z functions, which, a priori, are not known to us. Indeed, by getting the ionization right, we should be able to deduce what these two functions are.

So, what to do? The approach is essentially to use the RMHD to tell us what the prognostic variables $\rho(\mathbf{x}, t)$ and $e(\mathbf{x}, t)$ are, and how they evolve to the next time step, and concurrently to determine self-consistently what, $T(\mathbf{x}, t)$, $p^e(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ have to be. This is in some sense the determination of an "equation of state" for $p(\mathbf{x}, t)$ but with the necessity to carry along the temperature and the electron pressure as auxiliary diagnostic variables at each time step. So, in fact, we never will be able to write down a statement like

$$p(\rho, e) = \text{ some function}(\rho, e, T, p^e, \cdots)$$

but when the dust settles we will know ρ and e from the RMHD, and p, p^e , and T from the ionization algorithm.

To see how this works, we will break the problem into two separate pieces. And then it should be clear how you can combine them to deal with the full problem. *First* we will consider the case where our material consists *only* of Hydrogen, but allow for the formation of the anion of Hydrogen and the Hydrogen molecule. *Second*, we will permit an arbitrary admixture of additional elements, but will assume ionization only for every element including Hydrogen no molecules or anions.

α . Just Hydrogen

In stellar atmospheres, particularly cool stars, Hydrogen can exist in *five* different incarnations: H, H⁺, H⁻, H₂, H₂⁺, where H⁺ is just a bare proton, and H⁻ is the fascinating anion of Hydrogen. To each, we can assign a number density, and a partial pressure. The five number densities cannot be independent, but must give the correct mass density, at the current time and every position in the simulation:

$$\rho(\mathbf{x},t) = m_p N^{H^+} + m_H [N^H + N^{H^-}] + m_{H_2} [N^{H_2} + N^{H_2^+}] + m_e N^e .$$

The last term in this expression can usually be dropped.

Electron accounting provides a second relationship between the *six* number densities:

$$N^e = N^{H^+} + N^{H_2^+} - N^{H^-}$$

Next we observe that *each* of the following "chemical" reactions must come into local thermodynamic equilibrium:

$$H + e \leftrightarrow H^{-}$$
$$H^{+} + e \leftrightarrow H$$
$$H + H \leftrightarrow H_{2}$$
$$H + H^{+} \leftrightarrow H_{2}^{+}$$

meaning that the rates in each direction are the same and the number densities have equilibrated.

This in turn provides us with *four* independent relationships between the number densities of the constituents in each reaction, and the temperature T. So, we now have *six* equations for the *seven* unknowns—the seven being the temperature, T and the six number densities. The last required relationship is that we must have the correct internal energy per unit volume at the current time and every position in the simulation:

$$e(\mathbf{x}, t) = \frac{3}{2} \frac{p(\mathbf{x}, t)}{\rho(\mathbf{x}, t)} + e_{\text{dissociation}}(\mathbf{x}, t) + e_{\text{level occupation}}(\mathbf{x}, t) ,$$

$$e(\mathbf{x}, t) = e_{\text{thermal}}(\mathbf{x}, t) + e_{\text{dissociation}}(\mathbf{x}, t) + e_{\text{level occupation}}(\mathbf{x}, t) ,$$

where the last two term can be written explicitly in terms of the appropriate number densities and information about the energy levels and the dissociation energies of the two Hydrogen molecules, the Hydrogen atom, and the Hydrogen anion.

The first term is just the thermal kinetic energy with $(1/2)k_BT$ per translational degree of freedom, i.e.,

$$p(\mathbf{x},t) = [N^{H^+} + N^H + N^{H^-} + N^{H_2} + N^{H_2^+} + N^e]k_BT .$$

Therefore, with ρ and e given from the RMHD equations at a given time step, we can in principle solve this system of seven inhomogeneous equations in the seven unknowns, and then subsequently determine the total gas pressure from the last equation above. We can then advance the RMHD equations to the next time step, where this system of equations is solved anew.

A few remarks and observations will be helpful at this point. *First*, the expressions for the equilibrium number densities for the four reactions have been computed, tabulated and fit by various approximations. They are of the form, using the first reaction as an example,

$$\frac{N^H N^e}{N^{H^-} N_0} = \Upsilon^{H + e \leftrightarrow H^-}(T)$$

where the expression on the right side of this equation is a dimensionless function of the equilibrium temperature, T, and

$$N_0 \equiv 2 \frac{(2\pi m_e k_B T)^{3/2}}{h^3}$$

is a fiducial number density. Various fits for the four Υ 's are provided by Mihalas [M 5] and Vardya [V 1]. Unlike the other three equations, these four are nonlinear. Second, the capacity of the material to store energy in excited energy levels and through the binding energies of ionization and dissociation can have some very novel effects on the RMHD. If only the random thermal energy option existed, when a parcel of material is adiabatically compressed, the thermal energy, pressure and density all increase and act in a fashion to resist the compression. If instead the work done on the material goes into pumping up the population of internal energy levels overlying the ground state, then there may be little comparable increase in pressure. Similarly if the work done goes into dissociation, then each new particle adds a whopping $(3/2)k_BT$ to the pressure. Third, if LTE does not hold, then we are forced to carry along prognostic evolution equations for each of the six number densities which must be solved concurrently with the rest of the RMHD equations. Fourth, notice that we have left off the recombination reaction

$$H_2^+ + e \leftrightarrow H_2$$
.

Can you explain why?

β . Ionization Only

In this example, we will allow for a complete cosmic mix of all sort of elements and ions, but, to keep matters in hand, no molecules or anions will be permitted. The number densities we need to track now proliferate at an alarming rate, however, so do the number of equivalent Υ 's. And indeed, they keep pace in such a fashion that we will have as many equations as unknowns when all is said and done.

The additional information we need to supply a priori is the fractional abundance of each element. This can be approached in two equivalent ways. Either we give the fractional abundance relative to Hydrogen, in which case we have one fewer fractional abundance than elements, or, we give the fractional abundance relative to the total of all the elements, in which case we have as many fractional abundances as elements, however, they all have to add up to one. Both ways are equivalent, but, the actual fractional abundances are different, of course. The remainder of the information, ionization potentials, energy levels and so forth are in principle known in advance from the atomic physics, and we must simply access that information as we need it.

Anticipating that we will have to deal with some admixture of elements in our matter, we let $N^Z(\mathbf{x},t)$ be the number density of atoms/ions with Zprotons in the nucleus (we don't worry about isotopes, you can if you wish). So, Z=1 is Hydrogen, Z=2 is Helium, and so forth, or, we can also just use the atomic symbol, so $N^{He} \equiv N^2$ is the number density of Helium and $N^C \equiv N^6$ is the number density for Carbon. We shall also again need the number density of electrons in what follows, N^e . All of these capital N's have dimensions of cm⁻³.

A given element Z has Z states of ionization (including unionized or neutral). To distinguish them we add a subscript to obtain $N_j^Z(\mathbf{x}, t)$ for the number density of element Z in the *j*-the state of ionization. We let j = 0 denote neutral, j = 1 single ionized and so forth. (If we had an anion, we could use j = -1.) Hence our first result is simply bookkeeping:

$$N^Z = \sum_j N_j^Z \; ,$$

where j ranges over the allowed values. In practice, only j = 0 and j = 1 are usually necessary in the solar photosphere or chromosphere, because the higher stages of ionization cost too much energy. This is not true in stellar coronae.

Next we must be aware that each ion contributing to N_j^Z can be in any one of a number of internal energy levels described by several quantum numbers. For our purposes it suffices to lump them into a single index α which can be used to number the energy levels in increasing order above the ground state. The ground state will be denoted by $\alpha = 0$ and $\alpha = 1$ is the first excited state, and so forth. Since there are degeneracies several combinations of quantum numbers may in fact contribute to the same α and this can be accounted for by a numerical factor, called the *statistical weight* $g_{j,\alpha}^Z$ of the atomic level with energy $\varepsilon_{j,\alpha}^Z$ [dimensions: erg] above the ground state. By convention, $\varepsilon_{j,0}^Z \equiv 0$. Our second result is again simply bookeeping:

$$N_j^Z = \sum_{\alpha} N_{j,\alpha}^Z(\mathbf{x}, t) \; ,$$

the number densities in all the available energy levels added together must give the number density of the element Z in its j-th state of ionization.

Admittedly at this point we have a *vast* collection of number densities to track. But now we get some help.

We are now ready for our first nontrivial result, which is, in LTE, the ratio of the number densities in adjacent energy levels is given by Boltzmann's Equation:

$$\frac{N_{j,\alpha+1}^Z}{N_{j,\alpha}^Z} = \frac{g_{j,\alpha+1}^Z}{g_{j,\alpha}^Z} \exp\left(\frac{\varepsilon_{j,\alpha}^Z - \varepsilon_{j,\alpha+1}^Z}{k_B T}\right) \;,$$

where $T(\mathbf{x}, t)$ is the common temperature of the gas and the radiation. Notice that the right side of this equation depends only on the temperature (which is currently unknown of course, as it was for the pure Hydrogen example above), and atomic structure information which *is* known to us.

Since the satistical weights and the energy level spacings are all tabulated, once we know the temperature we know the *relative* populations. Next we want to find the ratios relative to the ground state instead of adjacent levels. To do this we daisy-chain this formula as many times as required to obtain

$$\frac{N_{j,\alpha+1}^Z}{N_{j,0}^Z} = \left(\frac{N_{j,\alpha+1}^Z}{N_{j,\alpha}^Z}\right) \left(\frac{N_{j,\alpha}^Z}{N_{j,\alpha-1}^Z}\right) \cdots \left(\frac{N_{j,2}^Z}{N_{j,1}^Z}\right) \left(\frac{N_{j,1}^Z}{N_{j,0}^Z}\right) \ ,$$

which "telescopes" to the simple result

$$\frac{N_{j,\alpha+1}^Z}{N_{j,0}^Z} = \frac{g_{j,\alpha+1}^Z}{g_{j,0}^Z} \exp\left(-\frac{\varepsilon_{j,\alpha+1}^Z}{k_B T}\right)$$

Again, the right side of this equation depends only upon the (unknown) temperature and the (known) atomic parameters.

Using this result in our bookkeeping sum we obtain

$$N_j^Z = \sum_{\alpha} N_{j,\alpha}^Z = \frac{N_{j,0}^Z}{g_{j,0}^Z} \sum_{\alpha} g_{j,\alpha}^Z \exp\left(-\frac{\varepsilon_{j,\alpha}^Z}{K_B T}\right) \equiv \frac{N_{j,0}^Z}{g_{j,0}^Z} U_j^Z[T] ,$$

which serves to define $U_j^Z[T]$, which is called the *partition function*. It too is tabulated for a range of temperatures and popular values of Z and the lowest values (generally 0 and 1) of j.

Therefore we have our final result

$$\frac{N_{j,\alpha+1}^Z}{N_j^Z} = \frac{g_{j,\alpha+1}^Z}{U_j^Z} \exp\left(-\frac{\varepsilon_{j,\alpha+1}^Z}{k_B T}\right) \equiv f_{j,\alpha+1}^Z[T],$$

which is the *fraction* of the population that lives in the $\alpha + 1$ energy level! Notice that at the appropriate time, this will allow us to compute $e_{\text{level occupation}}$.

So far we haven't ionized anything, but that comes next, and this detour was helpful to introduce the concept of the partition function and telescoping. The analog of Boltzmann's Equation for ionization is Saha's Equation:

$$\frac{N_{j+1}^Z}{N_j^Z} \frac{N^e}{N_0} = \frac{U_{j+1}^Z}{U_j^Z} \exp\left(-\frac{\varepsilon_{j\to j+1}^Z}{k_B T}\right)$$

Here, $\varepsilon_{j \to j+1}^Z$ is the energy required to ionize from the ground state ($\alpha = 0$) of the atom in the *j*-th state of ionization to the ground state of the ion in the j + 1-th state of ionization. N^e is the electron number density, and

$$N_0 \equiv 2 \frac{(2\pi m_e k_B T)^{3/2}}{h^3}$$

is a fiducial number density. The new wrinkle here is that in addition to the temperature we also need to know the electron number density to actually compute anything. This was not needed to determine the energy level populations. In fact the last step of our process will be to solve for the electron number density. However, as before, the right side of this equation still depends only upon the (unknown) temperature and the (known) atomic parameters.

We can again make use the telescoping concept to obtain

$$\frac{N_{j+1}^Z}{N_0^Z} = \left(\frac{N_{j+1}^Z}{N_j^Z}\right) \left(\frac{N_j^Z}{N_{j-1}^Z}\right) \cdots \left(\frac{N_2^Z}{N_1^Z}\right) \left(\frac{N_1^Z}{N_0^Z}\right) ,$$

or

$$\frac{N_{j+1}^Z}{N_0^Z} = \frac{U_{j+1}^Z}{U_0^Z} \left(\frac{N_\star}{N^e}\right)^{j+1} \exp\left(-\frac{\varepsilon_{0\to j+1}^Z}{k_BT}\right) \;. \label{eq:N_j_j}$$

The right side now depends upon *two* unknows, the temperature and the electron number density.

The bookkeeping requirement yields

$$N^Z = \sum_j N_j^Z \; ,$$

and an ionization analogue of the partition function, say $V^{Z}[T, N^{e}]$:

$$\frac{N_{j+1}^Z}{N^Z} = \frac{U_{j+1}^Z}{V^Z} \left(\frac{N_\star}{N^e}\right)^{j+1} \exp\left(-\frac{\varepsilon_{0\to j+1}^Z}{k_B T}\right) \equiv f_j^Z[T, N^e] \;.$$

One does not find tables of $V^{Z}[T, N^{e}]$ anywhere because it is a simple polynomial in N^{e} . The nontrivial temperature dependences are in the $U_{j}^{Z}[T]$ partition functions.

Now we are set, because if the *only* thing going on is ionization (non-negative values of j) and we have no molecules to worry about, it follows that

$$N^e = \sum_Z N^Z \sum_{j=1}^Z j f_j^Z [T, N^e]$$

provides the required equation for N^e , if the temperature is specified and we know the relative abundances of the various elements. For example if N^A is the number density of atoms of all types, then

$$N^A = \sum_Z N^Z \equiv N^A \sum_Z f^Z$$

in terms of fractional abundances of the elements, f^Z , which we must supply. Which leaves just N^A as the remaining unknown. But it can be related back to the (unknown) gas pressure and the (known) density by

$$p(\mathbf{x},t) = (N^e + N^A)k_BT$$

and

$$\rho(\mathbf{x},t) = m_e N^e + N^A \sum_Z m_Z f^Z \ .$$

Finally the very last equation needed to close the system is, as before,

$$e(\mathbf{x},t) = \frac{3}{2} \frac{p(\mathbf{x},t)}{\rho(\mathbf{x},t)} + e_{\text{dissociation}}(\mathbf{x},t) + e_{\text{level occupation}}(\mathbf{x},t) ,$$

or

$$e(\mathbf{x}, t) = e_{\text{thermal}}(\mathbf{x}, t) + e_{\text{dissociation}}(\mathbf{x}, t) + e_{\text{level occupation}}(\mathbf{x}, t)$$
.

11. Appendix C: RMHD's 58 Terms

The *energy density* of the material is

$$\frac{1}{2}\rho|\mathbf{u}|^2 + \rho e$$

and the *energy flux* is

$$\mathbf{u} \cdot \left(\frac{1}{2}\rho |\mathbf{u}|^2 + \rho e + p - \sigma\right) - \kappa \cdot \nabla T \ .$$

The *energy density* of the gravitational field is

$$\frac{2-\gamma}{2}\rho\Phi$$

where $\gamma=1$ if self-gravity is ignored and 0 if the Newton-Poisson Equation

$$\nabla^2 \Phi = 4\pi G \rho$$

is retained, and the energy flux vector for the gravitational field is

$$\rho \Phi \mathbf{u} + \gamma \mathbf{G}$$
.

The energy exchange with the material is

$$\dot{\mathcal{E}}^{M \to G} - \dot{\mathcal{E}}^{G \to M} = -\rho \mathbf{u} \cdot \mathbf{g} = \rho \mathbf{u} \cdot \nabla \Phi$$
.