

# Consistent approximate equations of state

A realistic equation of state for stellar interiors involves a number of different features, such as partial ionization from temperature and ‘pressure’ effects, Coulomb interactions, volume effects, etc. These must be included in the calculation of the thermodynamical quantities, such as density, internal energy and thermodynamical derivatives such as specific heats and adiabatic exponents, for a given pressure  $P$ , temperature  $T$  and composition, or other choices of the basic variables used to describe the thermodynamical state. Apart from the difficulties in characterizing these different components, a major concern is to ensure that they are included consistently everywhere in the thermodynamical description, so that the full set of quantities are derivable from a single equation of state. This will often not be the case if one simply adds bits to the expressions for, for example, the pressure and internal energy of the gas. The result will unavoidably be inconsistencies in the resulting models. For general reviews of these issues, see for example Christensen-Dalsgaard & Däppen (1992) and Däppen & Guzik (2000).

A specific issue, discussed by Kippenhahn & Weigert (1990), is the recombination that occurs in the inner parts of the star if the simple Saha equation is used. Kippenhahn & Weigert discuss this in a qualitative way based essentially on the perturbation of the atomic energy levels by neighbouring atoms, which is assumed eventually to ensure full ionization in stellar interiors, which is then generally assumed. This clearly glosses over some very complex processes in the interactions between atoms, ions and electrons in the plasma, and almost certainly does not satisfy constraints of thermodynamic consistency. A closely related problem is the obvious divergence of the partition function (Kippenhahn & Weigert, Eq. 14.3) if the full infinity of atomic states is included in the sum. This is sometimes avoided by making the opposite approximation, which in practice often works reasonably well, that all the atoms and ions are in their ground state.

In older stellar evolution codes, which generally form the basis for Kippenhahn & Weigert, some of these problems were suppressed by dealing separately with the stellar envelope and the stellar interior, as implied by the discussion of the boundary conditions in their Chapter 10. In this case the equation of state would be treated in detail in the envelope, while the interior would be assumed to be fully ionized. A significant argument in these early calculations was that this reduced the computing time. However, it obviously leads to potential subtle discontinuities at the matching point. Thus more modern codes probably in general make a full treatment of the equation of state in the entire model; this is certainly the case in the Aarhus code (ASTECC; Christensen-Dalsgaard 2008).

One way to avoid the problems with the equation of state is by considering the system as a combination of nuclei and electrons, interacting through their Coulomb potential, but with no *a priori* assumption about the presence of atoms and ions in the gas. Formally, the state of the gas is obtained by solving the Schrödinger equation for this combination. In practice, this is done through cluster analysis which then naturally leads to the formation of atoms and ions, but includes their interaction with other constituents in the gas. This has been called the *physical picture*.

Here I discuss a more intuitive ‘cook-book’ approach, known as the *chemical picture*. As in the straightforward, and likely inconsistent, procedures one proceeds from a collection of atoms, ions, etc., and include various physical effects in a largely heuristic fashion. The trick that ensures consistency is to do so in terms of the free energy  $F$  (e.g., Graboske, Harwood & Rogers 1969; Däppen 1980), related to the entropy  $S$  and the internal energy  $U$  by

$$F = U - TS . \tag{1}$$

$F$  is traditionally expressed as a function  $F(T, V, \{N_\nu\})$  of temperature  $T$ , volume  $V$  and the number  $N_\nu$  of the different constituents of the gas, a constituent being for example an ion in a given

ionization state and a given excitation state. For given  $T, V$  the equilibrium thermodynamic state is defined by the resulting set  $\{N_\nu\}$ , for example giving the degrees of ionization. This equilibrium is obtained as that configuration  $\{N_\nu\}$  that minimizes  $F$ , under the so-called *stoichiometric constraints*, e.g., the constraints that the total number of free electrons and the total number of any given nucleus is constant. As discussed, e.g., by Däppen & Guzik (2000) this in simple cases leads to the familiar form of the Saha equation.

Given this equilibrium  $F$  as a function of  $T$  and  $V$ , other thermodynamic quantities can be obtained by differentiation:

$$P = - \left( \frac{\partial F}{\partial V} \right)_T, \quad S = - \left( \frac{\partial F}{\partial T} \right)_V, \quad U = -T^2 \left( \frac{\partial}{\partial T} \frac{F}{T} \right)_V. \quad (2)$$

Similarly, other thermodynamic quantities are determined by higher derivatives, e.g. specific heat at constant volume:

$$c_V = - \frac{T}{\rho} \left( \frac{\partial^2 F}{\partial T^2} \right)_V. \quad (3)$$

The physics of the equation of state is defined by the specification of  $F(T, V, \{N_\nu\})$ ; given that, thermodynamic consistency is ensured if the remaining thermodynamic quantities are obtained through differentiation of  $F$ , as indicated.

An additional advantage of this formalism is that  $F$  can be expressed as a sum over individual contributions, each corresponding to a physical effect:

$$F = F_e + F_{\text{trans}} + F_{\text{int}} + F_{\text{rad}} + F_{\text{conf}}. \quad (4)$$

Here

- $F_e$ : contribution from free electrons (including effects of degeneracy, as appropriate)
- $F_{\text{trans}}$ : contribution from the motion of heavy particles
- $F_{\text{int}}$ : contribution from the internal states in atoms and ions
- $F_{\text{rad}}$ : contribution from radiation
- $F_{\text{conf}}$ : the ‘configuration’ contribution, resulting from the finite size of atoms and ions, and the Coulomb interaction.

Other effects may be included, as they are found to be required; the influence on  $P, U$ , etc. of such a change  $\Delta F$  to  $F$  can be obtained from equations (2). From the minimization of the free energy it is obvious that such a correction may also affect the ionization balance. It may be shown that the result is to modify the Saha equation to

$$\frac{n_{r+1}}{n_r} n_e = \frac{u_{r+1}}{u_r} 2 \frac{(2\pi m_e k_B T)^{3/2}}{h^3} e^{-\chi_r/k_B T + \Delta\mu} \quad (5)$$

( $k_B$  being Boltzmann’s constant), including the correction  $\Delta\mu$  to the electron chemical potential given by

$$\Delta\mu = - \frac{1}{k_B T} \left( \frac{\partial \Delta F}{\partial n_e} \right)_{T, V}. \quad (6)$$

This correction is often forgotten in *ad hoc* modifications of the equation of state.

A detailed discussion of the various components of  $F$  is clearly beyond the scope of these notes; some details are discussed by Graboske et al. (1969), Däppen (1980), Däppen et al. (1988), and references therein. However, a few points might be mentioned.

For a ‘classical’ gas the contribution from the internal states can be written as

$$F_{\text{int}} = -k_{\text{B}}T \sum_k \sum_j \ln \left[ \sum_i g_{ijk} \exp(-E_{ijk}/k_{\text{B}}T) \right], \quad (7)$$

where  $k$  sums over elements and  $j$  sums over the ionization states of each element, whereas  $i$  sums over the bound states of that particular ionization state. As usual,  $g_{ijk}$  is the statistical weight and  $E_{ijk}$  is the excitation energy. This is clearly closely related to the partition functions and share with them the problem of divergence when the sum extend over the infinite number of bound states in an isolated atom or ion. As suggested by Hummer & Mihalas (1988) (see also Däppen & Guzik 2000) this can be avoided by introducing into equation (7) a set of weights  $w_{ijk}$  giving the probability that the given state still exists, despite the perturbations from neighbouring constituents of the gas. Thus equation (7) is replaced by

$$F_{\text{int}} = -k_{\text{B}}T \sum_k \sum_j \ln \left[ \sum_i w_{ijk} g_{ijk} \exp(-E_{ijk}/k_{\text{B}}T) \right]. \quad (8)$$

The weights obviously depend on the detailed physical description of the interactions, and they are functions of  $T, V$  and  $\{N_\nu\}$ ; however, it is still possible to obtain the thermodynamic state through the minimization of  $F$ . This is the main ingredient of the so-called MHD (for Mihalas, Hummer and Däppen) equation of state (see Däppen et al. 1988).

The configuration term  $F_{\text{conf}}$  contains a part  $F_{\text{FV}}$  from the finite volume of the atoms and ions in the gas which clearly prohibits compression to arbitrary densities unless the gas is fully ionized. This term effectively takes care of the ‘pressure ionization’. The second contribution arises from the Coulomb effect, often described in the *Debye-Hückel approximation*,

$$F_{\text{DH}} = -\frac{k_{\text{B}}TV}{12\pi r_{\text{D}}^3}, \quad (9)$$

where  $r_{\text{D}}$  is the Debye length. This is approximately given by

$$r_{\text{D}} \simeq \left[ \frac{k_{\text{B}}T}{4\pi(n_{\text{e}}e^2 + n_{\text{i}}e^2)} \right]^{1/2}, \quad (10)$$

where  $n_{\text{e}}$  and  $n_{\text{i}}$  are number densities of electrons and ions. (For further details, see Kippenhahn & Weigert 1990, §18.4.) Obviously, this term causes changes to the pressure, internal energy *and* the ionization balance, the latter being the dominant effect of the Coulomb interaction e.g. in the solar envelope.

As a final example I note that Eggleton, Faulkner & Flannery (1973) proposed a simple, but thermodynamically consistent equation of state which achieved full ionization in stellar interiors through the inclusion of a correction  $\Delta F_{\text{EFF}}$  to  $F$ , with a corresponding change  $\Delta\mu_{\text{EFF}}$  in the Saha equation (cf. eq. 6). Again, the corresponding changes to  $P, U$ , etc. are obtained as derivatives of  $\Delta F_{\text{EFF}}$ . (Note that in contrast simply imposing full ionization, without other modifications to the equation of state, would not be thermodynamically consistent.) The formulation used for  $\Delta F_{\text{EFF}}$  probably has little physical meaning but has the advantage that the equation of state can be expressed in simple analytical form. The resulting *EFF equation of state* has seen widespread use in stellar modelling; a version which in addition includes the Coulomb effect, the CEFF equation of state (cf. Christensen-Dalsgaard & Däppen 1992) is also in use.

## References

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