ON THE INFLUENCE OF THE TREATMENT OF HEAVY ELEMENTS IN THE EQUATION OF STATE ON THE RESULTING VALUES OF THE ADIABATIC EXPONENT $\Gamma_1$

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INTRODUCTION

Helioseismology and asteroseismology put high demands on the accuracy and consistent numerical realization of the equation of state (for a review see Däppen, these proceedings). This is explicitly illustrated by the helioseismic determination of the helium abundance of the solar convection zone in a recent investigation by Kosovichev et al. (1992). In that work it was observed that details of the treatment of the heavy elements matter more than is intuitively expected. Naively, one would expect an uncertainty of less than $10^{-4}$ in the key thermodynamic quantity, the adiabatic gradient $\Gamma_1$. This is because in material of solar composition the heavy-element abundance is less than about $1.5 \times 10^{-3}$ by number, and under solar conditions the dominant nontrivial contributions to the seismically relevant thermodynamic quantities predicted by modern equations of state agree to a few per cent, even for the much more abundant hydrogen and helium. However, Kosovichev et al. (1992) found that uncertainties in the treatment of the heavy elements translate into discrepancies in $\Gamma_1$ of the order of $10^{-3}$, which is enough to disturb the helioseismic helium-abundance determination significantly. We briefly present the reason below. A forthcoming paper will show more detailed results, though some further information can already be found in papers by Kosovichev et al. (1992) and Christensen-Dalsgaard & Däppen (1992).

Kosovichev et al. (1992) considered solar models based on different equation-of-state tables, computed with the MHD partition-function formalism (Hummer & Mihalas, 1988; Mihalas, Däppen & Hummer, 1988; Däppen et al., 1988). Such different sets of MHD tables were available from previous studies, which had, because of limited computing resources, a simplified treatment of the heavy elements. The simplification was accomplished either by reducing the number of heavy elements (but with a fixed overall mass fraction of 0.02) or by limiting
the number of atoms and ions of the heavy elements that were treated with full internal partition functions (the rest of them having ground states only). At first it would seem that the principal influence of the heavy elements is due to the type of mixture (i.e. the number of heavy elements and their distribution). However, it turned out that the resulting discrepancies in $\Gamma_1$ were really the result of the internal partition functions.

**THE EQUATION-OF-STATE TABLES**

Our nomenclature is the same as that of Kosovichev et al. (1992). We consider three sets of MHD tables, which all have the same mass fractions of the chemical elements H, He, C, N, O, Fe, but are different in their treatment of the internal partition functions of the heavy elements. While all three tables have full MHD partition functions for H, He and He$^+$, they are distinguished in the following way:

* MHD3: no detailed partition functions for C, N, O, Fe and all of their ions, (i.e. only ground-state contributions),
* MHD4: full MHD treatments for C, N, O and all of their ions, and for Fe and Fe$^+$; ground-state contributions for all other Fe ions,
* MHD5: full MHD treatment for all elements and their ions.

**RESULTS AND DISCUSSION**

Figure 1 shows, along a single thermodynamic path (provided by a solar model), the difference between $\Gamma_1$ computed with MHD3 and MHD5 (solid line) and the analogous difference between MHD4 and MHD5 (dashed line). Intuitively, one
might expect some sort of a continuous transition from MHD3 to MHD5 via MHD4. However, this appears to be far from the case, because the difference between MHD4 and MHD5 exhibits a sharp spike between $r/R = 0.95$ and 0.97 that is not evident in the difference between MHD3 and MHD5. The reason for this unexpected behaviour was found by systematically switching on and off all internal partition functions, thus moving smoothly between MHD3 and MHD5. In an ensemble of several heavy elements (and their ions), each ionization zone produces a small well known “dip” in $\Gamma_1$ (relative to the ideal-gas value of 5/3). Since each ionization zone has its characteristic location in the Sun, $\Gamma_1$ is composed of a string of such dips. In the transition from ground-state-only (MHD3) to fully fledged MHD partition functions, each zone of ionization is shifted downwards (see, e.g., Däppen, these proceedings), but the shifted string of all the $\Gamma_1$ dips still looks roughly the same. However, in the intermediate case (MHD4), the lower half of the dips (more precisely those belonging to Fe$^{++}$ to Fe$^{+++}$) is not shifted downwards. Therefore, at the transition (in our case between the ionization zones of Fe$^+$ and Fe$^{++}$) the upper and the lower halves of the string are pushed into each other, causing an artificial local dip from blending the inconsistently treated partition functions. This explains the spike at $r/R = 0.96$ in the dashed line of Figure 1.

CONCLUSION

In principle, it is clear that a full MHD treatment for only a part of the species can produce a certain unrealistic roughness in the thermodynamic quantities. The surprise of this study is the size of the effect. It is due to the strong shift of the ionization equilibrium of heavy elements caused by the MHD treatment. One should therefore definitely refrain from computing the equation of state without full partition functions for all species. Furthermore, since the treatment of bound states is controversial (see Däppen, these proceedings), the results shown in Figure 1 herald a diagnostic potential of helioseismology to probe this important issue of physics.

REFERENCES


