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J. Phys. A: Math. Theor. 42 (2009) 214006 (5pp)

doi:10.1088/1751-8113/42/21/214006

A smooth equation of state for solar and stellar abundance determinations

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Received 20 October 2008, in final form 26 November 2008 Published 8 May 2009 Online at stacks.iop.org/JPhysA/42/214006

Abstract

The modulation of the equation of state by the chemical composition leads to a natural method to determine the helium and heavy-element abundance in the sun and stars. For solar helium this has indeed become the only reliable method. However, one has to keep in mind that the result is only as good as the quality of the equation of state. So far, there are only theoretical formalisms, but no experiments, for the relevant physical conditions. It is obvious that sharp theoretical tools in the form of smooth thermodynamic (and opacity) quantities are crucial for the interpretation of the astrophysical data, both for abundance determinations and improvements of the theory. An emulator of the OPAL equation of state was developed, by which the OPAL equation of state can be applied directly in stellar models, without recourse to pre-computed tables.

PACS numbers: 51.30.+i, 52.25.Jm, 52.25.Kn, 96.60.Jw, 96.60.Ly, 97.10.Cv, 97.10.Tk

1. Introduction

Stellar modeling requires thermodynamic quantities that are smooth, consistent, valid over a large range of temperatures and densities, and incorporate the most important astrophysically relevant chemical elements. Suitable thermodynamic quantities were obtained from the two major opacity efforts that were undertaken in the last 30 years.

One of these efforts is the International Opacity Project (OP; see the books by Seaton 1995, Berrington 1997); it contains the so-called Mihalas–Hummer–Däppen equation of state (Hummer and Mihalas 1988, Mihalas *et al* 1988, Däppen *et al* 1988, Nayfonov *et al* 1999, Trampedach *et al* 2006); hereinafter MHD). It is realized in the so-called *chemical picture*, and it deals with *heuristic* concepts about the modification of atoms and ions in a plasma. Possible open parameters in MHD are therefore atomic and ionic radii (which can be chosen to match observations), and the strength of the assumed micro-field distribution.

1751-8113/09/214006+05\$30.00 © 2009 IOP Publishing Ltd Printed in the UK



Figure 1. Difference between the squared sound speed from inversion and two solar models. Figure by S Basu.

The other effort is being pursued at the Lawrence Livermore National Laboratory by the OPAL group (Iglesias and Rogers 1996, Rogers *et al* 1996); its equation of state is based on a detailed *systematic* method to include density effects in a plasma (Rogers 1977, 1986, Rogers and Nayfonov 2002). This so-called *physical picture* provides a systematic method to include nonideal effects. In OPAL, any effects of the plasma environment on the internal states are obtained directly from the statistical–mechanical analysis, rather than by assertion as in the chemical picture. But that also means that in the physical picture there is not much room for adjustable parameters. Both MHD and OPAL equations of state have been successfully tested in solar models, using observed solar-oscillation data (Däppen 2006). Figure 1 shows a typical result of such a numerical inversion of observed frequencies (Basu and Christensen-Dalsgaard 1997). It shows the relative difference (in the sense the sun model) between the squared sound speed obtained from inversion of oscillation data and that of a two standard solar models. The two solar models used are identical in all respects except the equation of state (MHD and OPAL, respectively).

2. The thermodynamic signature of element abundance

An important application of high-precision and high-accuracy equations of state is the determination of the chemical composition of the sun and stars. The idea is to determine chemical abundances directly through seismological observations, in contrast to calibration of models, was first proposed by Gough (1984) who realized that one can exploit the fact that the principal deviation of pressure-density relation from the simple classical ideal gas law is due to partial ionization. More precisely, in ionization zones the adiabatic exponent

 $\gamma_1 = (\partial \ln p / \partial \ln \rho)_{ad}$ (p and ρ being the pressure and density, respectively) is lowered from its ideal value 5/3. This lowering makes the determination of the abundance of every element possible, at least in principle.

For helium, this method is the only game in town: the sun's helium abundance cannot be reliably measured by alternative means. The helioseismic method revealed, somewhat surprisingly, that the helium abundance Y in the solar convection zone lies between 0.24 and 0.25, substantially lower than the calibrated values for the age-zero sun (Baturin *et al* 2000), for which typically Y is between 0.27 and 0.28. This depletion in the convection zone drew renewed attention to gravitational settling of helium and heavier elements. As a result, solar models with settling were taken seriously since they are in better agreement with helioseismological data. Now settling is a firm part of standard solar models (Christensen-Dalsgaard and Däppen 1996). The major drawback of this thermodynamic abundance determination is the entanglement of the abundance uncertainty with that of the equation of state. This entanglement is fundamental and difficult to overcome, unless our confidence in the equation of state were to rise considerably. To illustrate, we note that there is a key thermodynamic quantity found by (Gough 1984),

$$\Theta = \frac{1 - \gamma_1 - \gamma_{1,\rho}}{1 - \gamma_{1,c^2}},$$

with

$$c^2 = \gamma_1 \left(\frac{p}{\rho}\right), \qquad \gamma_{1,\rho} = \left(\frac{\partial \ln \gamma_1}{\partial \ln \rho}\right)_{c^2}, \qquad \gamma_{1,c^2} = \left(\frac{\partial \ln \gamma_1}{\partial \ln c^2}\right)_{\rho}.$$

The quantity Θ is a powerful tracer of the abundance of individual chemical elements. In an adiabatically stratified part of a star it can be calibrated using the sound-speed gradient, itself an observable quantity thanks to the seismology of the sun and stars (for more details, see Baturin *et al* 2000).

3. OPAL emulator

The computation of the aforementioned quantity Θ , which is based on third-order derivatives of the free energy, requires a very smooth thermodynamic formalism. The published, precomputed tables of the OPAL equation of state are only marginally adequate for the task. As a consequence, we have been motivated to develop an OPAL emulator. We admit that such an approach is purely phenomenological, and it does not contribute to the improvement of the science of the equation of state. However, our resulting tool can still be very useful in practical applications. The emulator has been realized in the intuitive free-energy-minimization approach, specifically with new terms added to MHD. These terms were directly borrowed from OPAL and have no natural foundation in the chemical picture, and so they were obviously missing in the original MHD equation of state. More precisely, the principal new ingredient added to MHD mimics the role of Coulomb wavefunctions for the free (scattering) states and the associated Planck-Larkin partition function (PLPF) (Rogers 1986). The most recent version (Mao 2008) is an upgrade of the pure-hydrogen work by Liang (2004) to a hydrogenhelium mixture. The quality of the emulator is illustrated in figure 2, for the conditions found in the envelope part of a standard solar model (location being identified by temperature T). Besides pressure, the adiabatic exponent $\gamma_1 = (\partial \ln p / \partial \ln \rho)_{ad}$, the strain coefficient $\chi_t = (\partial \ln p / \partial \ln T)_{\rho}$ and the isothermal compression coefficient $\chi_{\rho} = (\partial \ln p / \partial \ln \rho)_T$ are being compared.

As revealed by the figure, the match between OPAL and our emulator is not exact. Such an exact match is fundamentally impossible, since unlike OPAL our emulator formalism is not



Figure 2. Relative difference of thermal quantities (*a*) log *p*, (*b*) γ_1 , (*c*) χ_t and (*d*) χ_ρ in a solar model, in the sense old MHD—OPAL and new MHD—OPAL, respectively. The three curves represent: the original MHD model (+), an intermediary MHD with the PLPF (×) and finally the OPAL emulator (*). In the figure, by definition, OPAL is the dotted zero line. See the text for the definition of the thermodynamic quantities.

an activity expansion. However, although the emulator is not exact, its quality can be assessed none the less by considering the 'distance' between, on the one hand, the emulator, and on the other hand, either OPAL or its closest competitor for stellar modeling, MHD. Figure 2 makes it clear that compared with the difference between MHD and OPAL, the emulator lies one order of magnitude closer to the latter than to the former. Furthermore, a detailed study of the error of helioseismic inversions such as that underlying figure 1 (Basu and Christensen-Dalsgaard 1997) suggests that the remaining differences between the emulator and OPAL are smaller than the current observational astrophysical errors. Therefore, for practical purposes, our emulator and OPAL describe the same physics. Finally, we note in passing that some of the wiggles that show up in the difference between the emulator and OPAL are actually due to the OPAL tables themselves (and the interpolations therein) and not to our (smooth) emulator.

4. Conclusions

We have developed an emulator of the OPAL equation of state. It is especially suited for abundance determinations. It can be used directly in stellar models, without recourse to the official OPAL tables from the Lawrence Livermore National Laboratory. As long as the OPAL source code remains proprietary, this emulator is an attractive smooth alternative to the tables.

Acknowledgments

This work was supported by the grant AST-0307578 of the National Science Foundation.

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