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THE STELLAR OPACITIES

S. Turck-Chièze[1], D. Gilles[1], F. Gilleron[2], J.C. Pain[2] and the international OPAC consortium

Abstract. Opacities are fundamental ingredients of stellar physics. Helioseismology and asteroseismology have put in evidence anomalies that could be attributed to an insufficient knowledge of the photon-plasma interactions. We work on a revision of this plasma physics in the conditions where the anomalies have been found: the region of the iron opacity peak near log T= 5.2 and the inner radiative region of Sun and solar-like stars. The international OPAC consortium performs new calculations, compares them and looks for the origin of their differences. In parallel, experimental campaigns are realized, others are in preparation to validate some conclusions on the reliability of the new proposed calculations. New tables for astrophysics will be performed in the framework of the ANR OPACITY and their influence on seismic observables will be studied. We explicit here the difficulty of the computations together with some computation resources.

Keywords: helioseismology, atomic processes, diffusion, oscillations, plasma, radiative transfer

1 Introduction

Seismology of stars has the potential to be a driver for introducing dynamical processes in stellar modeling. Rotation profiles begin to be determined in different types of stars and the subsurface magnetism is now followed in time for the Sun. Precise neutrino fluxes will have in parallel the potential to catch deep motions in the solar core. Face to this tremendous progress, it is important to ensure the reliability of the microscopic physics and to begin to consider the interplay of macroscopic physics on microscopic one.

A new investment on the photon-plasma interaction is justified by some evident discrepancies between seismic observations and their predictions. Two of them are well known: the solar sound speed profile and the excitation of modes of SPB and β-Cephei stars. In this invited review, we show first the two astrophysical conditions that we would like to improve. Then we present the general strategy of computation of opacity spectra, the used codes, our different actions and results and finally the future plan and some computer performances.

2 The astrophysical facts

Helioseismology produces an exigent check of the standard solar model (SSM) hypotheses. Today a clear discrepancy exists between their respective sound speed profiles. This fact is confirmed by the marginal agreement between the neutrino flux predictions of SSM and their detections, but one has identified a very good agreement between helioseismology and neutrinos through a seismic model (Turck-Chièze & Couvidat 2011; Turck-Chièze 2013). So the hypotheses of the SSM are questioned and in particular the reliability of the opacity coefficients. Among others, two possibilities are proposed, a direct inaccurate photon plasma calculations or an indirect effect coming from an inaccurate central composition of the Sun. If the second solution is the good one, that means that one can question not only directly the opacity calculations but also the way one treats the slow gravitational settling and the joined radiative accelerations of each element, in particular the heavier ones: C, N, O, Fe. In the two cases, a detailed examination of the whole calculation of the transfer of radiation is required.

On the other side, asteroseismology observes now a large range of stars of different masses. In particular it has put in evidence some excited modes which were not predicted by stellar models, in SPB and β-Cephei. These modes are supposed to be excited by κ mechanism, involving the iron group opacity peak around log T =5.2, the main contributors are iron, nickel and chromium (Pamyatnykh 1999; Zdravkov & A. 2009). This

[1] SAp/IRFU/CEA, CE Saclay, 91191 Gif sur Yvette cedex, France
[2] CEA/DAM/DIF, 91297 Arpajon, France

fact has been observed for different metallicities (Salmon et al. 2012). So opacities have been suspected, more surprisingly in some specific cases, the OP tables were more predictive and in other cases, the OPAL tables have appeared more appropriate, creating a confusion on which tables are the good ones to use for these stars.

3 The strategy for performing new opacity tables

The mentioned difficulties complicate the interpretation of the seismic observations of Sun and intermediate-type stars. Stellar evolution equations use the mean Rosseland values $\kappa(T, \rho, X_i)$ in the radiative transfer equation but radiative accelerations use directly the spectral opacity $\kappa_\nu(T, \rho, X_i)$ (Turck-Chièze et al. 2009) so any progress needs not only to modify the used tables for Astrophysics but also to compute the whole energy spectra for individual elements and then tables for a required mixture. Three years ago, we have decided different actions and the formation of the international OPAC consortium * composed by astrophysicists, plasma physicists and experimentalists (Turck-Chièze et al. 2011a) to gather together all the useful specialities. We define thermodynamical conditions available in laboratory and useful for astrophysics. We compare new opacity calculations done by different groups of different institutes between them and with the existing tables to estimate the validity of the approximations which are generally used to limit the computation time (Turck-Chièze et al. 2011a), we perform experiments when it is possible to guarantee better calculations before delivering them to the astrophysical community (Turck-Chièze et al. 2011b, 2013), the objectives of the ANR OPACITY.

In the envelopes of SPB or β-Cephei, the $10^{-6} - 10^{-7}\mathrm{g/cm^3}$ density is too small for a foil of iron or nickel to be manufactured. So when the astrophysical conditions are not accessible to laboratory, we work on equivalent conditions, that means on conditions corresponding to the same distribution of ionic charges, typically slightly higher temperature and 2 or 3 orders of magnitude higher in density. Present laser facilities like LULI2000 in France deliver sufficient power to perform such experiments. For the solar radiative interior and for solar-like stellar conditions $\mathrm{T} = 2\,\mathrm{to}\,15\,10^6\,\mathrm{K}, \rho = 0.2\,\mathrm{to}\,150\,\mathrm{g/cm^3}$, one needs more energetic facilities like LMJ in France which will be operational in 2016 or the NIF in USA. A first tentative by Bailey et al. (2007) has been realized with the Z pinch at Albuquerque.

Such activities are useful for stellar physics but also for fusion research, inertial fusion in LMJ and magnetic fusion in ITER as in these three disciplines the interaction of photon with the plasma is required in very large thermodynamical conditions. The main difficulties come from the numerous calculations to compute and the related computer times. Ten years ago, the available machines were limited in computation capabilities and approximations were generally made. In addition to that problem, plasma effects play some role that only new experiments could confirm if one can reach high density and high temperature with laser facilities.

4 Rapid description of the used codes

The different codes of the collaboration use different approximations, which when justified, can tremendously reduce the number of transitions to perform, see Figure 1. The exact description of atomic structure relies on the fine structure calculation of electronic configurations, i.e. the determination of the energy levels (characterized by the total angular momentum J) connected by electric-dipole lines (DLA: detailed-line accounting). The numerous levels can be grouped into relativistic configurations, connected by spin-orbit-split arrays (SOSA) represented by Gaussian distributions whose strength, average energy and variance can be calculated analytically using Racah algebra. The relativistic configurations in turn can be grouped into non-relativistic configurations, connected by unresolved transition arrays (UTA) also represented by Gaussian distributions. If the number of configurations remains too large, they can be grouped finally into “superconfigurations” (a superconfiguration is an ensemble of configurations close in energy) connected by super-transition arrays (STA). The total opacity is the sum of photo-ionization, inverse Bremsstrahlung, scattering spectra and a photo-excitation spectrum relying on the following expression for the opacity:

$$\kappa\,(h\nu) = \frac{1}{4\pi\epsilon_0}\frac{\mathcal{N}}{A}\frac{\pi e^2 h}{mc}\sum_{X\to X'} f_{X\to X'}\mathcal{P}_X\Psi_{X\to X'}(h\nu)$$

*S. Turck-Chièze, J. E. Ducret, D. Gilles, M. Le Pennec, SAp/ CEA France, C. Blancard, T. Caillaud, P. Cossé, T. Blenski, J. Farriaut, G. Faussurier, F. Gilleron, J. C. Pain, M. Poirier, C. Reverdin, V. Silvert, F. Thais, B. Villette CEA France, F. Delahaye, C. Zeippen Obs. Meudon France, S. Bastiani Ecole Polytechnique France, M. Busquet, ARTEP, USA, J. Bailey, G. Loisel Albuquerque, USA, J. Guzik, J. Colgan, D.P. Kilcrease, N.H. Magee, Los Alamos, USA, and J. W. Harris AWE England.

where h is Planck constant, $\mathcal{N}$ the Avogadro number, ϵ_0 the vacuum polarizability, m the electron mass, A the atomic number and c the speed of light. $\mathcal{P}$ is a probability, f an oscillator strength, $\Psi(h\nu)$ a profile. The sum $X \to X'$ runs over lines, UTAs or STAs of all ion charge states present in the plasma. Special care is taken to calculate the probability that can be either a level, a relativistic configuration, a non-relativistic configuration or a superconfiguration as it is the starting point for different transitions (DLA, SOSA, UTA, STA).

We rapidly describe some codes of the collaboration, others are also described in Turck-Chièze et al. (2011a).

The SCO-RCG opacity code (Porcherot et al. 2011) combines DLA calculations (when they are tractable and useful) with statistical approaches (UTA, SOSA and STA) when the DLA calculation is impossible from a computational point of view or if the lines coalesce into unresolved structures due to physical broadening mechanisms.

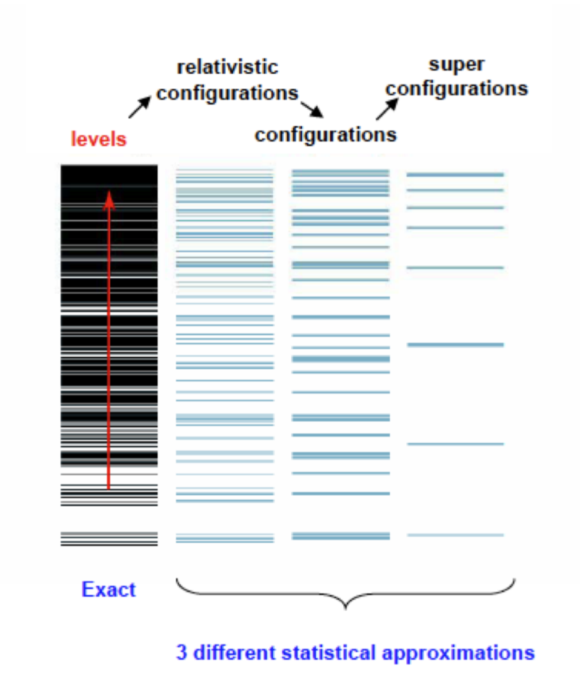

Fig. 1. : The different approximations generally found in opacity calculations.

OP (Opacity Project) is an on-line atomic database used in astrophysics (Badnell et al. 2005; Seaton 2007). TOPbase contains the most complete dataset of LS-coupling term energies, f-values and photoionization cross sections for the most abundant ions (Z = 126) in the universe. They have been computed in the close-coupling approximation by means of the R-matrix method with innovative asymptotic techniques. TOPbase also contains large datasets of f-values for iron ions with configurations 3sx 3px 3dx, referred to as the PLUS-data, computed with the atomic structure code SUPERSTRUCTURE.

The OPAS code (Blancard et al. 2012) calculates radiative opacity in LTE. Based on the average atom model SCAALP, it combines detailed configurations and level accounting treatments. The bound-bound opacity uses detailed line accounting and/or statistical methods. The bound-free opacity neglects the configuration level splitting. In warm dense matter, plasma and many-body effects can be important, the free-free opacity is obtained by interpolating between the Drude-like opacity and the opacity derived from the Kramers formula including a Gaunt factor and an electron degeneracy effect correction. Photon scattering by free electrons includes collective effects and relativistic corrections.

ATOMIC is a multi-purpose code (Colgan et al. 2013), developed in Los Alamos, that generates LTE or non-LTE quantities at various levels of approximation. Just now, they compute new LTE opacity data for elements from H to Zn. The tables up to Ne are complete, and a new Fe opacity table will be available soon. The calculations include fine-structure details and represent a systematic improvement over the LEDCOP legacy code. They incorporate atomic structure data from the CATS code, based on Cowan's atomic structure codes, and photoionization cross section data computed from the Los Alamos ionization code GIPPER. They use a new equation-of-state (EOS) model based on the chemical picture. ATOMIC incorporates some physics packages from LEDCOP and improved free-free cross sections and additional scattering mechanisms.

HULLAC code has been developed by Bar-Shalom et al. (2001). It is a powerful fine-structure relativistic code able to generate thousands of configurations and billions of lines and to compute LTE and non-LTE spectra. But the number of levels to be treated in full CI mode often give dramatic increase of the computation time. The flexibility of HULLAC-v9 (Busquet et al. 2006) allows to see the role of different terms or CI approximations. In the full CI mode the computation of fine structure levels is chosen for defined groups of levels (GRL), see Busquet & al (2012). Selecting the CIinNRC mode, HULLAC-v9 computes the usual Relativistic CI (RCI) between all levels of one Non Relativistic Configuration (NRC). The diagonalisation of the Hamiltonian matrix for all levels of same J is performed in a GRL. It is also possible to turn off the CI calculation using sub mode NoCI. Other GRL can be selected.This code is used in Saclay (Gilles et al. 2011, 2012).

HULLAC, OP and ATOMIC are the only calculations that introduce full CI, i.e. CI between all levels (Bar-Shalom et al. 1999). So these codes are extremely useful for some specific checks of the different approximations. They are also used to calculate precisely the interaction when the other codes are insufficient. OPAS, SCO-RCG are interesting to qualify the deep interiors.

5 Present results, next s

First comparisons between codes has been done for iron and nickel (T = 15 eV and 27 eV, and ρ = 3-5 mg/cm^3) using OP, LEDCOP, OPAS, STA, SCO-RCG codes. They correspond to conditions similar to the iron opacity bump that excites the intermediate-type stellar oscillations. Detailed comparisons are given in Gilles et al. (2011); Turck-Chièze et al. (2013) including ionic distribution, spectra and mean Rosseland and Planck values. Figure 2 summarizes this study in showing the compared spectra that present very different behaviors, in particular for nickel. The Rosseland values vary by more than 30% for iron and up to a factor 3 for nickel. So a complementary investigation of the differences has been realized with detailed HULLAC and ATOMIC codes.

5.1 First conclusions

The HULLAC and ATOMIC codes help us to understand the discrepancies between OP and OPAL in the iron bump which excites the modes observed in β-Cephei and SPB stars. We note that iron opacities are better estimated by OP calculations than by OPAS, LEDCOP, SCO-RCG ones because the interaction of configuration reduces the spectral opacity between 40-60 eV (so not too far from the maximum of the mean Rosseland values) (Gilles et al. 2012). But OP nickel opacities are not correct in the two conditions shown in Figure 2. Indeed the differences for nickel have a different origin: the OP calculations have been incorrectly extrapolated from iron calculations. ATOMIC full CI and HULLAC predict values between the OP and OPAL results. In that case, the interaction of configuration is located at lower energy and has a smaller impact on the mean Rosseland values. The inappropriate OP nickel spectra have been confirmed by the first experiment performed at LULI2000 (Turck-Chièze et al. 2013), see also Loisel (2010) for the description of the experimental set up. The second campaign shows that all the other calculations are in better agreement than OP. These facts are not in contradiction with the assumptions of Salmon et al. (2012).

The iron group peak varies strongly with stellar age, mass and composition, so the opacities of the different elements of the iron group (chromium, iron, nickel) need to be precisely calculated on a range of T and Ne that we are determining (Le Pennec & Turck-Chièze 2013). News tables are in construction thanks to HULLAC and ATOMIC codes. Then, radiative acceleration and non LTE-conditions will also be investigated.

5.2 Work in progress

In parallel to this activity, another one is dedicated to solar-like stars, both on new spectra from OPAS and the preparation of new tables and on the preparation of experiments on large facilities in order to focus first on the region of transition between radiative and convective zones.

6 Performances of the calculations

It is important to consider the consuming time to perform the astrophysical tables. We give here some estimates of the spectra calculations for individual elements.

Let first consider the Sun and OPAS calculations that are not detailed calculations. These calculations are done in CEA/DAM on 2PC 8CPU, 16 Goctets RAM, the calculations for Z < 10 are done in several seconds as

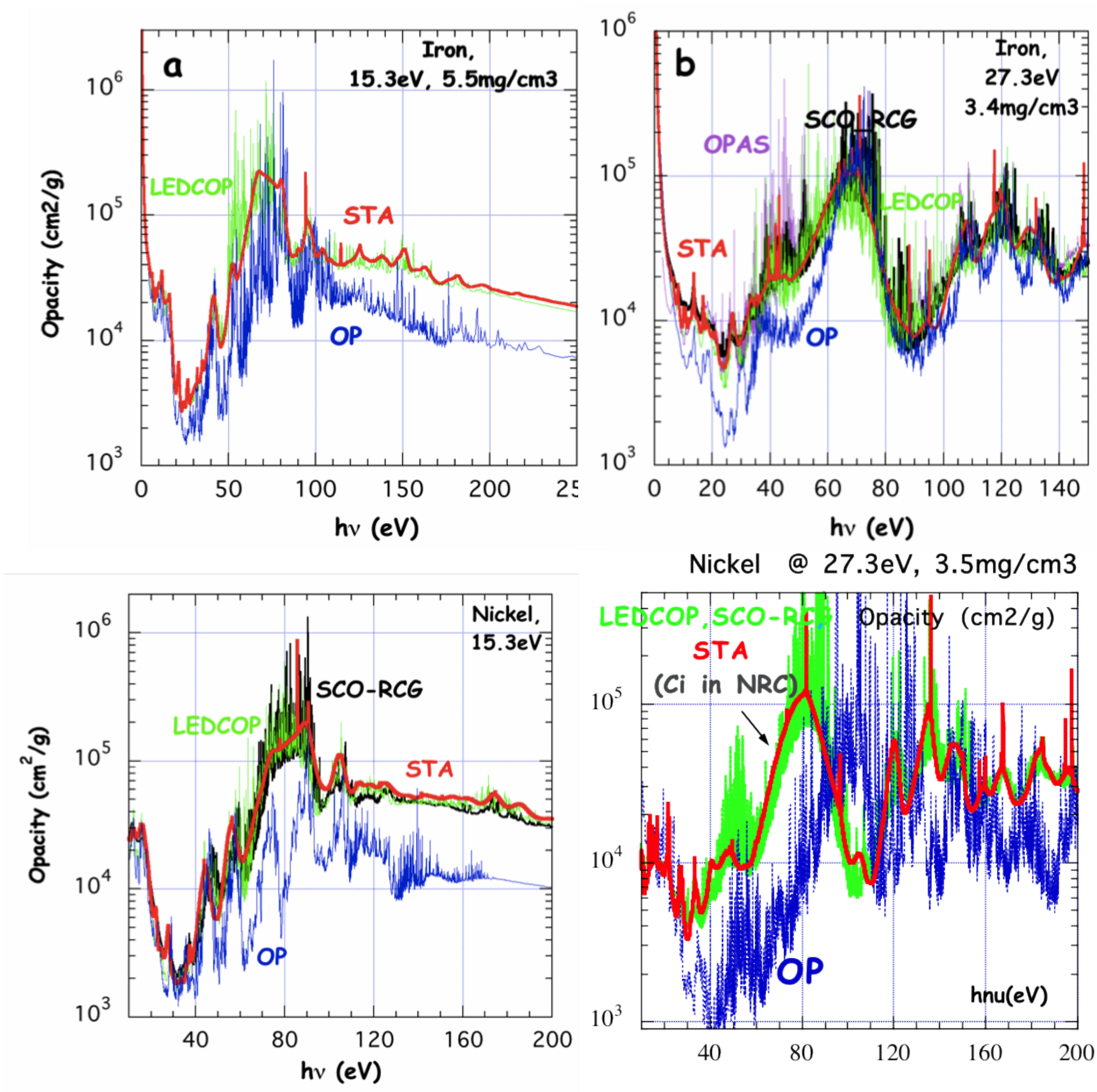

Fig. 2. : Comparison of calculations for iron and nickel in conditions near the realized LULI experiments, equivalent conditions of the opacity iron bump of the envelopes of intermediate-type stars. From Gilles et al. (2011)

these elements are totally ionized, for Z= 20, several seconds at the center (this element is also totally ionized), but 6 mn at the base of the convective zone (BCZ). In the case of iron, 20s at the center and 40h at the BCZ. These performances have been obtained on the basis of 100 Goctets of stored fundamental information to speed up these calculations.

For envelopes of stars, the ionic distribution is extremely unfavorable and the number of levels tremendous (see Figure 3), the OP calculations take several months for one condition. The HULLAC calculations are performed on Intel computer with 20 cores, 64 Goctets RAM and more than 1 Tera of stored memory. For the mentioned conditions discussed previously, the main contributors come from ions Fe IV (Z^*= 3) to Fe XII (Z^*=13) where Z^* is the number of free electrons. The size of the matrixes depends on the number of levels NI included in the atomic description which depends itself on the number of active electrons Ne defined as Ne = Z-Z^*-10 for M shell transitions with closed shells n=1 and n=2. Moreover the full CI treatment involves also a large number of coefficients NCI which can be so large that the calculation can be hardly tractable, so extreme care and strategy must be developed to lead to accurate results. For example, for FeV one counts Nl= 301610, NCI= 3 061 241 715; for FeX Nl= 117427, NCI= 493 527 664, which requires a computer time of 425 h to be

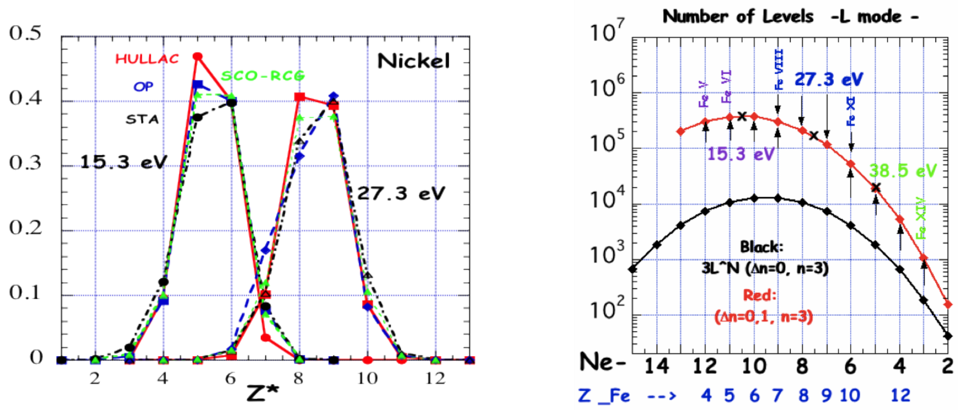

Fig. 3. Left: Ionic distribution of nickel obtained by different calculations for the two thermodynamical conditions, idem for iron. **Right:** Number of levels considered in HULLAC in function of the number of active electrons, the red curve corresponds to the transitions n=3 to n= 4, and the black curve to n=3 n=3.

performed. For Fe IX, Nl= 210 631, NCI = 1 488 790 396, so one needs to properly choose the transitions to calculate to converge in the calculation. In these conditions it is important to compare different codes to take the adopted decision in function of the range of photon energy that one considers and the accuracy we need to get.

In the ANR OPACITY, we hope to distribute new tables which have been largely discussed and for which we have decided when approximations are relevant. In parallel we continue to prepare new experiments to validate some choices.

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