High-precision equation-of-state formalisms for solar and stellar modeling

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or...

Here comes the Sun!
Observations!
Helioseismology: “Looking” into the Sun’s interior!

Discovery:

- 1960 Leighton, Noyes & Simon
- Irregular, quasi-periodic motion

\[ v \approx 100 \, \frac{\text{m}}{\text{s}} \]

\[ P \approx 5 \, \text{min} \]

- Hence name: “5-minute oscillations”
State of the art

- High spatial resolution (>1024 X 1024)
- Measure line-of-sight velocity at every pixel, at least once every 30s
- Doppler effect on given absorption line:
Single Dopplergram
(30-MAR-96 19:54:00)

SOI / MDI
Stanford Lockheed Institute for Space Research
4 typical oscillation modes

\[ l=2 \quad m=0 \quad l=10 \quad m=5 \quad l=20 \quad m=0 \quad l=100 \quad m=100 \]
Analogy (2-D): bell (from G. Houdek)

1342.3 Hz
1469.7 Hz
2605.9 Hz
Time dependence of a single mode

- Project the velocity pattern on a single mode, for each fixed \( l \) and \( m \) (analogous to Fourier coefficient)

\[
c_{lm}(t) := \int_{\text{Sun}} v(\theta, \phi) Y_l^m(\theta, \phi) d\Omega
\]
Interlude: no Sun at night!

What is to be done? Что делать?

South Pole
Networking (GONG)
Space (SOHO)
South Pole
GONG Stations
SOHO Instrument
SOHO Launch (Dec 2, 1995)
SOI to be launched later this year!
End of interlude
Time-series of one oscillation mode

Source: SOHO/MDI instrument
Power spectrum after Fourier transform

From: SOHO/GOLF instrument
More than $10^7$ modes observed

Single mode velocity tiny: $\approx 0.1 - 1 \ \text{m/s}$

Incoherently, the amplitudes add up to the observed total velocity of $\approx 100 \text{m/s}$

Data represented in so-called $\nu - \ell$ diagrams

High Q value (weeks of coherence!)
Modern $\nu - \ell$ diagram

Source SOHO/MDI instrument
Modeling!
Forward problem

Nobody does it in this way (!), but ...

\[
\left[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\frac{1}{\rho} \nabla p - \nabla \phi
\]

\[
\left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] = 0
\]

\[
\left[ \frac{\partial s}{\partial t} + \mathbf{v} \cdot \nabla s \right] = -\frac{1}{T} \epsilon_{\text{nucl}} - \frac{1}{\rho T} \nabla \cdot \nabla F
\]

\[
\Delta \phi = 4\pi G \rho
\]

... let’s illustrate the method, using the **same equations**, both for the equilibrium and the oscillation problem
First: the equilibrium solution

- Put all red stuff to 0!
- Obtain the usual equilibrium equations (for simplicity assume (i) spherical symmetry; (ii) no convection)

\[
\frac{dp}{dr} = -\frac{GM_r \rho}{r^2}
\]

\[
L_r = 4\pi r^2 F
\]

\[
\frac{dL}{dr} = 4\pi r^2 \rho \epsilon_{\text{nucl}}
\]

\[
\frac{dT}{dr} = -\frac{3\kappa \rho L}{64\pi \sigma r^2 T^3}
\]
Material properties are mandatory!

- So far all equations the same for all stars
- Wealth of different stars only enters with the constituent equations

\[
\begin{align*}
\rho &= \rho(T, \rho, X) \\
\kappa &= \kappa(T, \rho, X) \\
\epsilon &= \epsilon_{\text{nuc}}(T, \rho, X) \\
s &= s(T, \rho, X) \\
F &= K(\nabla T; T, \rho, X) \\
(Diffusive radiation: \; F &= -\frac{16\sigma T^4}{3\kappa\rho} \nabla T)
\end{align*}
\]
BTW: Not only for variety!

Material properties are essential for the (parametric) evolution of stars!
Second: oscillation equations

Once equilibrium model found, solve red part by putting black part $= 0$

\[
\left[ \frac{\partial v}{\partial t} + v \cdot \nabla v \right] = -\frac{1}{\rho} \nabla p - \nabla \phi = 0
\]

\[
\left[ \frac{\partial \rho}{\partial t} + \text{div}(\rho v) \right] = 0
\]

\[
\left[ \frac{\partial s}{\partial t} + v \cdot \nabla s \right] = -\frac{1}{T} \epsilon_{\text{nucl}} - \frac{1}{\rho T} \text{div}F = 0
\]

If appropriate, use linearization, spherical harmonics, adiabatic $\Rightarrow \nu_{n\ell}$
Result: model frequencies

Figure: J. Christensen-Dalsgaard
Apply “O-C Diagrams”

- O = “Observation”
- C = “Computation”

(Q_{nl} is a scale factor. Details see: Christensen-Dalsgaard & Däppen 1992, A&A Rev. 4, 267)
Impact: two similar solar models...

- Identical models, except for their equations of state. One is with Debye-Hückel screening, one without. Their adiabatic exponents are:

Dashed: with screening  
Solid: without screening

From: Christensen-Dalsgaard & Däppen 1992, A&A Rev. 4, 267
There is DH in the Sun...

Christensen-Dalsgaard, Däppen & Lebreton 1988, Nature 336, 634
The physicists were not overwhelmed!
Result of the “helium-hump” method (and similar techniques, e.g., by Dziembowski, Thompson, Vorontsov, Antia, Basu…)

\[ Y = 0.24 \ldots 0.25 \]

inside the solar convection zone
Whatever the value of Y thus obtained, the result is entangled with the 
uncertainty in the equation of state!
Now we have a heavy-element abundance problem: 
$Z=0.018$ or $Z=0.012$??

Helioseismology and EOS work shall solve it!!
Major EOS Efforts
Two main approaches: introduction

- Free-energy minimization
  - Chemical picture
  - Intuitive, but highly practical

- Grand-canonical expansions
  - Physical picture
  - Systematic method for non-ideal corrections
Chemical picture

- Treat compounds as fundamental entities
- Reactions \( (H \leftrightarrow H^+ + e^-) \), etc.
- Constraints \( (N_H + N_p = \text{const.}) \), etc.
- Minimize \( F(T, V, N_H, N_p, N_{e-}, ...) \)
  
  \[ F_{\text{tot}} = F_{\text{nuc}} + F_e + F_{\text{interactions}} + ... \]

- In practice, cook a free energy (intuition!)

- Consistent (formally!) \( p = -\left(\frac{\partial F}{\partial V}\right)_T \), etc.
Example: MHD

- Fairly conventional realization (chemical picture)
- Key ingredient: **occupation probabilities**


\[ Z_{jk}^{\text{int}} = \sum_i w_{ijk} g_{ijk} \exp \left( -\beta E_{ijk} \right) \]

\[(w_{ijk})_{\text{neutral}} = \exp \left[ -\left( \frac{4\pi}{3V} \right) \sum_{j',k'} N_{j'k'} (r_{ijk} + r_{1j'k'})^3 \right] \]

\[(w_{ijk})_{\text{charged}} = \exp \left\{ - \left( \frac{4\pi}{3V} \right) 16 \left[ \frac{(Z_{jk}+1)^{1/2}e^2}{K_{ijk} x_{ijk}} \right]^{3/2} \sum_{j',k'} N_{j'k'} Z_{j'k'}^{3/2} \right\} \]
Physical picture

- Only electrons and nuclei are fundamental
- No reactions
- Quantum mechanics and statistical mechanics dealt with simultaneously
- Nothing to minimize
- Consistent (not just formally!)
Example: OPAL/ACTEX

- First **successful stellar modeling** with an equation of state in the physical picture (LLNL)


- Key points: **systematic expansions**
  
  \( z = \text{activity} \)

  \[
  \frac{p}{k_B T} = z + z^2 b_2 + z^3 b_3 + \ldots ; \quad \rho = \frac{z}{k_B T} \frac{\partial p}{\partial z}
  \]

  Planck-Larkin Partition Function

  \[
  \text{PLPF} = \sum_{nl} (2l + 1) \left[ \exp\left(-\frac{E_{nl}}{kT}\right) - 1 + \frac{E_{nl}}{kT} \right]
  \]
$c^2$ Inversions (numerical; Sun-Model)

Basu & Christensen-Dalsgaard
Intrinsic $\gamma_1$ inversions (Sun-Model)

- Filled (1-4): chemical picture (MHD)
- Open (5-8): physical picture (ACTEX)

Details in:
S. Basu,
W. Däppen,
A. Nayfonov, 1999
OPAL fares better than MHD...

- Why? Likely answer:
  - There is no PLPF in MHD
  - There are no scattering states in MHD

- Open question: is it fundamentally impossible to find PLPF entirely from within the chemical picture?
Try emulating OPAL!

- **OPAL simulator** for a quantitative study, which brings the OPAL program to **public domain** for the first time (so far H-He only, but more to come)
- Incorporating **scattering-state terms and PLPF** into MHD
- Comparing **thermodynamic quantities** of the modified MHD formalism with OPAL results
Numerical results (Mao, 2008)
Tool for the community

- To get rid of the ugly interpolation errors of OPAL, incorporate emulator into an in-line formalism (work in progress by USC group)
There are exact density expansions, for instance the Feynman-Kac [FK] path-integral computations [1] or Green-function calculations [2],

The coefficients in these expansions are exact,

Problem is the domain of applicability; thus, exact yes, but only for very simple compositions.

\[
\beta P = \sum_\alpha \rho_\alpha - \frac{\kappa_D^3}{24\pi} \\
+ \frac{\pi}{6} (\ln 2 - 1) \sum_{\alpha, \beta} \beta^3 e_\alpha^3 e_\beta^3 \rho_\alpha \rho_\beta \\
- \frac{\pi}{\sqrt{2}} \sum_{\alpha, \beta} \rho_\alpha \rho_\beta \lambda_{\alpha\beta}^3 Q(x_{\alpha\beta}) - \frac{\pi}{3} \beta^3 \sum_{\alpha, \beta} \rho_\alpha \rho_\beta e_\alpha^3 e_\beta^3 \ln (\kappa_D \lambda_{\alpha\beta}) \\
+ \frac{\pi}{\sqrt{2}} \sum_{\alpha} \frac{(-1)^{2\sigma_\alpha + 1}}{(2\sigma_\alpha + 1)} \lambda_{\alpha\alpha}^3 \rho_{\alpha}^2 E(x_{\alpha\alpha}) \\
- \frac{3\pi}{2\sqrt{2}} \beta \sum_{\alpha, \beta} e_\alpha e_\beta \kappa_D \rho_\alpha \rho_\beta \lambda_{\alpha\beta}^3 Q(x_{\alpha\beta}) \\
- \frac{\pi}{2} \beta^4 \sum_{\alpha, \beta} \rho_\alpha \rho_\beta e_\alpha^4 e_\beta^4 \kappa_D \ln (\kappa_D \lambda_{\alpha\beta}) \\
+ \frac{3\pi}{2\sqrt{2}} \beta \sum_{\alpha} \frac{(-1)^{2\sigma_\alpha + 1}}{(2\sigma_\alpha + 1)} \lambda_{\alpha\alpha}^3 \rho_{\alpha}^2 e_{\alpha}^2 \kappa_D E(x_{\alpha\alpha}) \\
+ \frac{1}{16} \sum_{\alpha} \frac{\beta^2 \hbar^2 e_\alpha^2}{m_\alpha} \kappa_D^3 \rho_\alpha + \pi \left(\frac{1}{3} - \frac{3}{4} \ln 2 + \frac{1}{2} \ln 3\right) \times \\
\sum_{\alpha, \beta} \beta^4 e_\alpha^4 e_\beta^4 \kappa_D \rho_\alpha \rho_\beta \\
+ C_1 \sum_{\alpha, \beta, \gamma} \beta^5 e_\alpha^3 e_\beta^4 e_\gamma^3 \kappa_D^{-1} \rho_\alpha \rho_\beta \rho_\gamma \\
+ C_2 \sum_{\alpha, \beta, \gamma, \delta} \beta^6 e_\alpha^3 e_\beta^3 e_\gamma^3 e_\delta^3 \kappa_D^{-3} \rho_\alpha \rho_\beta \rho_\gamma \rho_\delta
\]
Extension of FK to higher terms & creation of in-line tool:

Papers II & III in progress

Collaborators:
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Katie Mussack, Los Alamos
Exact Option (in another sense...)

SAHA-S
SAHA-S EOS

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• References:
SAHA-S is part of a larger solar-modeling effort [ISTC 3705]. It is a serious alternative to OPAL (and MHD). It is based on a systematic development, and it contains a modified Planck-Larkin partition function.

Many participants and collaborators: Loboda-Shadrin et al., Baturin-Ayukov et al., Redmer group, Christensen-Dalsgaard, USC group, etc.
Very promising first results:
Inversion in solar convection zone (Baturin et al.)

Preliminary results of $\Gamma_1(r)$ inversion, performed by S.V.Vorontsov, 2009 (private communication), using two evolutionary models with different EOS as base model.
Conclusion

**THERE IS A GOOD CHOICE OF EQUATIONS OF STATE FOR HIGH-PRECISION SOLAR MODELING!**
Finally, let’s not forget the physical issues in the equation of state

- Various smaller competing - but relevant - effects, among other:
  - Existence and population of excited states
  - Diffraction and exchange terms
  - Parametric “size” in hard-spheres
  - Relativistic correction for electrons
To illustrate: a small effect - relativistic electrons in the Sun

- Relativistic corrections are expected to be small, central temperature

\[ kT \approx 1 \text{ keV} \ll 511 \text{ keV}(= m_e c^2) \]

- And yet: the effect can be observed!!
Models with and without relativistic electrons (MHD; same result with then-OPAL)

Figures from:
Elliot, J.R. & Kosovichev, A.G.
SAHA-S EOS

• Basic features

Based on “chemical picture” of plasma, what means the free energy is represented as a sum “ideal-gaseous” terms and further contributions from interactions between these particles.

\[ F(V, T, N_i) = \sum F_{\text{id}}^{(id)} + F_e^{(id)} + F_{\text{rad}}^{i, e, i, e} + \ldots \]

“Ideal” terms are correspond to atoms, molecules and ions, “free” electrons. Chemicals included - H, He, C, N, O, Ne, Si, Fe, also selected molecules. Number of “free” electrons is according to the Saha equations.

Ideal terms, electrons

\[ F_{e}^{(id)} = 2Vk_B T \pi^{-1/2} \hat{\alpha}_e^{-3} \left[ \alpha_e I_{1/2}(\alpha_e) - \frac{2}{3} I_{3/2}(\alpha_e) \right] \]

\[ \alpha_e = \mu_e / k_B T ; \quad n_e \hat{\lambda}_e^3 = \frac{\sqrt{\pi}}{2} I_{1/2}(\alpha_e) \]

ions

\[ F_{i}^{(id)} = \sum_{j=1}^{L} N_j k_B T \left[ \ln \left( \frac{n_j \hat{\lambda}_j^3}{Q_j} \right) - 1 + \frac{A_j}{k_B T} \right] ; \]

\[ Q_j = \sum_{i} g_i \omega(n_i, T) \exp \left[ -\frac{\varepsilon_i}{k_B T} \right] \]

Nonideal terms, Coulomb corrections

\[ \frac{\Delta P^{(Coul)}}{n_e kT} = -\frac{\Gamma_D^3}{24\pi n_e f^3}, \]

where \( \Gamma_D^2 = 4\pi f^3 \sum \frac{Z_i^2 n_i}{1 + Z_i^2 \frac{f}{T_D/2}} \) and \( f \equiv e^2 / kT \)

Planck-Larkin partition function

\[ \omega_{i}^{PL}(T) = 1 - (1 + \tilde{E}_i) e^{-\tilde{E}_i}, \text{ where } \tilde{E}_i \equiv \varepsilon_i / kT \]

modified by Starostin & Rorich, 2003
SAHA-S EOS

• **Advantages**
  1. Rich chemical mixture. In next version we plan to extend up to 10 heavy elements. One can interpolate EOS data in respect to individual component of Z.
  2. Good and stable results for conditions of “low-temperature” ionization, i.e. \( I/kT_{ion} \ll 1 \)
  3. Explicit parameters of “free” electrons \( N_e \) or \( \mu_e \). It is allowing to extend EOS-data besides given tables. E.g. produce ionization state of arbitrary element, not included originally.
  4. High internal consistency, providing tiny ionization “features” in \( \Gamma_1 \)

• **Possible limitations**
  1. Some arbitrary way to estimate partition function of ions, which are not hydrogen-like. It maybe important for high-temperature ionization.
  2. Inconsistency with significant degeneracy in respect of ionization and Coulomb corrections.