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

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Los Angeles

or...

Here comes the Sun!

# Observations!

# Helioseismology: "Looking" into the Sun's interior!

## Discovery:

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

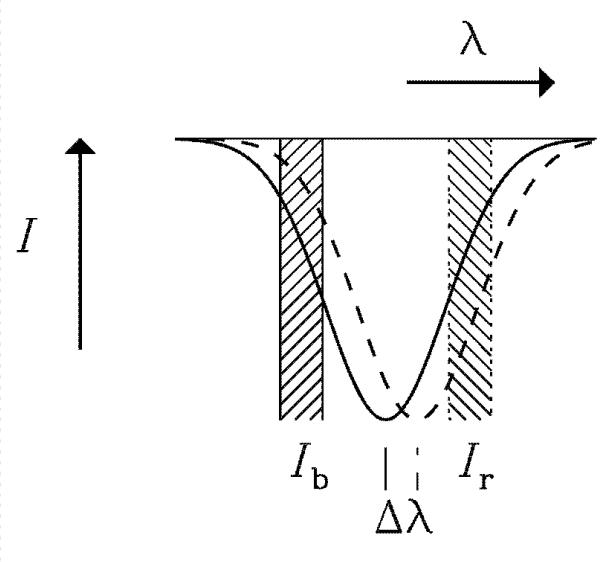
$$v \approx 100 \ \frac{\mathrm{m}}{\mathrm{s}}$$

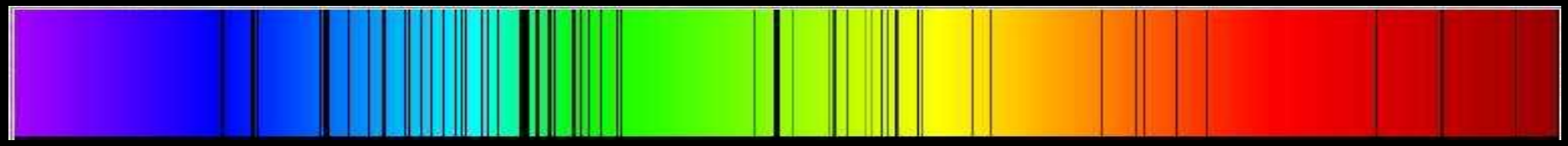
$$P \approx 5 \ \mathrm{min}$$

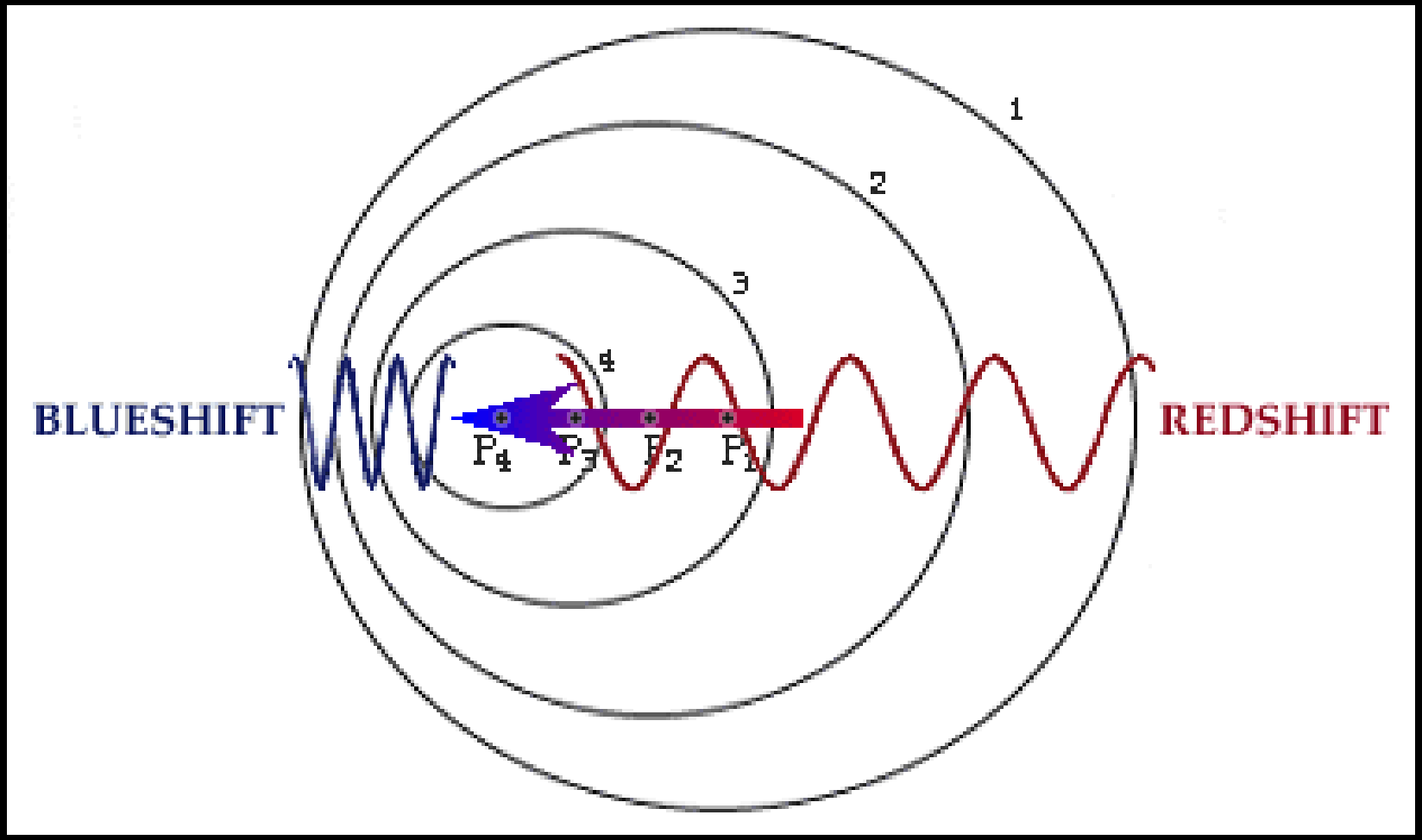
- Hence name: "5-minute oscillations"

# 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:

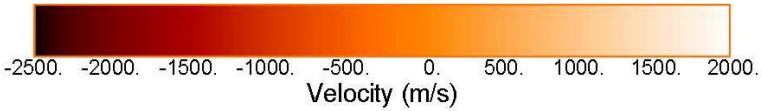





1
2
3
4
BLUESHIFT
REDSHIFT
P4
P3
P2
P1

# Single Dopplergram

(30-MAR-96 19:54:00)

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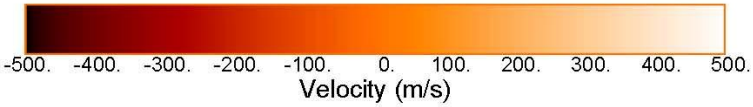
# Single Dopplergram Minus 45 Images Average

(30-MAR-96 19:54:00)

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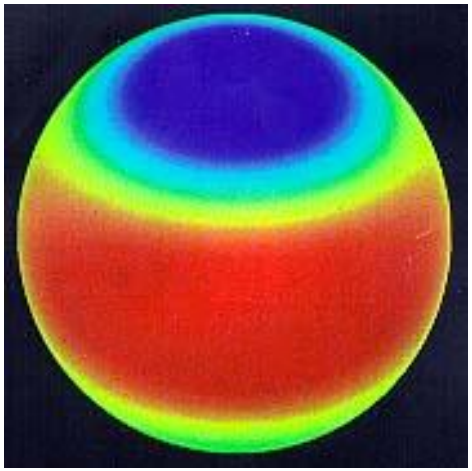
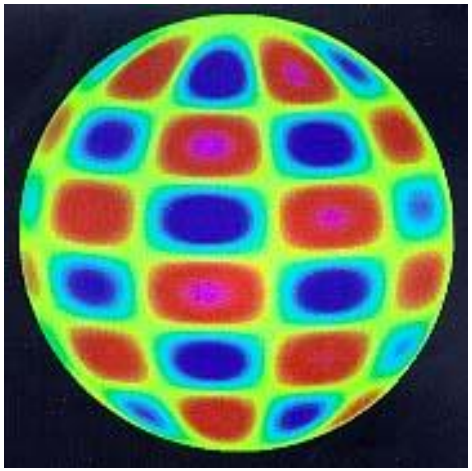
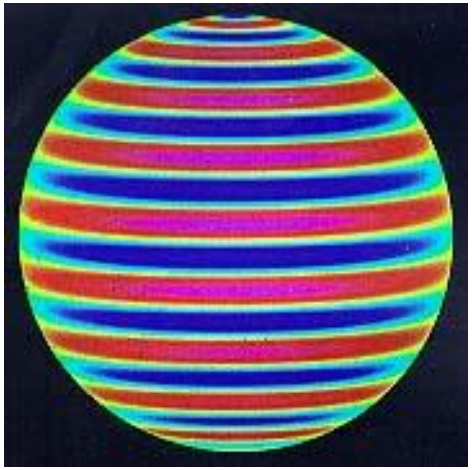
# 4 typical oscillation modes



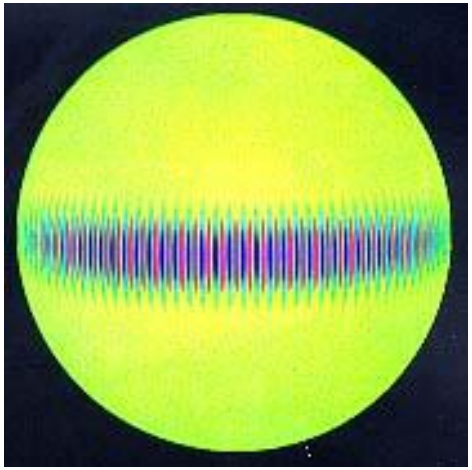
*l*=2 *m*=0



*l*=*10* *m*=5



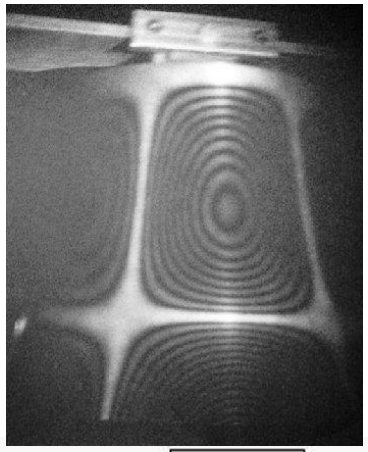
*l*=20 *m*=0



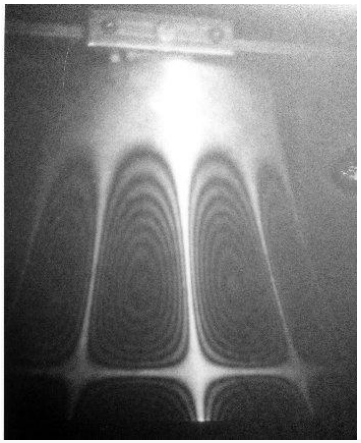
*l*=100 *m*=100

# Analogy (2-D): bell (from G. Houdek)

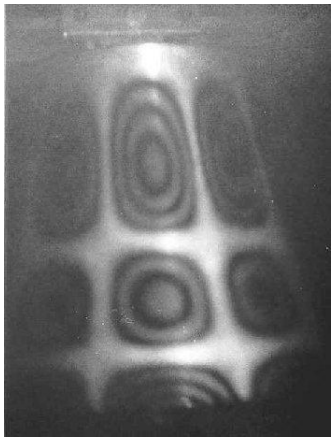
1342.3 Hz

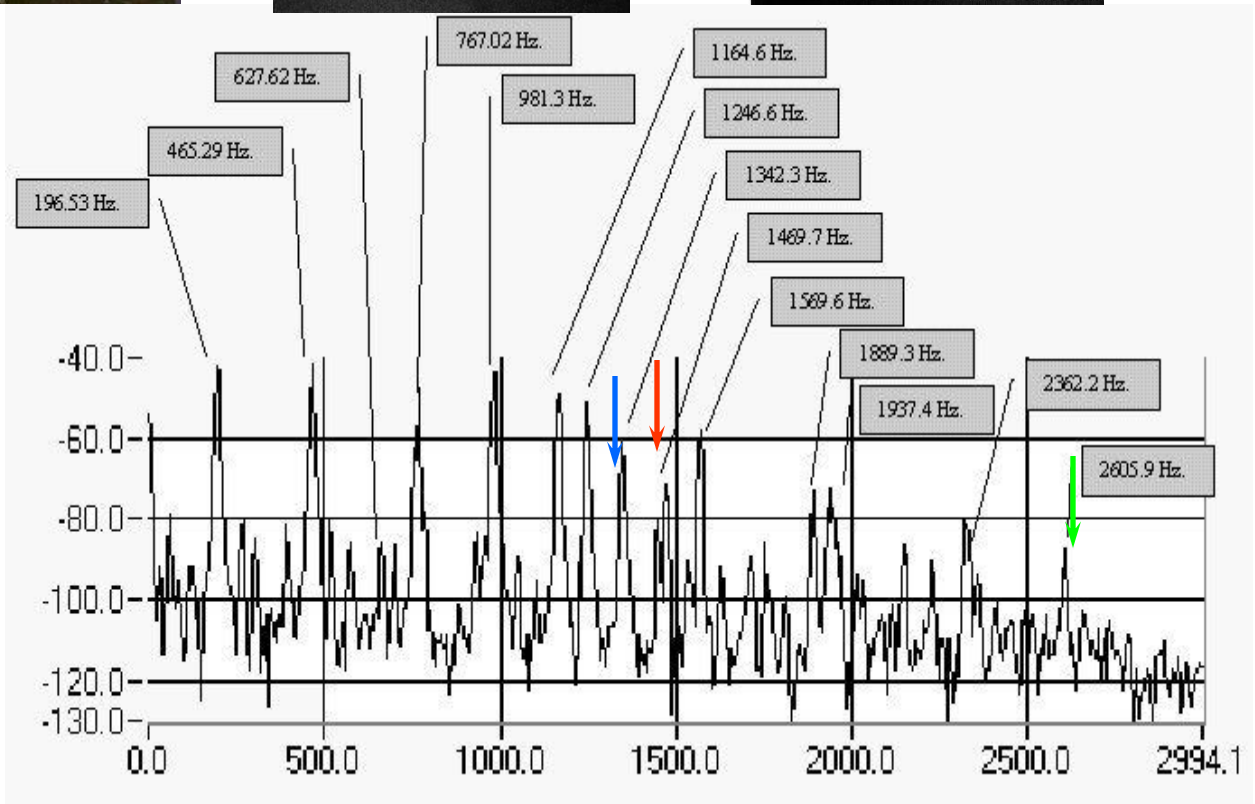


1469.7 Hz



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?

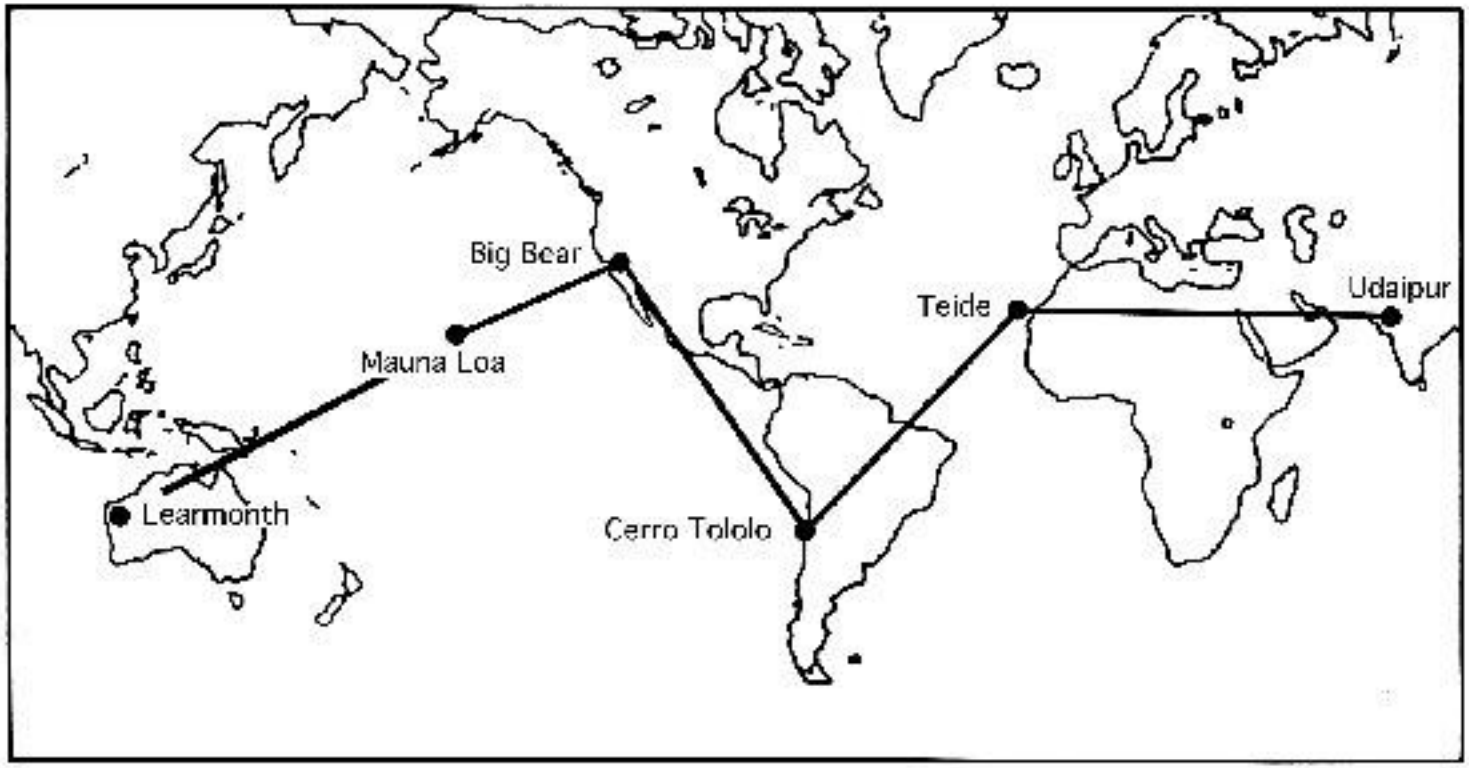
South Pole

Networking (GONG)

Space (SOHO)

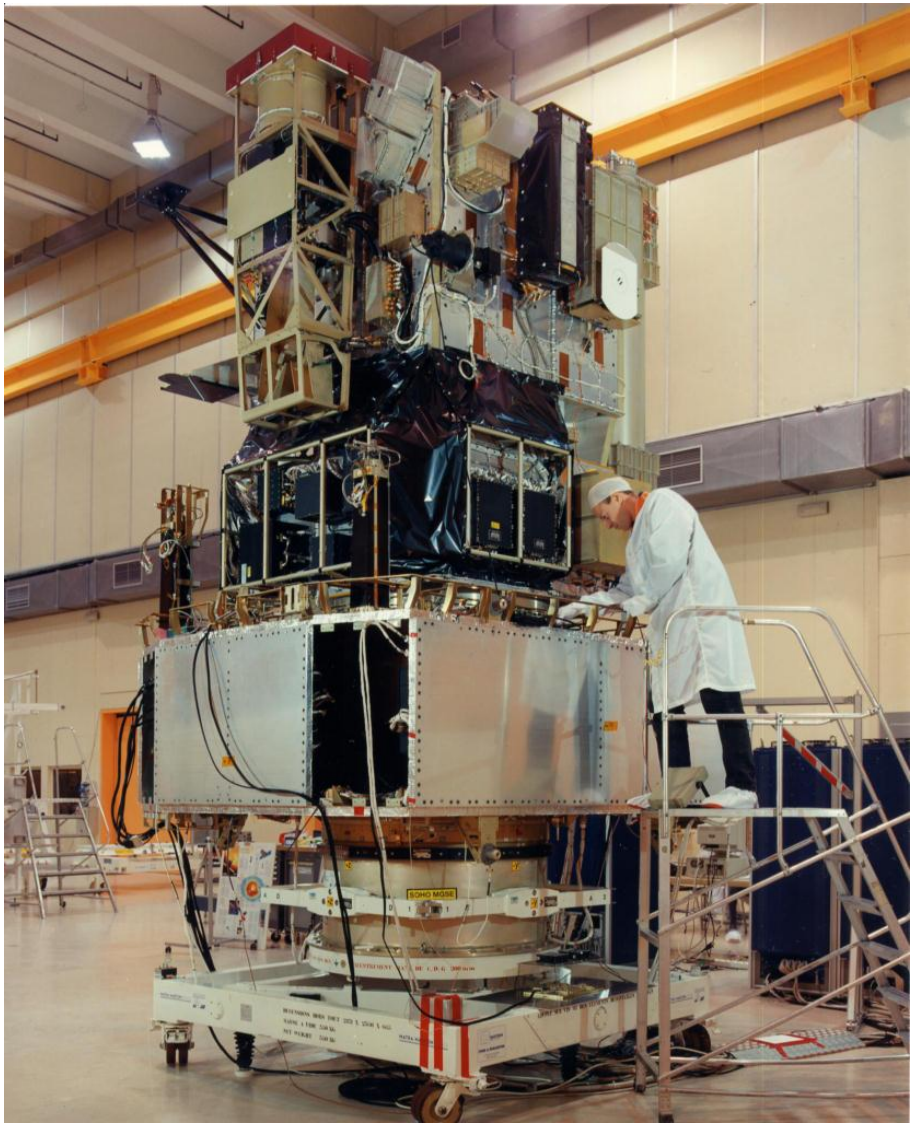
# South Pole

# GONG Stations



# GONG Instruments

# SOHO Instrument

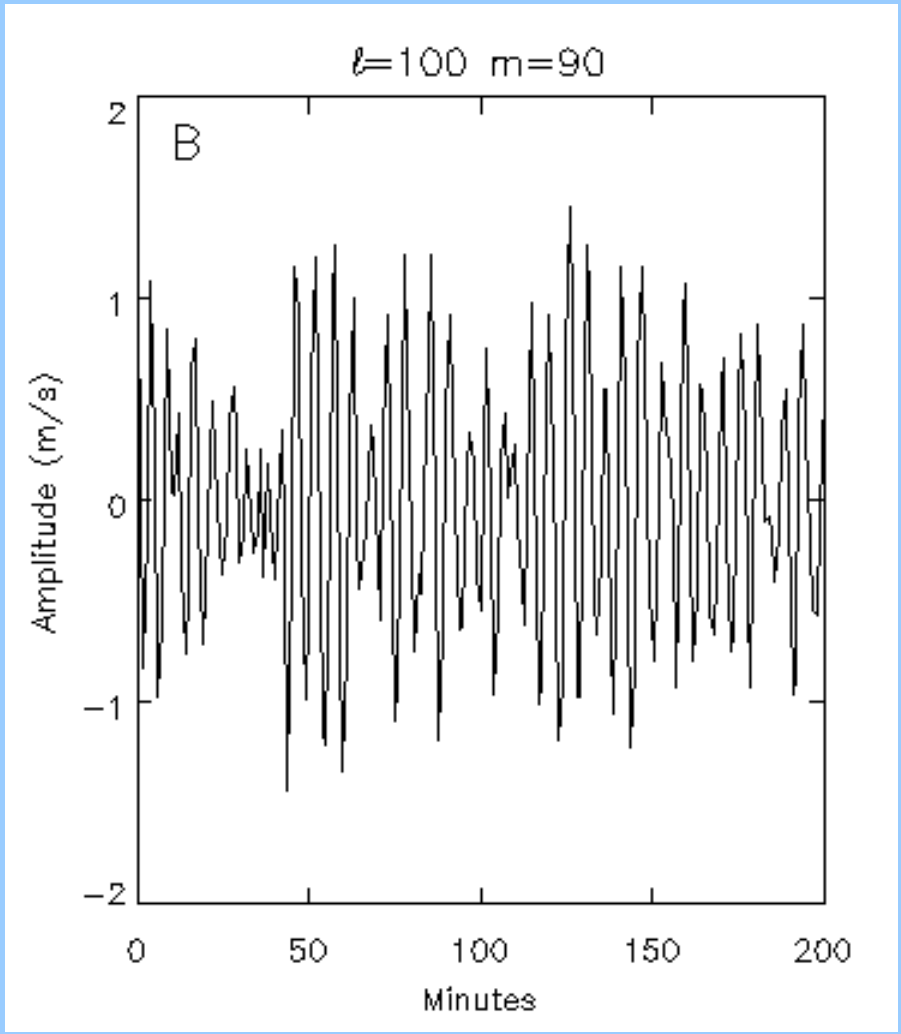


# SOHO Launch (Dec 2, 1995)

SOI to be launched later this year!

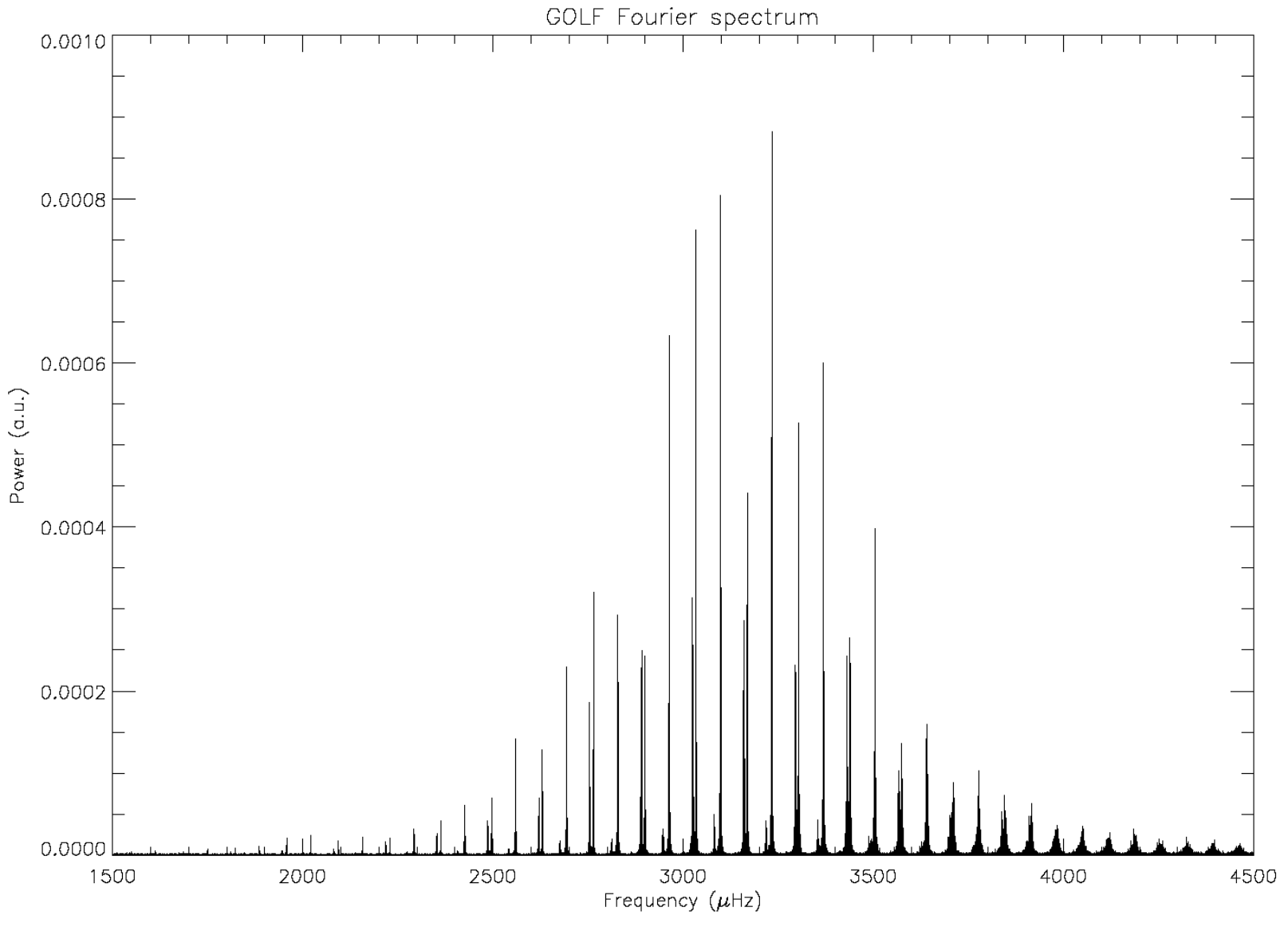
End of interlude

# Time-series of one oscillation mode




Source: SOHO/MDI instrument

# Power spectrum after Fourier transform

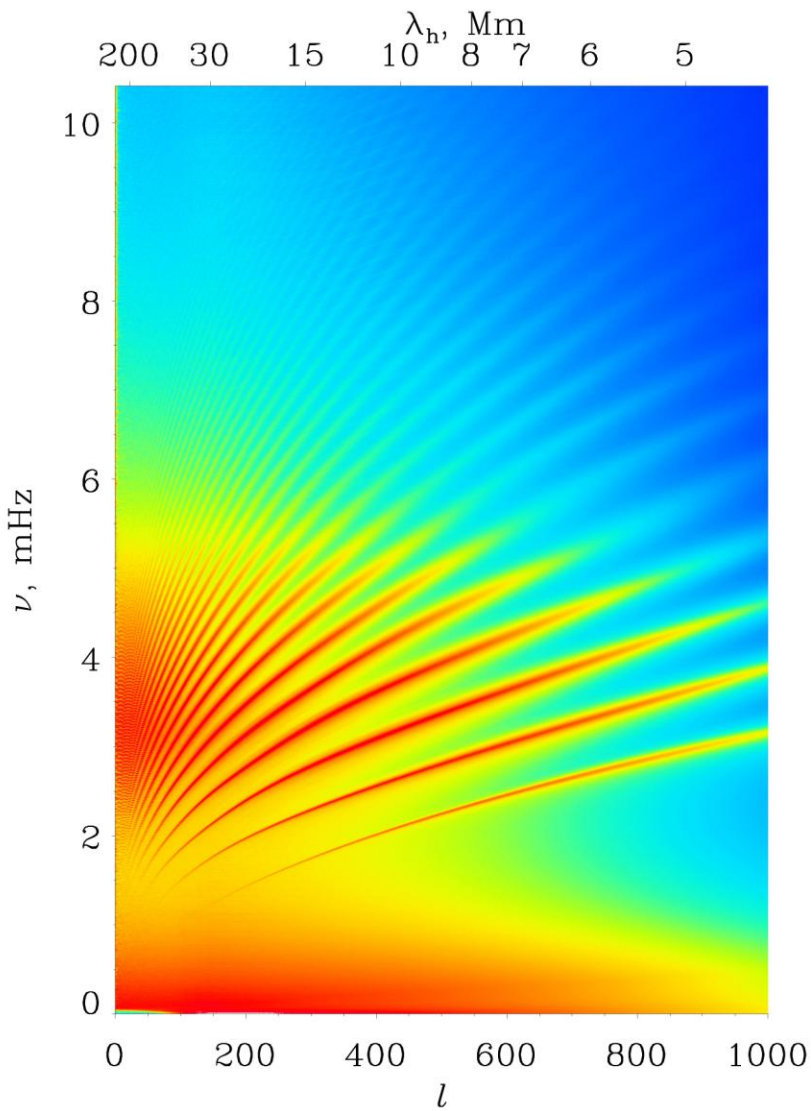



From: SOHO/GOLF instrument

# Mode frequencies: properties

- More than $10^7$ modes observed
- Single mode velocity tiny: $\approx 0.1 - 1\ \frac{\mathrm{m}}{\mathrm{s}}$
- Incoherently, the amplitudes add up to the observed total velocity of $\approx 100 \frac{\mathrm{m}}{\mathrm{s}}$
- 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 …

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

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

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

$$\Delta\phi = 4\pi G\rho$$

**… 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)**

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

$$L_r = 4\pi r^2 F$$

$$\frac{dL}{dr} = 4\pi r^2 \rho \epsilon_{\mathrm{nuc}}$$

$$\frac{dT}{dr} = -\frac{3\kappa\rho L}{64\pi\sigma r^2 T^3}$$

# Material properties are mandatory!

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

$$\rho = \rho(T, p, \mathbf{X})$$

$$\kappa = \kappa(T, \rho, \mathbf{X})$$

$$\epsilon = \epsilon_{\mathrm{nuc}}(T, \rho, \mathbf{X})$$

$$s = s(T, \rho, \mathbf{X})$$

$$\mathbf{F} = \mathbf{K}(\nabla T; T, \rho, \mathbf{X})$$

$$\left(\text{Diffusive radiation}: \quad F = -\frac{16\sigma T^4}{3\kappa\rho}\nabla T\right)$$

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

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

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

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

- If appropriate, use linearization, spherical harmonics, adiabatic $\Rightarrow \nu_{n\ell}$

# Result: model frequencies

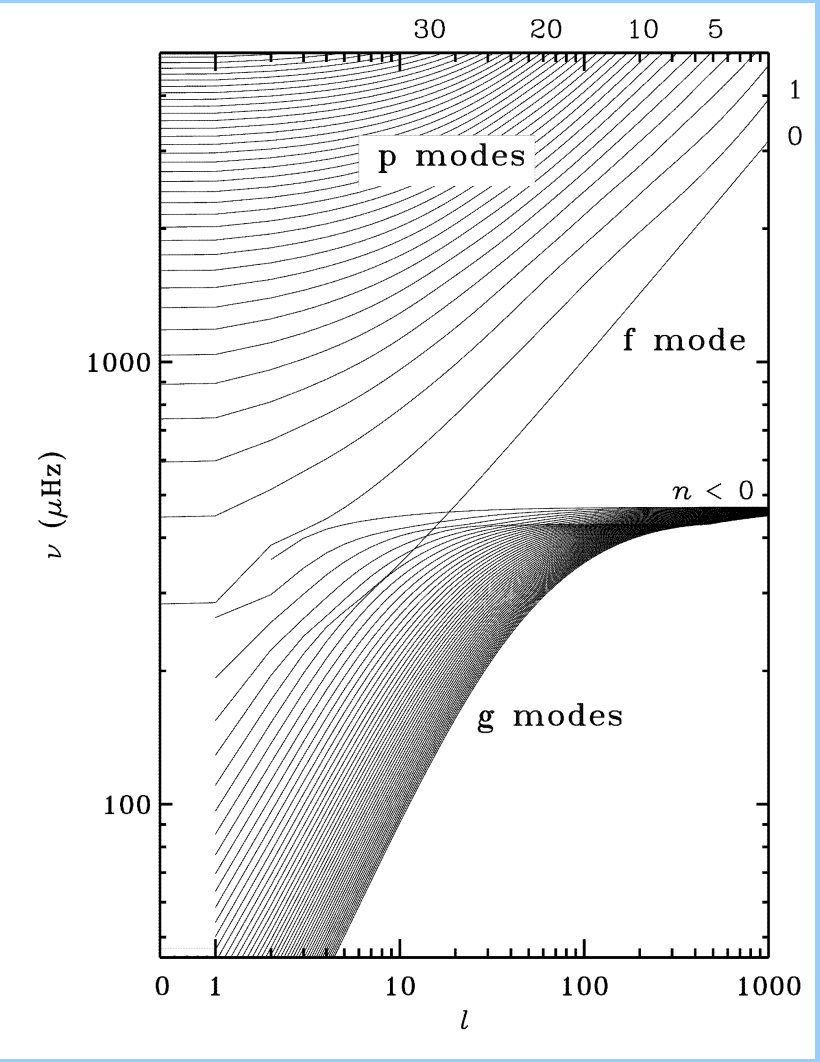
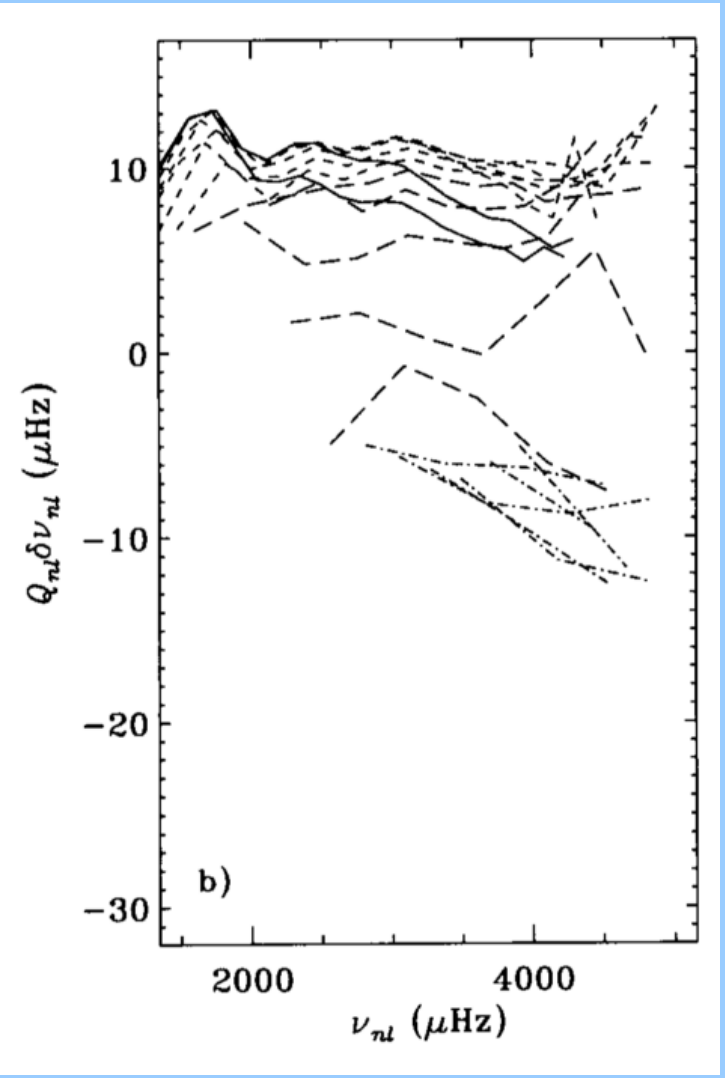



Figure:

J. Christensen-Dalsgaard

# Apply "O-C Diagrams"

- O = "Observation"
- C = "Computation"

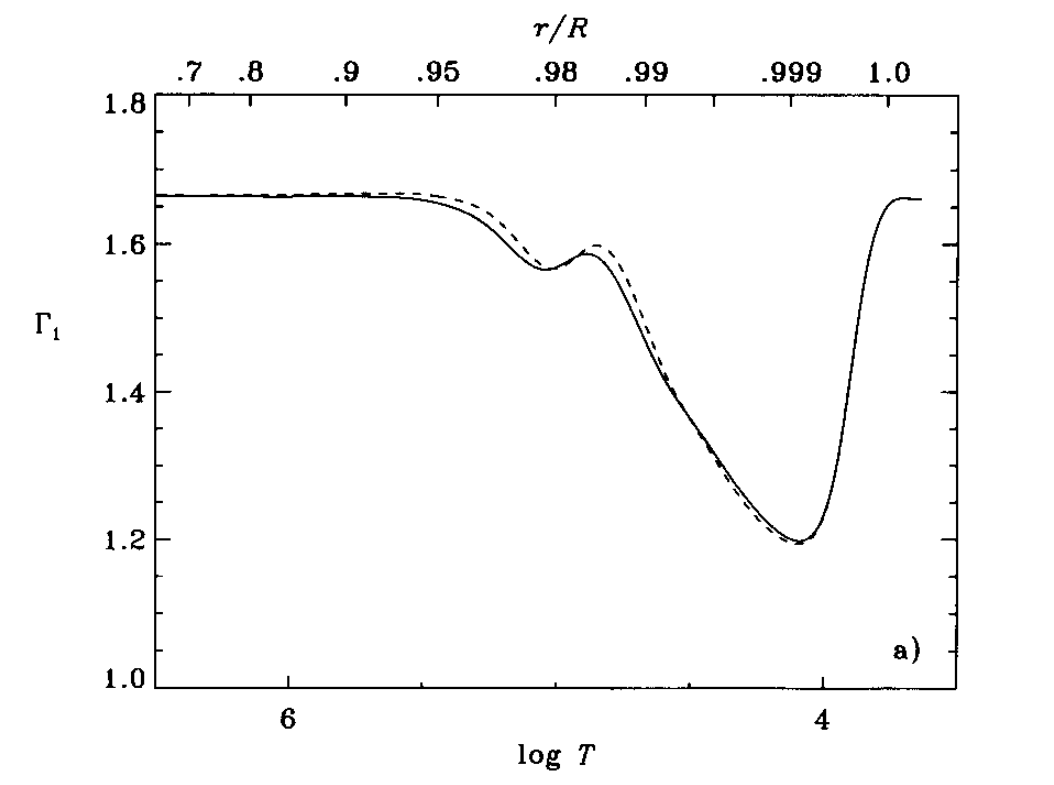



($Q_{nl}$ is a scale factor. Details see: Christensen-Dalsgaard & Däppen 1992, A&A Rev. **4**, 267)

# Impact: two similar solar models…

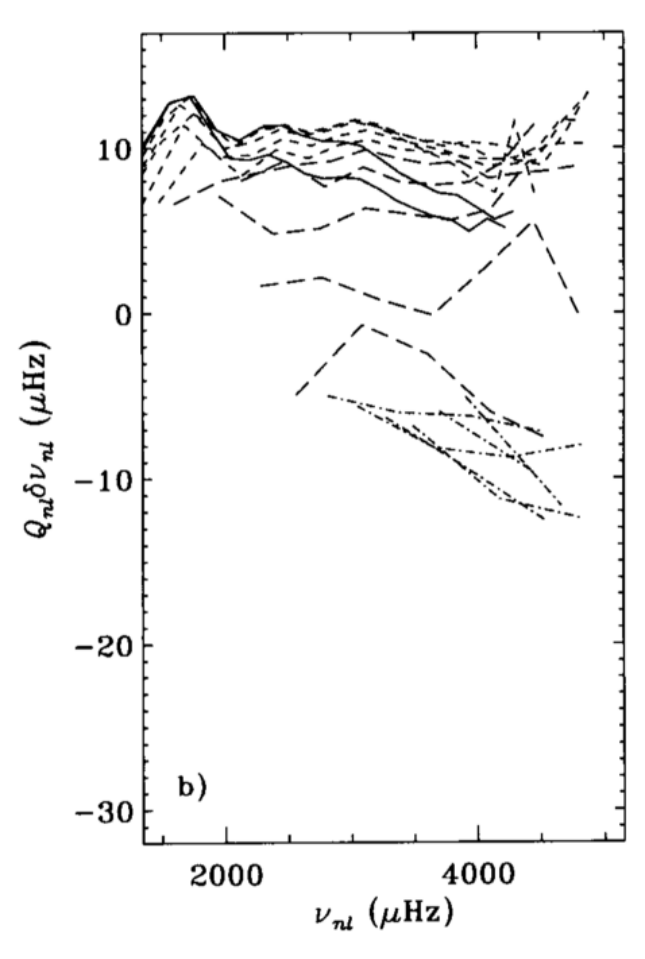
- **Identical models, except for their equations of state. One is with Debye-Hückel screening, one without. Their adiabatic exponents are:**

**Dashed: with screening**
**Solid: without screening**

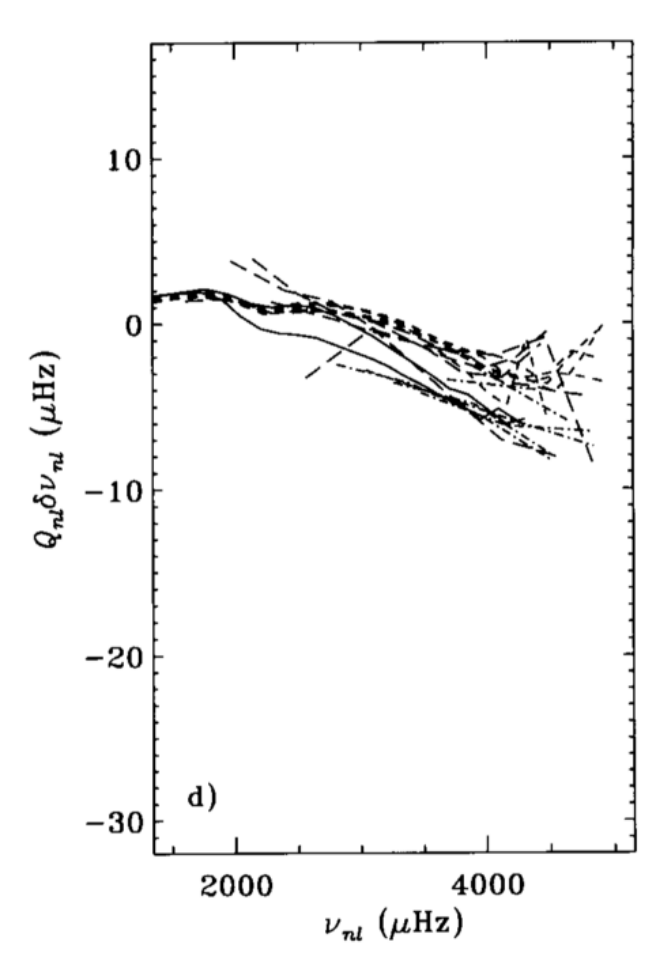



From: Christensen-Dalsgaard & Däppen 1992, A&A Rev. **4**, 267

# There is DH in the Sun…




**without screening**




**with screening**

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…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 $(\mathrm{H} \leftrightarrow \mathrm{H}^{+} + \mathrm{e}^{-}\ ,\ \text{etc.})$
- Constraints $(N_{\mathrm{H}} + N_{\mathrm{p}} = \text{const.}\ ,\ \text{etc.})$
- Minimize $F(T, V, N_{\mathrm{H}}, N_{\mathrm{p}}, N_{\mathrm{e}^-}, \ldots)$

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

$$F_{\mathrm{tot}} = F_{\mathrm{nuc}} + F_{\mathrm{e}} + F_{\mathrm{interactions}} + \ldots$$

- Consistent (formally!) $p = -(\frac{\partial F}{\partial V})_T\ ,\ \text{etc.}$

# Example: MHD

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

Hummer, D.G. & Mihalas, D.M. 1988, *ApJ* **331**, 794;
Mihalas, D.M., Däppen, W. & Hummer, D.G. 1988, *ApJ* **331**, 815
Däppen,W., Mihalas, D.M., Hummer, D.G. & Mihalas, B.W. 1988, *ApJ* **332**, 261

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

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

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

# 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)**

  Rogers, F.J. 1986, *ApJ* **310**, 723;
  Rogers, F.J., Swenson, F.J. & Iglesias, C.A. 1996, *ApJ* **456**, 902
  Rogers, F.J. & Nayfonov, A. 2002, *ApJ* **576**, 1064

- **Key points: systematic expansions**

  **(z = activity)**

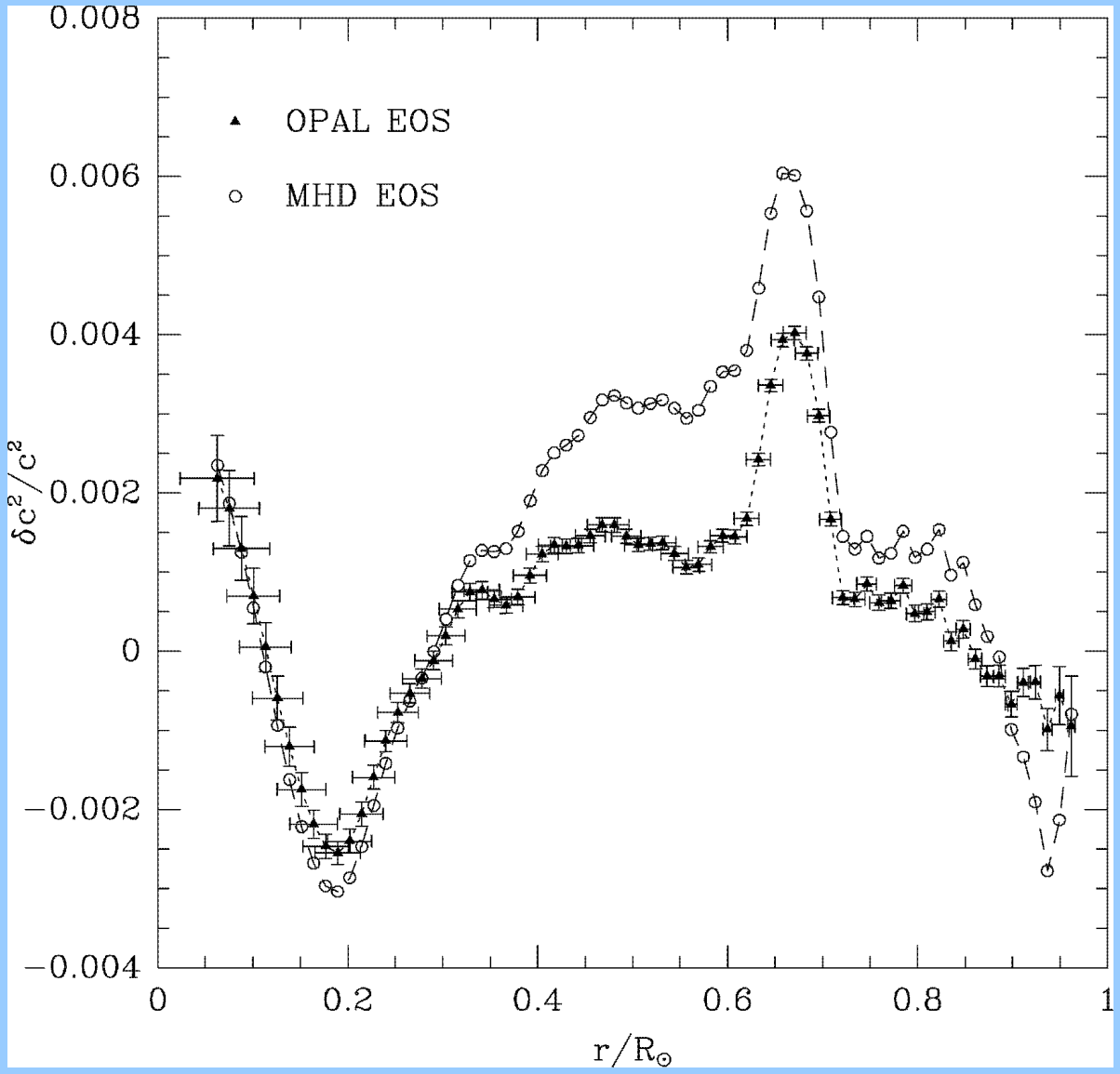
$$\frac{p}{k_B T} = z + z^2 b_2 + z^3 b_3 + \ldots \; ; \quad \rho = \frac{z}{k_B T}\left(\frac{\partial p}{\partial z}\right)$$

Planck-Larkin Partition Function

$$\mathrm{PLPF} = \sum_{nl}(2l+1)\left[\exp\left(-\frac{E_{nl}}{kT}\right) - 1 + \frac{E_{nl}}{kT}\right]$$

# MHD vs. OPAL

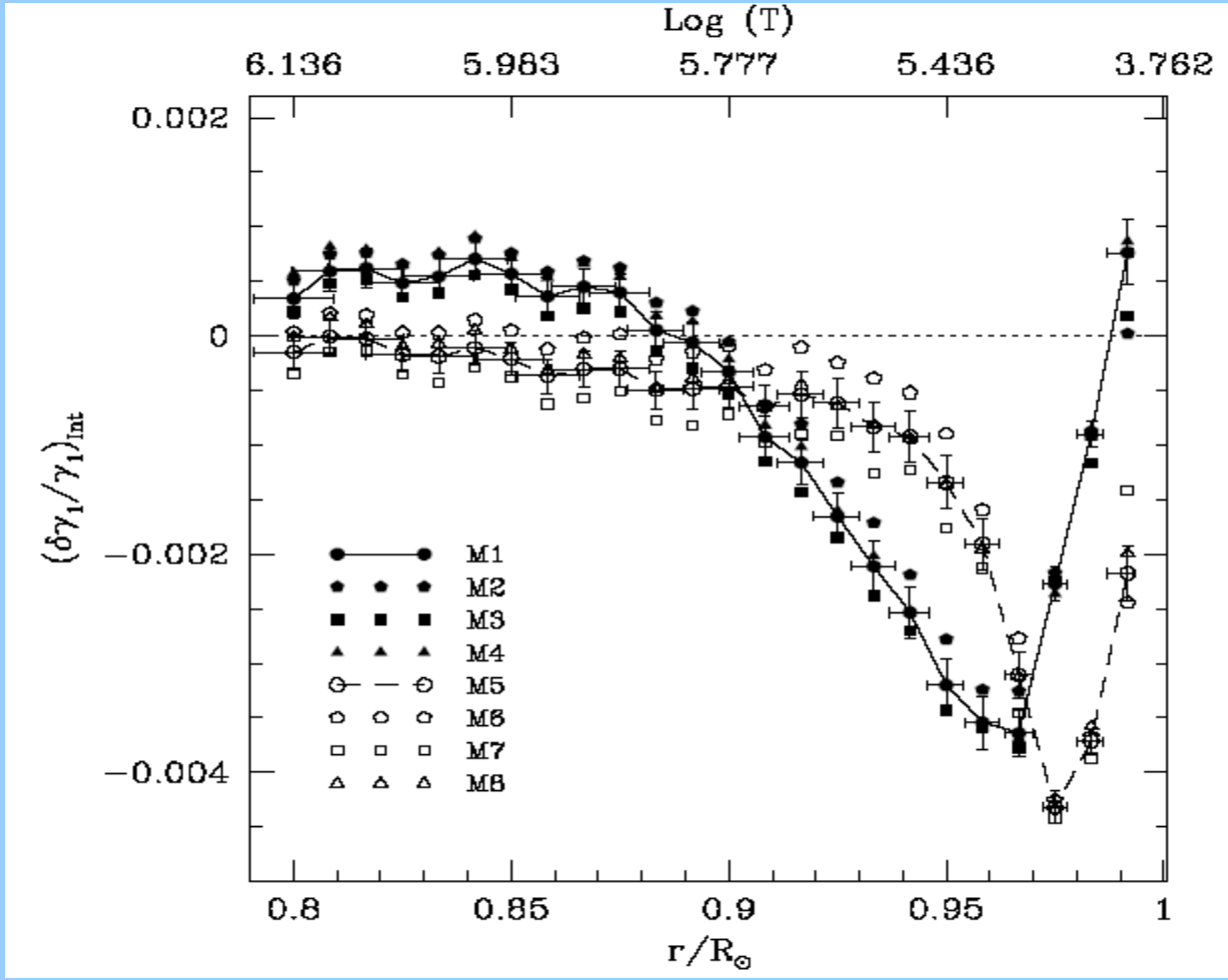
# $c^2$ Inversions (numerical; Sun-Model)




Basu & Christensen-Dalsgaard 1997, A&A **322**, L5

# 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
*ApJ*, **518**: 985

# OPAL fares better than MHD…

- Why? Likely answer:

- There is no PLPF in MHD
- There are no scattering states in MHD

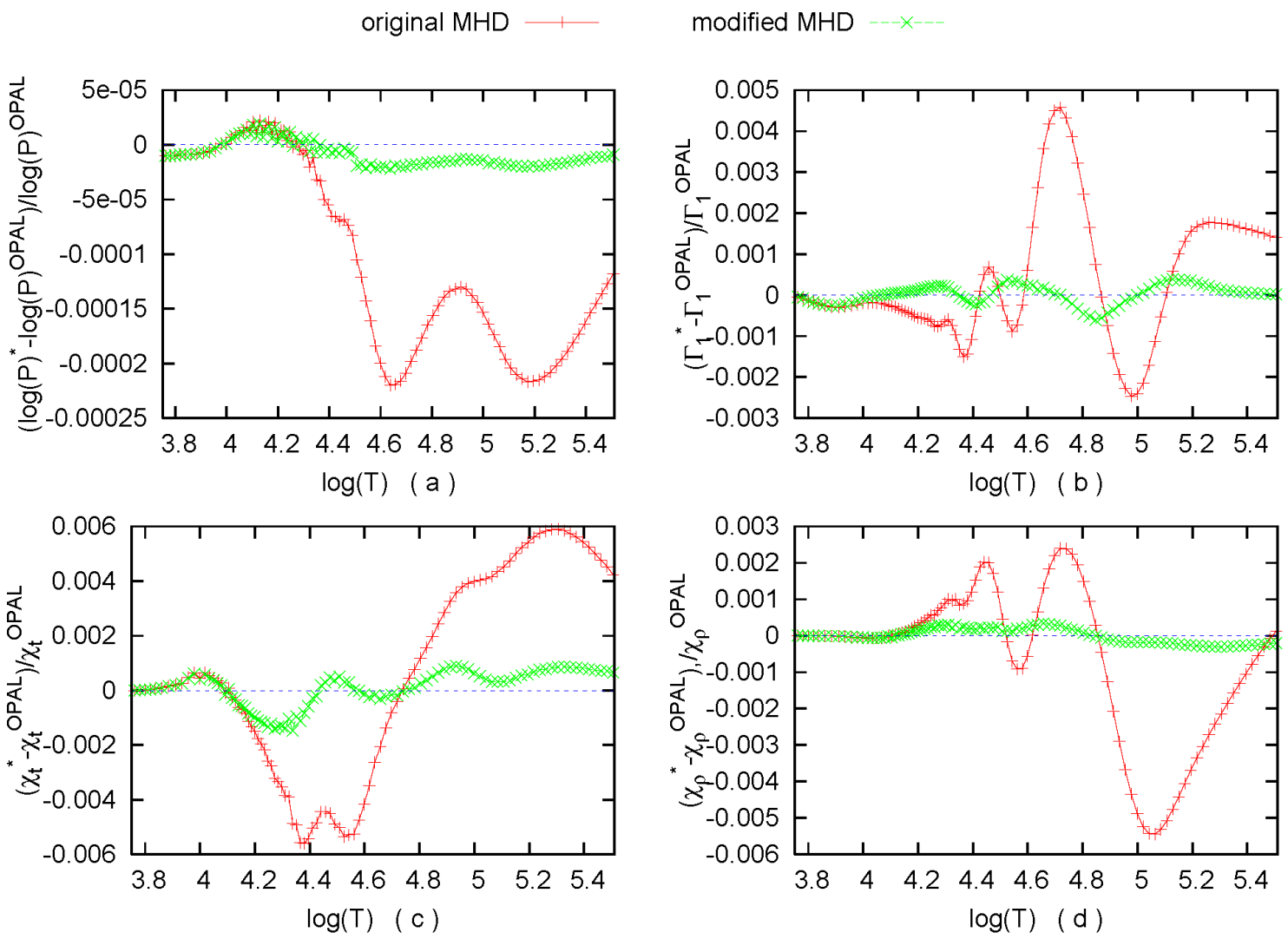
- Open question: is it fundamentally impossible to find PLPF entirely from within the chemical picture?

# 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)

# Exact Option (in a sense…)

- 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.

[1] Alastuey, A. & Perez, A. 1992, Europhys.Lett., 20, 19
[2] Kraeft, W.-D., Kremp, D., Ebeling,W., Röpke, G., 1986, Quantum Statistics of Charged Particle Systems (Plenum)

$$
\begin{aligned}
\beta P \;=\; & \sum_{\alpha} \rho_\alpha - \frac{\kappa_D^3}{24\pi} \\
& + \frac{\pi}{6}(\ln 2 - 1) \sum_{\alpha,\beta} \beta^3 e_\alpha^3 e_\beta^3 \rho_\alpha \rho_\beta \\
& - \frac{\pi}{\sqrt{2}} \sum_{\alpha,\beta} \rho_\alpha \rho_\beta \lambda_{\alpha\beta}^3 Q(x_{\alpha\beta}) - \frac{\pi}{3}\beta^3 \sum_{\alpha,\beta} \rho_\alpha \rho_\beta e_\alpha^3 e_\beta^3 \ln(\kappa_D \lambda_{\alpha\beta}) \\
& + \frac{\pi}{\sqrt{2}} \sum_{\alpha} \frac{(-1)^{2\sigma_\alpha+1}}{(2\sigma_\alpha+1)} \lambda^3{}_{\alpha\alpha} \rho_\alpha^2 E(x_{\alpha\alpha}) \\
& - \frac{3\pi}{2\sqrt{2}} \beta \sum_{\alpha,\beta} e_\alpha e_\beta \kappa_D \rho_\alpha \rho_\beta \lambda_{\alpha\beta}{}^3 Q(x_{\alpha\beta}) \\
& - \frac{\pi}{2}\beta^4 \sum_{\alpha,\beta} \rho_\alpha \rho_\beta e_\alpha^4 e_\beta^4 \kappa_D \ln(\kappa_D \lambda_{\alpha\beta}) \\
& + \frac{3\pi}{2\sqrt{2}} \beta \sum_{\alpha} \frac{(-1)^{2\sigma_\alpha+1}}{(2\sigma_\alpha+1)} \lambda_{\alpha\alpha}^3 \rho_\alpha^2 e_\alpha^2 \kappa_D E(x_{\alpha\alpha}) \\
& + \frac{1}{16} \sum_{\alpha} \frac{\beta^2 \hbar^2 e_\alpha^2}{m_\alpha} \kappa_D^3 \rho_\alpha + \pi\left(\frac{1}{3} - \frac{3}{4}\ln 2 + \frac{1}{2}\ln 3\right) \times \\
& \sum_{\alpha,\beta} \beta^4 e_\alpha^4 e_\beta^4 \kappa_D \rho_\alpha \rho_\beta \\
& + C_1 \sum_{\alpha,\beta,\gamma} \beta^5 e_\alpha^3 e_\beta^4 e_\gamma^3 \kappa_D^{-1} \rho_\alpha \rho_\beta \rho_\gamma \\
& + C_2 \sum_{\alpha,\beta,\gamma,\delta} \beta^6 e_\alpha^3 e_\beta^3 e_\gamma^3 e_\delta^3 \kappa_D^{-3} \rho_\alpha \rho_\beta \rho_\gamma \rho_\delta
\end{aligned}
$$

# Extension of FK to higher terms & creation of in-line tool:

Paper I: ***Astron. Astrophys.*** (in press)

Papers II & III in progress

Collaborators:

Asher Perez, Jerusalem & Strasbourg;
Hsiao-Hsuan Liang, Yung-Ching Liang, USC;
Katie Mussack, Los Alamos

# Exact Option (in another sense…)

**SAHA-S**

# SAHA-S EOS

- Authors:

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I.L.Iosilievskiy, *Moscow Institute of Physics and Technology, Dolgoprudnyi, Russia;*

A.N.Starostin*, Troitsk Institute for Innovation and Fusion Research, Troitsk, Russia;*

V.E.Fortov*, Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia;*

- References:

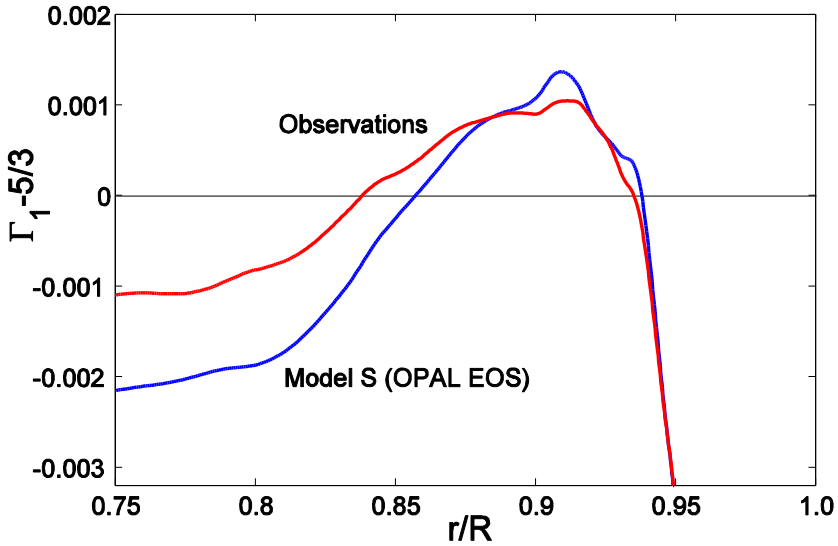
1. V.K.Gryaznov et al., *J. Phys.* A: Math. Gen. **39** (2006) p. 4459
2. S.V.Ayukov et al., *JETP Letters*, Vol. 80, No. 3, (2004) p. 141
3. V.K.Gryaznov et al. *in* «Equation-of-State and Phase-Transition Issues in Models of Ordinary Astrophysical Matter», Eds. V.Celebonovic, W.Dappen, D.Gough, AIP Conference Proceedings v. 731, (2004) p.147, and several papers *ibid*.

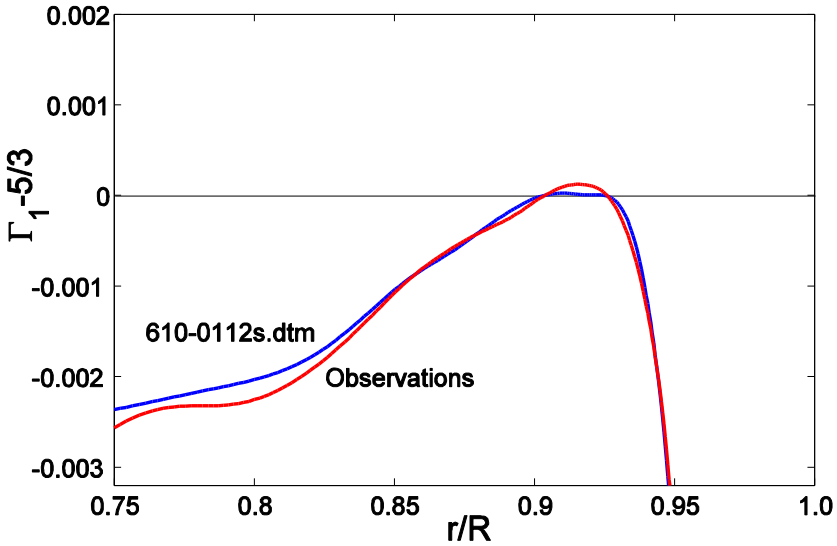
**SAHA-S is part of a larger solar-modeling effort [ISTC 3705].** It is a serious alternative to OPAL (and MHD). It is based on a systematic development, and it contains a modified Planck-Larkin partition function.

## 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

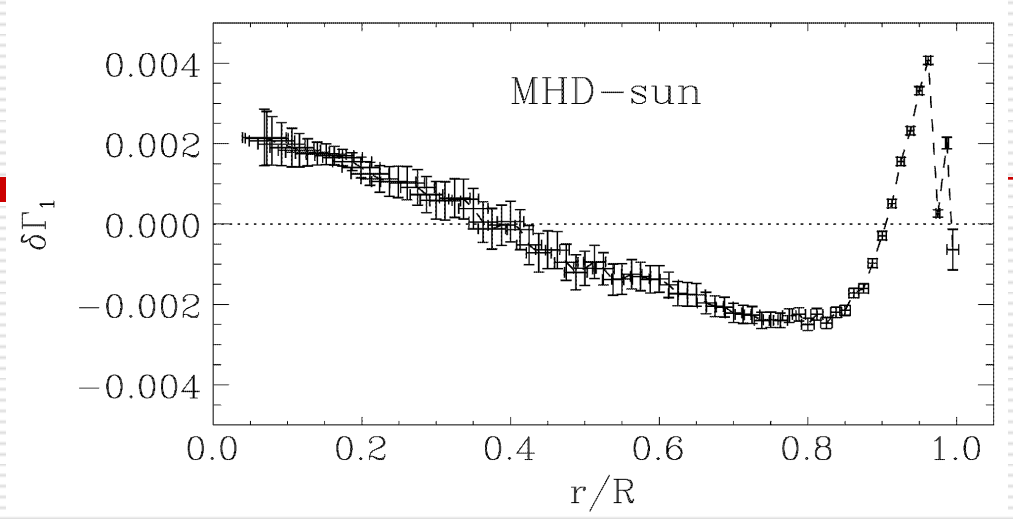
# To illustrate: a small effect - relativistic electrons in the Sun

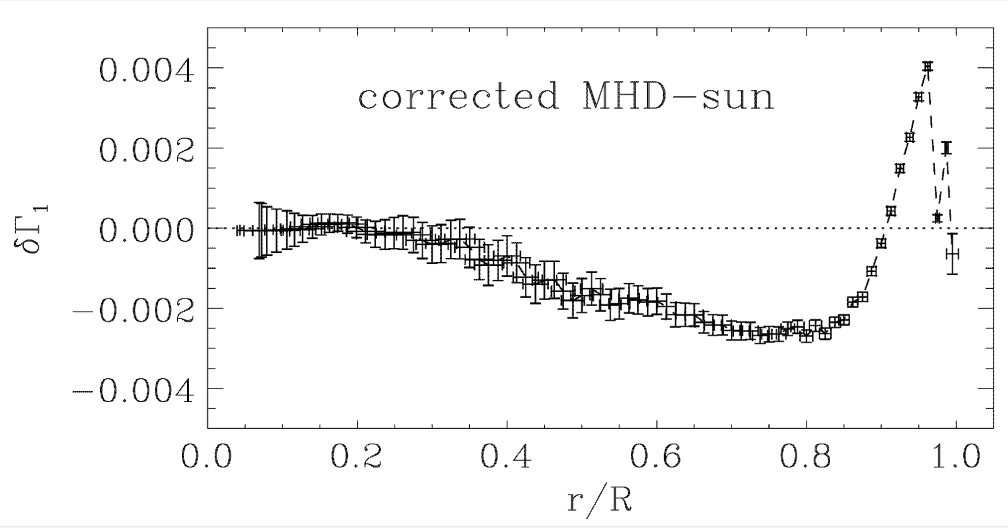
- Relativistic corrections are expected to be small, central temperature

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

- And yet: the effect can be observed!!
  (Elliot & Kosovichev 1998, ApJ, **500**

# Models with and without relativistic electrons (MHD; same result with then-OPAL)




Figures from:

Elliot, J.R. & Kosovichev, A.G. 1998, *ApJ*, **500** L199

# 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.

$$F(V,T,N_i)=\sum F_{ion}^{(id)}+F_e^{(id)}+F_{rad}+F_{ii,ee,ie}^{(\mathrm{int})}+\ldots$$

"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

$$F_e^{(id)}=2Vk_BT\pi^{-1/2}\lambda\!\!\!^{-}_e{}^{-3}\left[\alpha_e I_{1/2}(\alpha_e)\ -\ \frac{2}{3}I_{3/2}(\alpha_e)\right]$$

$$\alpha_e=\mu_e/k_BT;\quad n_e\lambda\!\!\!^{-}_e{}^{3}=\frac{\sqrt{\pi}}{2}I_{1/2}(\alpha_e)$$

ions

$$F_i^{(id)}=\sum_{j=1}^{L}N_jk_BT\left[\ln\left(\frac{n_j\lambda\!\!\!^{-}_j{}^{3}}{Q_j}\right)-1+\frac{A_j}{k_BT}\right];$$

$$Q_j=\sum_i g_i\omega(n_i,T)\exp\left[-\frac{\varepsilon_i}{k_BT}\right]$$

## Nonideal terms, Coulomb corrections

$$\frac{\Delta P^{(Coul)}}{n_ekT}=-\frac{\Gamma_D^3}{24\pi n_e f^3},$$

$$\text{where } \Gamma_D^2=4\pi f^3\sum_i\frac{Z_i^2n_i}{1+Z_i^2\Gamma_D/2} \text{ and } f\equiv e^2/kT$$

Planck-Larkin partition function

$$\omega_i^{PL}(T)=1-\left(1+\tilde{E}_i\right)e^{-\tilde{E}_i},\ \text{where } \tilde{E}_i\equiv\varepsilon_i/kT$$

modifed 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. $I/kT_{ion} \gg 1$
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.