HElio3Sei3smi3c Analysis of the Hydrogen Partition Function in the Solar Interior

Sarbani Basu, Werner Däppen, and Alan Nayfonov

Received 1998 October 6; accepted 1999 January 1

ABSTRACT

The difference in the adiabatic gradient $\gamma_1$ between inverted solar data and solar models is analyzed. To obtain deeper insight into the issues of plasma physics, the so-called intrinsic difference in $\gamma_1$ is extracted, that is, the difference due to the change in the equation of state alone. Our method uses reference models based on two equations of state currently used in solar modeling, the Mihalas-Hummer-Däppen (MHD) equation of state and the OPAL equation of state (developed at Livermore). Solar oscillation frequencies from the SOI/MDI instrument on board the SOHO spacecraft during its first 144 days in operation are used. Our results confirm the existence of a subtle effect of the excited states in hydrogen that was previously studied only theoretically (Nayfonov & Däppen). The effect stems from an internal partition function of hydrogen, as is used in the MHD equation of state. Although it is a pure hydrogen effect, it takes place in somewhat deeper layers of the Sun, where more than 90% of hydrogen is ionized, and where the second ionization zone of helium is located. Therefore, the effect will have to be taken into account in reliable helioseismic determinations of the astrophysically relevant helium abundance of the solar convection zone.

Subject headings: atomic processes — equation of state — Sun: interior — Sun: oscillations

1. INTRODUCTION

Helioseismology has proved to be an extremely powerful tool to study the solar interior. Helioseismic inversion techniques have been used to probe details of the solar structure (see, e.g., Gough et al. 1996; Basu et al. 1996; Kosovichev et al. 1997), abundances (see, e.g., Basu & Antia 1995; Kosovichev 1996; Antia & Chitre 1998), and rotation rate (see, e.g., Thompson et al. 1996; Schou et al. 1998). High-quality helioseismological data have allowed us for some time to go beyond studying solar structure and probe the properties of solar matter (see, e.g., Christensen-Dalsgaard et al. 1996). Here, we try to study the equation of state of solar matter using inversions of solar oscillation frequencies. Our inversions are differential, that is, they determine the solar values in terms of deviations from given reference models. For the present analysis two sets of reference models have been used. They are based on the two equations of state normally used to construct solar models (see § 2.2), the so-called Mihalas-Hummer-Däppen (MHD) equation of state (Hummer & Mihalas 1988; Mihalas, Däppen, & Hummer 1988; Däppen et al. 1988; Däppen, Anderson, & Mihalas 1987) and the OPAL equation of state developed at Livermore (Rogers 1986; Iglesias & Rogers 1995; Rogers, Swenson, & Iglesias 1996, and references therein), respectively.

The observed solar oscillation modes are standing acoustic waves; hence the quantity most obviously probed is sound speed. Since the oscillations are largely adiabatic (except very near the surface), the frequencies are determined predominantly by the local adiabatic sound speed $c$, which is a thermodynamic quantity. In addition, the frequencies depend on the distribution of the density $\rho$ in the Sun. Equivalently, adiabatic oscillation frequencies can also be determined from the distribution of density and the adiabatic gradient $\gamma_1$ in the Sun (see § 3.2 for more details). Since $\gamma_1$ is a dimensionless quantity, it is especially suited to study qualitative effects in the equation of state. In addition, for a high-precision diagnosis of the equation of state it is very fortunate that the Sun has a substantial convection zone, where equation of state effects show up independent of our uncertainty in the opacity. The reason is that in the bulk of the convection zone, the stratification is essentially adiabatic and thus determined by thermodynamics (Christensen-Dalsgaard & Däppen 1992).

Helioseismic equation-of-state studies have shown the necessity to include the leading Coulomb correction (expressed by the Debye-Hückel approximation) in order to meet the helioseismological constraints. This was recognized in the early 1980s, and models with more sophisticated equations of state were tried in helioseismic studies (see, e.g., Berthomieu et al. 1980; Lubow, Rhodes, & Ulrich 1980; Ulrich 1982; Ulrich & Rhodes 1983; Shibahashi, Noels, & Gabriel 1983, 1984; Noels, Scuflaire, & Gabriel 1984). With better data toward the end of the 1980s, a clearer picture emerged (Christensen-Dalsgaard, Däppen, & Lebreton 1988; Basu & Antia 1995; Christensen-Dalsgaard & Däppen 1992; Christensen-Dalsgaard et al. 1996). However, even those equations of state that do include the leading Coulomb correction differ from the solar data by more than the observational uncertainty. They also differ discernibly among themselves, thus revealing the importance of the treatment of the nonideal effects beyond the leading Coulomb term. The aforementioned studies were based on the forward approach, i.e., the comparison between observed and theoretically predicted solar oscillation frequencies. Equation-of-state studies based on inversions have also been attempted earlier (see, e.g., Dziembowski, Pamyatnykh, & Sienkiewicz 1992; Elliot 1996; Elliot & Kosovichev 1998), but they have been indirect. Those studies involved looking at either the sound-speed differences or differences in the adiabatic index $\gamma_1$, between the solar models and the Sun, both of which have...
coupling parameter in addition to contributions from the difference in the equation of state.

In this paper we use the method proposed by Basu & Christensen-Dalsgaard (1997) to study the difference in $\gamma_1^c$ between solar models that result from the differences in the equation of state alone, but not from the ensuing change in solar structure. To distinguish it from the total $\gamma_1$ difference $\delta\gamma_1$, we call this contribution the “intrinsic” $\gamma_1$ difference $(\delta\gamma_1)_{\text{iut}}$. An immediate target of the new observational technique is a subtle effect of the excited states in hydrogen (Nayfonov & Däppen 1998). So far, this effect has only been studied theoretically. We begin with a presentation of the equation-of-state issues in order to discuss the hydrogen partition function effect. The solar oscillation frequencies used for this work were obtained from the SOI/MDI instrument on board the SOHO spacecraft during its first 144 days in operation (Rhodes et al. 1997).

2. EQUATION-OF-STATE ISSUES

2.1. Ideal and Nonideal Plasmas

The simplest model is a mixture of nuclei and electrons, assumed fully ionized and obeying the classical perfect gas law. However, an “ideal gas” equation of state can be more general. It may include deviations from the perfect gas law, namely ionization, radiation, and degeneracy of electrons, as long as the underlying microphysics of these additional effects is still ideal, that is, as long as it does not contain interactions. The “particles,” however, can be classical or quantum, material or photonic. In such an ideal framework, bound systems (molecules, atoms, ions) are allowed to have internal degrees of freedom (excited states, spin). All such ideal effects can be calculated as exactly as desired. Incidentally, in a recent study by Elliot & Kosovichev (1998) it turned out that helioseismological accuracy demands inclusion of the relativistic effect in the electron gas, which has been neglected both in MHD and OPAL. Subsequently, both of these equations of state are now being upgraded to include a relativistic treatment of electrons. Interestingly, the simple but astrophysically useful Eggleton, Faulkner, & Flannery (1973, hereafter EFF) equation of state includes relativistic electrons.

One measure of nonideality in plasmas is the so-called coupling parameter $\Gamma$. In a plasma where particles have average distance $\langle r \rangle$ from each other, we can define $\Gamma$ as the ratio of average potential binding energy over mean kinetic energy $k_B T$ (in the simplest case of hydrogen; generalizations to other elements are straightforward)

$$\Gamma = \frac{\langle e^2 / r \rangle}{k_B T}. \quad (1)$$

Plasmas with $\Gamma \gg 1$ are strongly coupled, and those with $\Gamma \ll 1$ are weakly coupled. A famous example of strongly coupled plasmas is the interior of white dwarfs, where the coupling can become so strong as to force crystallization. Weakly coupled are the interiors of stars with masses ranging from the slightly subsolar ones to the largest.

As one can suspect, $\Gamma$ is the dimensionless coupling parameter according to which one can classify theories. Weakly coupled plasma lend to systematic perturbative ideas (e.g., in powers of $\Gamma$) and strongly coupled plasma need more creative treatments. Improvements in the equation of state beyond the model of a mixture of ideal gases are difficult. This has both conceptual and technical reasons. As a fundamental conceptual reason, we mention the fact that in a plasma environment already the idea of isolated atoms (and compound ions) must be abandoned. A technical reason is the difficulty encountered when specific nonideal effects are modeled. The three principal nonideal effects are related to (1) the internal partition functions of bound systems, (2) pressure ionization, and (3) collective interactions of the charged particles. The internal partition functions contain the difficult problem of excited states, where and how they are to be cut off. They are an important element in determining the ionization balances. Pressure ionization must be provided by nonideal interaction terms, because ideal gases would unphysically recombine in the central regions of stars.

2.2. Chemical and Physical Picture

There are two basic approaches to realize nonideal equations of state: the so-called chemical and physical pictures. In the chemical picture, one assumes that the notion of atoms and ions still makes sense, and ionization is treated like a chemical reaction. Modifications of atomic states by the surrounding plasma are expressed in a heuristic and intuitive way. A typical procedure is to find an expression for the probability that a given atomic state of an individual atom still exists. Examples of equations of state realized in the chemical picture are the MHD equation of state (see below), as well as the aforementioned simple EFF equation of state.

The physical picture provides a systematic method to include nonideal effects. The approach starts out from the grand canonical ensemble of a system of the basic constituents (electrons and nuclei) interacting through the Coulomb potential. Configurations corresponding to bound combinations of electrons and nuclei, such as ions, atoms, and molecules, arise in this ensemble naturally as terms in cluster expansions. 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. The only equation of state realized in the physical picture that has been applied to stellar interiors is the OPAL equation of state (see below).

2.2.1. Chemical Picture

Most realistic equations of state that have appeared in the last 30 yr belong to the chemical picture and are based on the free-energy minimization method. This method uses approximate statistical mechanical models (for example, the nonrelativistic electron gas, Debye-Hückel theory for ionic species, hard-core atoms to simulate pressure ionization via configurational terms, quantum mechanical models of atoms in perturbed fields, etc.). From these models a macroscopic free energy is constructed as a function of temperature $T$, volume $V$, and the particle numbers $N_1, \ldots, N_m$ of the $m$ components of the plasma. This free energy is minimized subject to the stoichiometric constraint. The solution of this minimum problem then gives both the equilibrium concentrations and, if inserted in the free energy and its derivatives, the equation of state and the thermodynamic quantities.

Obviously, this procedure automatically guarantees thermodynamic consistency. As an example, when the Coulomb pressure correction (to the ideal-gas contribution) is taken into account in the free energy (and not merely in the
pressure), it affects both the pressure and the equilibrium concentration, i.e., the degrees of ionization. In contrast, the mere inclusion of the pressure correction would be inconsistent with other thermodynamic quantities. In the chemical picture, perturbed atoms must be introduced on a more-or-less ad hoc basis to avoid the familiar divergence of internal partition functions (see, e.g., Ebeling, Kraeft, & Kremp 1976). In other words, the approximation of unperturbed atoms precludes the application of standard statistical mechanics, i.e., the attribution of a Boltzmann factor to each atomic state. The conventional remedy of the chemical picture against this is a modification of the atomic states, e.g., by cutting off the highly excited states in function of density and temperature of the plasma. A currently popular equation of state realized in the chemical picture is the MHD equation of state (Hummer & Mihalas 1988; Mihalas et al. 1988; Däppen et al. 1988, 1987), based on an occupation probability formalism. Specifically, the internal partition functions $Z_{\text{int}}^s$ of species $s$ adopted by MHD are weighted sums

$$Z_{\text{int}}^s = \sum_{i} w_{is} g_{is} \exp \left( - \frac{E_{is}}{k_B T} \right). \tag{2}$$

Here, the subscript $is$ labels states $i$ of species $s$. $E_{is}$ are their energies, and the coefficients $w_{is}$ are the occupation probabilities that take into account charged and neutral surrounding particles. In physical terms, $w_{is}$ gives the fraction of all particles of species $s$ that can exist in state $i$ with an electron bound to the atom or ion, and $1 - w_{is}$ gives the fraction of those that are so heavily perturbed by nearby neighbors that their states are effectively destroyed. Perturbations by neutral particles are based on an excluded-volume treatment and perturbations by charges are calculated from a fit to a quantum-mechanical Stark-ionization theory (for details see Hummer & Mihalas 1988).

### 2.2.2. Physical Picture

It is clear from the preceding subsection that the advantage of the chemical picture lies in the possibility to model complicated plasmas and to obtain numerically smooth and consistent thermodynamic quantities. Nevertheless, the heuristic method of the separation of the atomic-physics problem from that of statistical mechanics is not satisfactory, and attempts have been made to avoid the concept of a perturbed atom in a plasma altogether. This has suggested an alternative description, the physical picture. In such an approach one expects that no assumptions about energy-level shifts have to be made. On the contrary, properties of energy levels and the partition functions should come out from the formalism.

There is an impressive body of literature on the physical picture. Important sources of information with many references are the books by Ebeling et al. (1976, 1991) and Kraeft et al. (1986). However, the majority of work on the physical picture was not dedicated to the problem of obtaining a high-precision equation of state for stellar interiors. Such an attempt was made for the first time by the OPAL group at Livermore (Rogers 1986; Iglesias & Rogers 1995; Rogers et al. 1996, and references therein).

To explain the advantages of this approach for partially ionized plasmas, it is instructive to discuss the activity expansion for gaseous hydrogen. The interactions in this case are all short ranged, and pressure is determined from a self-consistent solution of the equations

$$\frac{P}{k_B T} = z + z^2 b_2 + z^3 b_3 + \cdots. \tag{3}$$

$$\rho = \frac{z}{k_B T} \left( \frac{\partial P}{\partial z} \right) \tag{4}$$

(Rogers 1981), where $z = \exp(z^2 - 1)$ is the activity, $\lambda \equiv \hbar/(2\pi m_e k_B T)^{1/2}$ is the thermal (de Broglie) wavelength of electrons, $\mu$ is the chemical potential, and $T$ is the temperature. The $b_n$ are cluster coefficients such that $b_2$ includes all two particle states, $b_3$ includes all three particle states, etc.

In contrast to the chemical picture, which is plagued by divergent partition functions, the physical picture has the power to avoid them altogether. An important example of such a fictitious divergence is that associated with the atomic partition function. This divergence is fictitious in the sense that the bound-state part of $b_2$ is divergent, but the scattering state part, which is omitted in the chemical-picture approach, has a compensating divergence. Consequently, the total $b_3$ does not contain a divergence of this type (Ebeling et al. 1976; Rogers 1977). A major advantage of the physical picture is that it incorporates this compensation at the outset. A further advantage is that no assumptions about energy-level shifts have to be made (see the previous subsection); it follows from the formalism that there are none.

As a result, the Boltzmann sum appearing in the atomic (ionic) free energy is replaced with the so-called Planck-Larkin partition function (PLPF), given by (see, e.g., Ebeling et al. 1976; Kraeft et al. 1986; Rogers 1986, and references therein)

$$\text{PLPF} = \sum_{nl} (2l + 1) \left[ \exp \left( - \frac{E_{nl}}{k_B T} \right) - 1 + \frac{E_{nl}}{k_B T} \right]. \tag{5}$$

Here, the $E_{nl}$ denote the energies of states with principal quantum number $n$ and angular degree $l$. The PLPF is convergent without additional cutoff criteria, as are required in the chemical picture. We stress, however, that despite its name, the PLPF is not a partition function, but merely an auxiliary term in a virial coefficient (see, for example, Däppen et al. 1987).

### 2.3. Coulomb Correction and the Debye-Hückel Approximation

The Debye-Hückel (DH) theory is based on the replacement of the long-range Coulomb potential by a screened potential (see, e.g., Ebeling et al. 1976). This interaction leads to a negative pressure correction to the ideal-gas value. Under solar conditions, the relative correction culminates at about 8% in the outer part of the convection zone, and it has another local maximum of about 1% in the core. Originally, the DH formalism included an additional ingredient of a fixed size for positive ions, inside of which the electrostatic potential is assumed to be constant. In astrophysical applications such as MHD, this so-called $\tau$-correction has been adopted in the form given by Harris, Roberts, & Trulio (1960; see also Gabriel 1994; Baturin et al. 1996). The systematic OPAL equation of state, however, comes close to the unmodified DH results under solar condition. This makes any $\tau$-correction rather implausible,
especially since in comparisons with observational data, OPAL seems to fare better than MHD (Christensen-Dalsgaard et al. 1996), at least below the helium ionization zones where perhaps other effects, related to excited states, might dominate (see § 4).

We would like to emphasize that close attention to the DH theory is warranted, because it describes the main truly nonideal effect under solar conditions. It was suggested in a number of early papers (see, e.g., Berthomieu et al. 1980; Ulrich 1982; Ulrich & Rhodes 1983; Shibahashi et al. 1983, 1984; Noels et al. 1984) that improvements in the equation of state can reduce discrepancies between theory and observations. Later, Christensen-Dalsgaard et al. (1988) showed that the MHD equation of state reduced these discrepancies significantly for a large range of oscillation modes. It turned out that the Coulomb term is the dominant nonideal correction in the hydrogen and helium ionization zones. This discovery led to an upgrade of the simple, but astrophysically useful, EFF equation of state through the inclusion of the Coulomb interaction term (Christensen-Dalsgaard 1991; Christensen-Dalsgaard & Däppen 1992).

2.4. Beyond the Debye-Hückel Correction

Due to the relatively high temperature inside the Sun, the potential energy of the Coulomb interaction is small compared to the kinetic energy of particles, which allows us to believe that the DH theory makes quantitative sense, at least asymptotically. But to estimate the possible error we need a physically based expression for the next terms in the corresponding expansion. The OPAL equation of state contains such higher terms. An alternative is the path-integral–based Feynman-Kac formalism of Alastuey & Perez (1992, 1996) and Alastuey, Cornu, & Perez (1994, 1995). Its application to solar models is in progress (Perez & Däppen 1999).

New insight beyond DH might come through the equivalent description of the DH correction as a self-energy of electrons and nuclei. A first study has revealed that the thermodynamic consequence of screened bound-state energies and a shifted continuum is hypersensitive to the details of the screening and the method with which the thermodynamic quantities are evaluated. No conclusion has been reached thus far, but a preliminary study has shown that static screening alone comes close to the observational data, leaving little room for any thermodynamic influence of dynamic screening (Arndt, Däppen, & Nayfonov 1998). Screening has also been considered in connection with nuclear reaction rates, more specifically those responsible for the solar neutrino flux (see, e.g., Brüggen & Gough 1997, and references therein).

Very recently, Nayfonov & Däppen (1998) examined the signature of the internal partition function in the equation of state. That study has revealed interesting features about excited states and their treatment in the equation of state. The MHD equation of state, with its specific, density-dependent occupation probabilities (see § 2.2.1), is causing a characteristic “wiggle” in the thermodynamic quantities, most prominently in $\gamma_1$, where perhaps other effects, related to excited states, might manifest in the differences between MHD and MHD$_{GS}$. Density is implied but not shown in the figure (for more details and different thermodynamic variables and chemical compositions, see Nayfonov & Däppen 1998). Five cases were considered: (1) MHD (standard MHD occupation probabilities of Hummer & Mihalas 1988); (2) MHD$_{GS}$ (standard MHD internal partition function of hydrogen but truncated to the ground state term); (3) OPAL and OPAL tables (1996 November version of Rogers et al. 1996); (4) MHD$_{PL}$ (MHD internal partition function of hydrogen, but replaced by the PLPF, eq. [5]); and (5) MHD$_{PL,GS}$ (MHD$_{PL}$ truncated to the ground state term). The effect of the inclusion of the excited states in the internal partition function is manifest in the differences between MHD and MHD$_{GS}$, and between MHD$_{PL}$ and MHD$_{PL,GS}$, respectively. The effect of

![Fig. 1a](image-url)

**Fig. 1a**—(a) Absolute values of $\gamma_1$ for solar temperatures and densities of a hydrogen-only plasma; MHD (asterisks), MHD$_{GS}$ (dashed lines), MHD$_{PL}$ (dotted-dashed lines), MHD$_{PL,GS}$ (dotted lines), and OPAL (solid lines). (b) Relative differences with respect to MHD$_{GS}$, in the sense $[\gamma_1 - \gamma_1(MHD_{cal})/\gamma_1(MHD_{cal})]$, using the same line styles as in (a). The horizontal solid zero line, representing MHD$_{GS}$, is also shown. See text for the definitions of the different MHD versions.
the different occupation probability of the ground and excited states shows up in the difference between MHD and MHD$_{PL}$, and between MHD$_{GS}$ and MHD$_{PL,GS}$. It was found that the presence of excited states is crucial. Also, the wiggle, which is a genuine neutral-hydrogen effect, is present despite the fact that most of the hydrogen is already ionized. The qualitative picture does not change when helium is added (Nayfonov & Däppen 1998).

3. INVERTING THE DATA

3.1. Introduction

We have performed differential inversions with respect to given reference models. We examine the influence of the equation of state by choosing two sets of models, one with the MHD and the other with the OPAL equation of state. Because of its differential nature, our inversion procedure is more reliable for reference models close to the real solar structure. Since diffusion has now become part of the standard solar model (Christensen-Dalsgaard et al. 1996), it is included in our reference models M1–M8 (see Table 1). For a study with artificial data, we have also considered a reference model without diffusion (M9). We use it to demonstrate that our inversion procedure applied to the theoretical frequencies of model M9 is able to reconstruct the intrinsic $\gamma_1$ difference with respect to the reference model (M5). We found that this is indeed the case even for the relatively bad model M9, which is most likely farther away from the true solar structure than each of the reference models M1–M8 used for the real data. In addition, we have tested the robustness of the inferred results despite uncertainties in solar model inputs by using a number of different solar models. Comparing the results of inversions that are made with respect to different reference models with the directly evaluated difference of the models themselves is a powerful tool to assess the quality of the inversions.

3.2. Method

An inversion for solar structure (see, e.g., Dziembowski, Pamyatnykh, & Sienkiewicz 1990; Däppen et al. 1991; Antia & Basu 1994; Dziembowski et al. 1994) generally proceeds through a linearization of the equations of stellar oscillations around a known reference model. The differences between the structure of the Sun and the reference model are then related to the differences in the frequencies of the Sun and the model by kernels. Nonadiabatic effects and other errors in modeling the surface layers give rise to frequency shifts (Cox & Kidman 1986; Balmforth 1992; Guenther 1994; Rosenthal et al. 1995, 1999) which are not accounted for by the variational principle. In the absence of any reliable formulation, these effects have been taken into account in an ad hoc manner by including an arbitrary function of frequency in the variational formulation (Dziembowski et al. 1990). Thus the fractional change in frequency of a mode can be expressed in terms of fractional changes in the structure of the model and a surface term.

When the oscillation equation is linearized—under the assumption of hydrostatic equilibrium—the fractional change in the frequency can be related to the fractional changes in two of the functions that define the structure of the models. Thus,

$$\frac{\delta \omega_i}{\omega_i} = \int K_{e,\rho}(r) \frac{\delta c^2(r)}{c^2(r)} \, dr + \int K_{\rho,\rho}(r) \frac{\delta \rho(r)}{\rho(r)} \, dr + \frac{F_{\text{surf}}(\omega_i)}{E_i}$$

(6)

(see, e.g., Dziembowski et al. 1990). Here $\delta \omega_i$ is the difference in the frequency $\omega_i$ of the $i$th mode between the solar data and a reference model. The functions $c$ and $\rho$ are the sound speed and density. The kernels $K_{e,\rho}$ and $K_{\rho,\rho}$ are known functions of the reference model that relate the changes in frequency to the changes in $c^2$ and $\rho$, respectively; and $E_i$ is the inertia of the mode, normalized by the photospheric amplitude of the displacement. The term $F_{\text{surf}}$ results from the near-surface errors.

The conversion of the kernels for $(c^2, \rho)$ to those of the set $[(\gamma_1)]_{\text{int}}$, $u$, $Y$, $u_Y$, $Y_u$, where $u = P/\rho$, $P$ being the pressure and $Y$ the helium abundance, is discussed in Basu & Christensen-Dalsgaard (1997). After the conversion, equation (6) can be written as

$$\frac{\delta \omega_i}{\omega_i} = \int K_{1,\gamma_1}(r) \frac{\delta \gamma_1}{\gamma_1} \, dr + \int K_{1,u}(r) \frac{\delta u}{u} \, dr + \int K_{1,Y}(r) \delta Y \, dr + \frac{F_{\text{surf}}(\omega_i)}{E_i}.$$  

(7)

We use the technique of Optimally Localized Averages (OLA) to carry out the inversion. The purpose of the OLA technique (Backus & Gilbert 1968; Kosovichev 1995) is to construct appropriate linear combinations, $\sum_i c(r_0)\delta \omega_i / \omega_i$, of the data with coefficients $c(r_0)$ so that the result represents a localized average of the quantity $(\delta \gamma_1 / \gamma_1)_{\text{int}}$ at the radius $r_0$. This is possible since the $(\gamma_1)_{\text{int}}$ averaging kernel

\[\text{TABLE 1}
\]

Properties of the Solar Models Used in Figures 2a, 2b, and 4

| Model | Equation of State | Radius (Mm) | Convective Flux | $Y_e$ | $r_{\text{eq}}/R_0$ |
|-------|------------------|-------------|-----------------|------|-----------------|
| M1    | MHD              | 695.78      | CM              | 0.2472 | 0.7145 |
| M2    | MHD              | 695.99      | CM              | 0.2472 | 0.7146 |
| M3    | MHD              | 695.51      | CM              | 0.2472 | 0.7145 |
| M4    | MHD              | 695.78      | MLT             | 0.2472 | 0.7146 |
| M5    | OPAL             | 695.78      | CM              | 0.2465 | 0.7134 |
| M6    | OPAL             | 695.99      | CM              | 0.2465 | 0.7135 |
| M7    | OPAL             | 695.51      | CM              | 0.2466 | 0.7133 |
| M8    | OPAL             | 695.78      | MLT             | 0.2465 | 0.7135 |
| M9    | OPAL             | 695.78      | CM              | 0.2646 | 0.7268 |

* See text.

b CM: Canuto & Mazitelli 1991. MLT: mixing length theory.
The parameters $c_i$ control the effect of data noise. The function $K_i$ is a unimodular function localized at $r = r_0$, and the sums $\sum_i c_i(r_0)K_i^b \delta u/u$, $\sum_i c_i(r_0)K_i^b \delta Y$, and $\sum_i c_i \tilde{F}_{surf}(\omega_i)/E_i$ are small.

This objective is achieved by minimizing

$$
\int \left[ \sum_i c_i(r_0)K_i^{b\text{int}} \right]^2 (r - r_0)^2 dr + \beta_1 \int \left[ \sum_i c_i w(r)K_i^b \right]^2 dr + \beta_2 \int \left[ \sum_i c_i w(r)K_i^b \right]^2 dr + \mu \sum_{i,j} c_i c_j E_{ij},
$$

with the constraint that the averaging kernel be unimodular, i.e.,

$$
\sum_i c_i(r_0) \int K_i^{b\text{int}}(r) dr = 1.
$$

Here, $E_{ij}$ is the covariance matrix of errors in the data. The parameters $\beta_1$ and $\beta_2$ control the contributions of $\delta u/u$ and $\delta Y$, respectively, and $\mu$ is a trade-off parameter that controls the effect of data noise. The function $w(r)$ is a suitably chosen, increasing function of radius, which ensures that the contributions from the second and third terms from the surface layers are suppressed properly. To reduce the influence of near-surface uncertainties, we apply the additional constraints that

$$
\sum_i c_i(r_0) \Phi_i(\omega_i) = 0, \quad \lambda = 0, \ldots, \Lambda,
$$

where the $\Phi_i$ are B-splines with a suitably scaled argument (see, e.g., Däppen et al. 1991).

### 3.3. Reference Models

We have constructed a set of calibrated solar models, all of which have either the MHD or the OPAL equation of state. All models use OPAL opacities (Iglesias & Rogers 1996), which are supplemented by the low-temperature opacities of Kurucz (1991). Since one of the most uncertain aspects of solar modeling is the formulation of the convective flux, we use two different convective flux formalisms—

the standard mixing length theory and that of Canuto & Mazzitelli (1991). The two formalisms give fairly different stratifications in the outer regions of the Sun where $\gamma_1$ differences are also likely to be the largest. All models have $Z/X = 0.0245$ (see, e.g., Grevesse & Noels 1993).

A major source of uncertainty in the inversion results is the solar radius. Until recently, the standard value of 695.99 Mm was used unquestioningly. However, new $f$-mode data suggests that the radius is actually smaller (see, e.g., Schou et al. 1997; Antia 1998). A difference in the radius between the solar models used as a reference model for inversions and the Sun can lead to a large error in the inversion results (see, e.g., Basu 1998a). Thus we have constructed models with the standard radius as well as the $f$-mode radius of 695.78 Mm (see, e.g., Antia 1998). Recent observations to determine the solar radius (see, e.g., Brown & Christensen-Dalsgaard 1998) suggest that the solar radius is even lower, 695.508 Mm. Some of the relevant properties of the models are listed in Table 1. All models, except M9, assume the gravitational settling of helium and heavy elements. The composition profiles for models M1–M8 are the ones obtained from helioseismological inversions by Antia & Chitre (1998). For model M9, the profile from the no-diffusion model of Bahcall & Pinsonneault (1992) was used.

Note that the surface helium abundances and convection zone depths of all models except M9 are consistent with the helioseismically determined helium abundance and depth of the convection zone of the solar envelope (see, e.g., Basu & Antia 1997; Basu 1998a).

### 3.4. Test Results

To test the inversion procedure, we have inverted models M1 and M9 using model M5 as the reference model. The purpose of inverting model M1 is to show that we can invert for the intrinsic $\gamma_1$ differences between two models (Fig. 2a). We see that we are indeed successful in inverting...
for the intrinsic $\gamma_1$ difference between MHD and OPAL models. The structure and helium abundance of the models M1 and M5 are very similar, hence the $\gamma_1$ difference between models with different equations of state is dominated by differences in the equation of state, rather than differences in structure.

In a parallel test, model M9 is inverted with respect to reference model M5 in order to show that we are indeed inverting just for the equation of state part of the $\gamma_1$ difference $|\delta\gamma_1|_{\text{int}}$. We deliberately choose for this test the relatively bad solar model M9 without diffusion to show insensitivity to the quality of the reference model. Importantly for this test, model M9 has the same equation of state as the reference model M5. Using theoretically computed frequencies of model M9, our inversion procedure gives the intrinsic difference of between models M5 and M9. Since the equation of state is the same in the two models, we should obtain essentially zero for the intrinsic difference. This is indeed the case (see Fig. 2b).

The small deviations from zero can be explained mainly as contributions in the solution because of the large difference in the helium abundance (i.e., the third term in eq. [7]), although there can also be a contribution from the neglected differences in the heavy-element abundances. Increasing the parameter $\beta_2$ helps in getting better inversion results, but it degrades the quality of the inversion. However, this is not a concern for inversion of the solar data with models M1–M8, since the difference in the helium abundance between these models and the Sun is an order of magnitude less than the helium-abundance difference between models M9 and M5. For comparison, Figure 2b also shows total $\gamma_1$ difference. Note that the total $\gamma_1$ inversion captures the difference in total $\gamma_1$ to within the limits of the resolution.

The mode set and errors used for the test were the same as that of the SOI/MDI set mentioned above (Rhodes et al. 1997). We are quite successful in constructing localized kernels until fairly close to the solar surface. A sample of the averaging kernels is shown in Figure 3. The use of the observational mode set and errors ensures that the inversion properties (see, for example, resolution of the averaging kernels, propagated errors, etc.) will remain the same when solar data are inverted.

4. RESULTS AND CONCLUSION

The result obtained by inverting solar data using models M1–M8 are shown in Figure 4. We show inversions with respect to a deliberately large number of reference models having different parameters. By doing so we demonstrate that in the chosen technique only the equation of state matters.

Note that the results of all of the MHD models are very similar despite differences in radius and stratification. However, these are very different from the OPAL models that form a distinct group. The differences between the two equations of state and the Sun are fairly large in the outer layers of the Sun.

In contrast to earlier results (Basu & Christensen-Dalsgaard 1997), which could only resolve the somewhat deeper layers of the Sun, the present focus on the 20% uppermost layers confirms the aforementioned effect of excited states as included in the MHD equation of state (§ 2.4). The results also confirm that the OPAL equation of state is better for $r < 0.97 R_\odot$ (Christensen-Dalsgaard et al. 1996), but the situation is reversed in the top 2%–3% of the radius.

Since the difference in $\gamma_1$ between MHD and OPAL is the wiggle of Figure 1, the observed preference of the MHD model in the upper region could indicate the correctness of an MHD-like treatment of the excited states. Again, we emphasize that Figure 4 confirms earlier results that below the wiggle region OPAL fares better than MHD (Christensen-Dalsgaard et al. 1996). There, the internal par-
tition functions of OPAL à la the PLPF and the absence of a $r$-correction (§ 2.3) seem to be the better choice.

The reversal of fortune in favor of MHD in the upper part of the Sun (above $0.97 \, R_\odot$) could be because of the different implementations of many-body interactions in the two formalisms. Since density decreases in the upper part, OPAL, by its nature of a systematic expansion, inevitably becomes more accurate; but MHD might, by its heuristic approach (and by luck!), have incorporated even finer, higher order effects.

The helioseismic helium-abundance determination procedure is quite sensitive to the details of internal partition functions. Since the wiggle is located in the second ionization zone helium, although it is a pure hydrogen effect (see § 2.4), it has a very important bearing on the astrophysically relevant helioseismic helium-abundance $Y$ determination in the solar convection zone. In principle, the asymptotic analysis by Basu & Antia (1995), which leads to $Y = 0.249$ for OPAL and $Y = 0.246$ for MHD, could be taken as an indication that the equation of state does not matter in the result for $Y$. However, other studies came to a different conclusion. In independent inversions, Kosovichev (1997) obtained $Y = 0.23$ for MHD and $Y = 0.25$ for OPAL, Richard et al. (1998) $Y = 0.242$ for MHD and $Y = 0.248$ for OPAL, and Basu (1998b) $Y = 0.248$ for OPAL and $Y = 0.251$ for MHD. In an entropy calibration by Baturin & Ayukov (1997), the result was $Y = 0.23$ for OPAL and $Y = 0.25$ for MHD. In the latter two, the sign of the change is reversed compared to the three former.

The confirmation of the excited-states effect in solar data makes helium-abundance determinations based on the MHD equation of state more plausible than the ones based on OPAL, but the various current techniques do not yet allow a consensus. We note in passing that the helium-abundance values given in Table 1 should not be confused with the aforementioned inversion results. Table 1 lists the result of calibrations in which the helium parameter compensates for other effects as well, and the relative stability of the helium parameter in M1–M8 is no indication for its absolute correctness. Inversions can, in principle, isolate the helium abundance from other effects, but an absolutely accurate equation of state is required. As we mentioned, any quantitative conclusions about the value of $Y$ would be premature. However, since the MHD equation of state appears to describe reality in the helium-ionization zone better, it might be the preferable equation of state in helium-abundance determinations.

Let us add a word of caution. It could appear tempting to produce a “combined” solar equation of state, with MHD for the top part and OPAL for the lower part. However, such a hybrid solution is fraught with danger. For instance, it is known that patching together equations of state can introduce spurious effects (Däppen et al. 1993). It seems that the right way is to improve MHD and OPAL in parallel and independently, guided by the progress of helioseismology.

We thank Jørgen Christensen-Dalsgaard and Forrest Rogers for stimulating discussions and valuable advice. W. D. and A. N. are supported by grant AST 96-18549 of the National Science Foundation. W. D. acknowledges additional support from the SOHO Guest Investigator grant NAG 5-6216 of NASA, a grant extended to the University of Southern California by the Theory Group of Lawrence Livermore National Laboratory, and from the Danish National Research Foundation through its establishment of the Theoretical Astrophysics Center. S. B. is supported by funds from the Institute for Advanced Study. SOHO is a project of international cooperation between ESA and NASA.

REFERENCES

Christensen-Dalsgaard, J., & Lebreton, L. 1988, Nature, 336, 634
 Cox A. N., & Kidman R. B. 1986, in Theoretical Problems in Stellar Stability and Oscillations (Lége: Institut d’Astrophysique), 259
 Däppen, W., Mihalas, D. 1997, ApJ, 498, 349
 Ebeling, W., Kraft, W. D., & Kremp, D. 1976, Theory of Bound States of Southern California by the Theory Group of Lawrence Livermore National Laboratory, and from the Danish National Research Foundation through its establishment of the Theoretical Astrophysics Center. S. B. is supported by funds from the Institute for Advanced Study. SOHO is a project of international cooperation between ESA and NASA.

We thank Jørgen Christensen-Dalsgaard and Forrest Rogers for stimulating discussions and valuable advice. W. D. and A. N. are supported by grant AST 96-18549 of the National Science Foundation. W. D. acknowledges additional support from the SOHO Guest Investigator grant NAG 5-6216 of NASA, a grant extended to the University of Southern California by the Theory Group of Lawrence Livermore National Laboratory, and from the Danish National Research Foundation through its establishment of the Theoretical Astrophysics Center. S. B. is supported by funds from the Institute for Advanced Study. SOHO is a project of international cooperation between ESA and NASA.

REFERENCES

Christensen-Dalsgaard, J., Däppen, W., & Lebreton, L. 1988, Nature, 336, 634
Cox A. N., & Kidman R. B. 1986, in Theoretical Problems in Stellar Stability and Oscillations (Lége: Institut d’Astrophysique), 259
Däppen, W., Mihalas, D. 1997, ApJ, 498, 349
Ebeling, W., Kraft, W. D., & Kremp, D. 1976, Theory of Bound States and Ionization Equilibrium in Plasmas and Solids (Berlin: Akademieverlag)
Eggleton, P. P., Faulkner, J., & Flannery, B. P. 1973, Astron. Astrophys. Trans. 23, 325
Elliot, J. R. 1996, MNRAS, 280, 1244
Elliot, J. R., & Kosovichev, A. G. 1998, ApJ, 500, L199
Gabriel, M. 1994, Astron. Astrophys. Trans., 292, 281
Gough, D. O., Kosovichev, A. G., Toomre, J., & Global Oscillation Network Group Team. 1996, Science, 272, 1296
Grevesse, N., & Noels, A. 1993, in Origin and Evolution of the Elements, ed. N. Prantzos, E. Vangioni-Flam, & M. Cassé (Cambridge: Cambridge University Press), 15
Guenter, D. B. 1994, ApJ, 422, 400
Harris, G. M., Roberts, J. E., & Trulio, J. G. 1960, Phys. Rev., 119, 1832
Hummer, D. G., & Mihalas, D. 1988, ApJ, 331, 794
Iglesias, C. A., & Rogers, F. J. 1995, ApJ, 443, 460
Iglesias, C. A., & Rogers, F. J. 1996, ApJ, 464, 943
Kosovichev, A. G. 1995, in ASP Conf. Ser. 76, Helio- and Asteroseismology from the Earth and Space, ed. R. K. Ulrich, E. J. Rhodes, & W. Däppen (San Francisco: ASP), 89
———. 1996, Bull. Astron. Soc. India, 24, 355
———. 1997, in AIP Conf. Ser. 385, Robotic Exploration Close to the Sun: Scientific Basis, ed. S. R. Habbal (New York: AIP), 159
Kosovichev, A. G., et al. 1997, Solar Phys., 170, 43
Kraeft W. D., Kremp, D., Ebeling, W., & Röpke G. 1986, Quantum Statistics of Charged Particle Systems (New York: Plenum)
Kurucz R. L. 1991, in NATO ASI Series, Stellar Atmospheres: Beyond Classical Models, ed. L. Crivellari, I. Hubeny, & D. G. Hummer (Dordrecht: Kluwer), 441
Lubow, S. H., Rhodes, E. J., & Ulrich, R. K. 1980, in Lecture Notes in Physics, Vol. 125, Nonradial and Nonlinear Stellar Pulsation, ed. H. A. Hill & W. Dziembowski (Berlin: Springer), 300
Mihalas, D., Däppen, W., & Hummer, D. G. 1988, ApJ, 332, 815
Nayfonov, A., & Däppen, W. 1998, ApJ, 499, 489
Noels, A., Scuflaire, R., & Gabriel, M. 1984, Astron. Astrophys. Trans., 130, 389
Perez, A., & Däppen, W. 1999, ApJ, submitted
Rhodes, E. J., Kosovichev, A. G., Schou, J., Scherrer, P. H., & Reiter, J. 1997, Solar Phys., 175, 287
Richard, O., Dziembowski, W. A., Sienkiewicz, R., & Goode, P. R. 1998, Astron. Astrophys., 338, 756
Rogers, F. J. 1977, Phys. Rev. Lett., A61, 358
———. 1981, Phys. Rev., A24, 1531
———. 1986, ApJ, 310, 723
Rogers, F. J., Swenson, F. J., & Iglesias, C. A. 1996, ApJ, 466, 943
Rosenthal, C. S., Christensen-Dalsgaard, J., Houdek, G., Monteiro, M., Nordlund, Å., & Trampedach, R. 1995, in Proc. 4th SOHO Workshop, ed. J. T. Hoeksema, V. Domingo, B. Fleck, & B. Battrick (Noordwijk: ESA), 459
Rosenthal, C. S., Christensen-Dalsgaard, J., Nordlund, Å., Stein, R., & Trampedach, R. 1999, A&A, submitted
Schou, J., et al. 1998, ApJ, 505, 390
Shibahashi, H., Noels, A., & Gabriel, M. 1984, Astron. Astrophys. Trans., 130, 389
Thompson, M. J., Toomre, J., Anderson, E. R., & Global Oscillation Network Group Team. 1996, Science, 272, 1300
Ulrich, R. K. 1982, ApJ, 258, 404
Ulrich, R. K., & Rhodes, E. J. 1983, ApJ, 265, 551