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2006 J. Phys. A: Math. Gen. 39 4459

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Solar plasma: calculation of thermodynamic functions and equation of state

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Received 19 September 2005, in final form 4 January 2006

Published 7 April 2006

Online at stacks.iop.org/JPhysA/39/4459

Abstract

Calculations of thermodynamic properties for the solar plasma are presented. Effects of Coulomb interaction, exchange and diffraction effects, free electron degeneracy, relativistic corrections and radiation pressure contributions are taken into account. Calculations of the equation of state of the solar plasma with different element compositions are carried out. The contribution of various plasma effects and chemical element abundance to thermodynamic functions and in particular Γ_1 is discussed.

PACS numbers: 51.30.+i, 96.60.–j, 96.60.Ly

1. Introduction

A great number of high precision observation data on eigenfrequencies of solar oscillations obtained during the last decade [1, 2] provides detailed information on physical conditions in the interior of the Sun and permits us to develop more precise models of its inner structure. To build an adequate model of the Sun one needs a very accurate equation of state (EOS hereafter) of the solar plasma together with other microphysical parameters (opacity, nuclear reaction rate, etc). Modern EOS models of the solar plasma now in use [3, 4] reproduce the sound velocity with high accuracy over the whole temperature range, but there are some issues which have to be clarified. Among them are the level of accuracy of theoretical estimations for adiabatic exponent Γ_1 in the lower part of the convection zone and the possible effect in the EOS of nonideal plasma corrections on the profile of Γ_1 . We intend to discuss the adiabatic exponent profile inside the Sun, using a comparison of the values for different EOS models, which successively include different plasma effects.

2. Thermodynamic model

The SAHA-S EOS is based on the so-called chemical picture of plasmas [5, 6] which starts from the representation of the free energy as a sum of the zero approximation terms $F^{(\text{id})}$, corresponding to the ‘ideal-gas’ mixture with varying composition of a wide spectrum of simple and complex particles—electrons and ions, atoms and molecules and so on—and of further contributions stemming from interaction between these particles. Historically, the free energy formulation in the EOS procedure has been written in [7]. Generally, complex particles have internal degrees of freedom—excited states, being in thermodynamic equilibrium with the system as a whole, i.e. with its translational degrees of freedom:

$$F(\{N_i\}, V, T) = \sum_i F_i^{(\text{id})} + F_e^{(\text{id})} + F^{(\text{rad})} + \Delta F_{ii,ee,ie}^{(\text{int})}(\{N_i\}, V, T). \quad (1)$$

The first term of the Helmholtz free energy (1) is the contribution of the ideal gas of ‘heavy’ particles, atoms, ions and molecules and represents the Boltzmann ideal-gas expression for a mixture of particles of various species:

$$F_i^{(\text{id})} = \sum_{j=1}^L N_j k_B T \left(\ln \frac{n_j \lambda_j^3}{Q_j} - 1 \right). \quad (2)$$

Here k_B is the Boltzmann constant, $\lambda_j = \sqrt{\frac{2\pi\hbar^2}{m_j k_B T}}$ is the thermal de Broglie wavelength and Q_j is the partition function for a particle of species j , which uses the excited energy levels and statistical weights for isolated particles. For atoms and ions we use data from [8]. For diatomic molecules the partition functions correspond to the approximation of the non-rigid rotator—the non-harmonic oscillator with the data from [9] with restriction for energies $\varepsilon_i \leq D - k_B T$, where D is the dissociation energy of a diatomic molecule.

The contribution of the electronic ideal gas to the Helmholtz free energy expression (1) is represented by the second term $F_e^{(\text{id})}$. The ideal gas of free electrons is considered as a partially degenerate Fermi gas [10].

The fourth term of the Helmholtz free energy (1) is responsible for inter-particle interaction. In this work, the main inter-particle interaction for the solar plasma is the Coulomb interaction between charged particles in the framework of the Debye approximation in the grand canonical ensemble, generalized for the case of multi-stage ionization (DGCE) [11]. To make the EOS of the solar plasma more precise, the electron exchange and diffraction corrections to the Coulomb interaction are taken into account. In accordance with [12], the Coulomb correction to the ideal-gas pressure with the exchange and diffraction effects has the form

$$\begin{aligned} \frac{\Delta P^{(\text{CoulExDif})}}{n_e k_B T} = & -\frac{\tilde{\Gamma}^3}{24\pi n_e f^3} - \frac{1}{4} \zeta_e \lambda_e^2 f \frac{\zeta_e}{n_e} + \frac{\lambda_e \zeta_e f^2}{4} \frac{\tilde{\Gamma}^2}{4n_e f^3} \\ & + \frac{\pi \lambda_e f^2 \zeta_e}{4} \frac{\zeta_e}{n_e} \left\{ \frac{(1 - \sqrt{2})}{\sqrt{2}} + \frac{1}{2} \sum_{i=1}^L \sum_{k=1}^L Z_i^2 Z_k^2 \frac{\zeta_i}{\zeta_e} \frac{\zeta_k}{\zeta_e} \frac{\lambda_{ik}}{\lambda_e} \right\}, \end{aligned} \quad (3)$$

where λ_e, ζ_e are the thermal de Broglie wavelength and activity ($\zeta_e = \exp(\mu_e/k_B T)/\lambda_e^3$) for the electrons and the same λ_i, ζ_i for the ions, and λ_{ik} is the thermal de Broglie wavelength with the reduced mass $m_{ik} = m_i m_k / (m_i + m_k)$; the summation in (3) is over ions only. In (3) all activities have to be expressed in terms of the particle densities using equations [12]

$$\begin{aligned} \zeta_e = & \frac{n_e}{1 + \frac{\tilde{\Gamma}}{2} + \frac{1}{4} \zeta_e \lambda_e^2 f - \frac{\lambda_e \tilde{\Gamma}^2}{f} - \frac{\pi \lambda_e f^2 \zeta_e}{4} [\sqrt{2} - 1]} \\ \zeta_i = & \frac{n_i}{1 + Z_i^2 \frac{\tilde{\Gamma}}{2} - \frac{\pi \lambda_e f^2 \zeta_e Z_i^2}{4} \left(1 + \sum_{k=2}^I Z_k^2 \frac{\zeta_k}{\zeta_e} \frac{\lambda_{ik}}{\lambda_e} \right)}. \end{aligned} \quad (4)$$

The parameter $\tilde{\Gamma}$ is defined from the equation

$$\tilde{\Gamma} = 4\pi f^3 \sum_{i=1}^L Z_i^2 \zeta_i. \quad (5)$$

Due to the high temperature values of plasma in the inner part of the sun, the relativistic effects in the electron motion and radiation pressure can affect the thermodynamics of the solar plasma. To understand how important these effects are, the relativistic corrections [10] were accounted for. It has to be noted that the first order correction to the pressure vanishes completely, but there are corrections to the internal energy of the same order,

$$\frac{\Delta E^{\text{rel}}}{k_B T} = \zeta_e \frac{15k_B T}{8m_e c^2}, \quad (6)$$

and the electronic chemical potential.

The radiation pressure and the internal energy contributions are taken in the form [10]

$$\Delta P^{(\text{Rad})} = \frac{\Delta E^{(\text{Rad})}}{3V} = \frac{4\sigma_{\text{SB}}}{3c} T^4; \quad \sigma_{\text{SB}} = \frac{\pi^2 k_B^4}{60\hbar^3 c^2}. \quad (7)$$

3. Results and discussion

Using the model (1)–(7), computations of composition and thermodynamic properties of the solar plasma have been carried out. All the calculations were performed by the computer code SAHA-S [13]. The ‘adiabatic exponent’ Γ_1 ,

$$\Gamma_1 = \left(\frac{\partial \ln P}{\partial \ln \rho} \right)_S, \quad (8)$$

one of the key thermodynamic values in helioseismology, is paid the main attention.

It is well known that models now in use [3, 4] demonstrate growing discrepancy with the results of helioseismic inversion [1] to temperatures corresponding to the bottom of the convection zone. To understand possible reasons for this discrepancy, computations of thermodynamics of solar plasmas taking into account various plasma effects along the solar trajectory were carried out.

The idea of these calculations consisted in successive switching of the plasma effects to the EOS to analyse the dependence of the thermodynamic functions on these effects. In this case, we used data of the model S for the solar trajectory, namely the dependence of the density on temperature, and the helium and heavy elements abundance. The first step consisted of calculations of the fully ionized ideal plasma of hydrogen and helium. In this case Γ_1 has to be exactly equal to 5/3. In the second step the fully ionized plasma of hydrogen and helium was considered with the Coulomb interactions in accordance with the DGCE [11]. Figure 1 demonstrates the shift of Γ_1 to higher values due to the contribution of the charged particle interactions.

In the third step, the calculations of plasma properties were carried out in which together with the Coulomb interactions the recombination of free charges was allowed. The contribution of bound states Q_j using the Planck–Larkin [14] formula to calculate the partition functions, as a first step, was considered. It is seen in figure 1 that in the region of lower temperature where the contribution of bound states is noticeable, the recombination effects lead Γ_1 to a steep falling down. Addition of degeneracy effects of free electrons does not change this picture, since the adiabatic exponent of the ideal electron gas is exactly equal to 5/3 [10].

The next step in our calculations consisted in the inclusion of heavy elements. The abundance of heavy elements corresponded to the model S and the distribution of mass

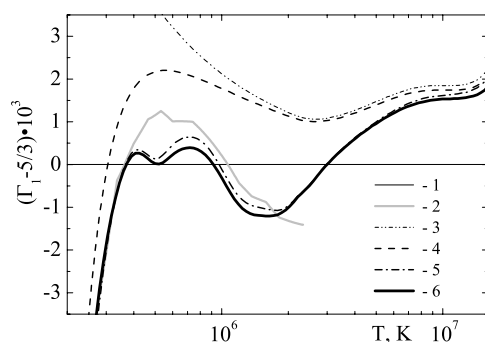


Figure 1. Adiabatic exponent of the ideal plasma of protons and alpha-particles (curve 1) is the present calculation, the results of inversion [1]. Curves 2, 3 represent the fully ionized plasma of hydrogen and helium with Coulomb interaction in the framework of the DGCE [11]; curve 4 represents the contribution of bound states of H and He to Γ_1 . Contribution of heavy elements and bound states with the Planck–Larkin [14] and Starostin–Roerich–More [15] partition functions.

fractions was C—0.190 6614, N—0.055 8489, O—0.542 9784, Ne—0.210 5114. All degrees of ionization for each chemical element were taken into account so as the diatomic molecules H_2 , H_2^+ , C_2 , N_2 , O_2 , CH, CN, CO, NH, NO. The partition functions of the excited states of atoms were calculated using for example the Planck–Larkin formula. The maxima of Γ_1 in the temperature range 400–700 kK are due to the ionization of inner electronic shells of heavy elements. The difference between the values of Γ_1 calculated with the Planck–Larkin [14] and Starostin–Roerich–More [15] formulae for the partition functions of atoms and ions Q_j can be seen in the same figure. The maximal difference between the calculation results with two partition functions is of factor 4 at very high temperature [15], but for the solar plasma the maximal effect occurs at the temperatures of about 500 kK, which is due to the contribution of the abundance of bound states in this temperature region. Whereas in the centre of the sun where temperature reaches maximum, this difference is not so high due to the full ionization of the main chemical elements of the solar plasma, H and He. The difference between Γ_1 with and without the radiation effects is practically constant beginning from the temperature of about 1000 kK, which can be explained by the increase of the solar plasma density in the direction to the centre of the sun. A smallest effect is connected with additional quantum corrections (exchange and diffraction), which are given by (3)–(5).

Due to the very high temperature of the solar plasma in the zone deeper than the bottom of the convection zone, relativistic effects are quite noticeable (see [16]). Curve 5 in figure 2 for Γ_1 represents the calculation with all plasma effects considered above including the Coulomb interaction effects with quantum corrections, degeneracy of free electrons, radiation effects, relativistic effects and the partition functions of atoms and ions according to [15].

The last numerical experiment in the present work consisted of the variation of the composition of heavy elements, namely it was enriched with iron and silicon. The element composition of heavy elements (in the limits of the abundance of heavy elements within the model S) was as follows: C—0.1762, N—0.0516, O—0.5018, Ne—0.0967, Fe—0.0982, Si—0.0755. Other parameters of the calculation coincided with those demonstrated in figure 2, that is all plasma effects were taken into account.

The results of such calculations are represented in figure 3. It is seen that the enriched composition of heavy elements does not lead to a radical change in the Γ_1 behaviour and

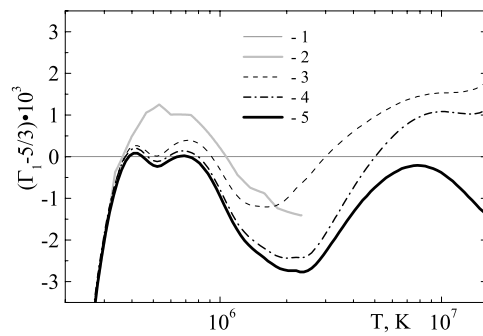


Figure 2. Contribution of radiation, exchange and diffraction effects (3) and relativistic effects (8) to Γ_1 . 1, 2, 3 are the same as 1, 2, 6 in figure 1.

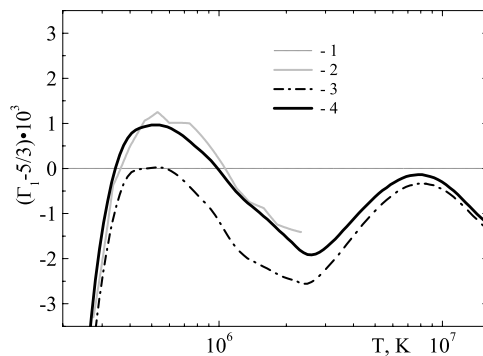


Figure 3. Influence of extension (3) of heavy element composition on the behaviour of Γ_1 ; 1, 2 are the same as 1, 2 in figure 2, 4 is the calculation with extended composition and double diminished Z .

becomes apparent by removing the two-peak structure in the 400–700 kK temperature range.

In the last step, the heavy element abundance was equal to $Z/2$, where Z was that corresponding to the model S value. The results of these calculations are also shown in figure 3. One can see this more than satisfactory accordance of these results with the data obtained from the procedure of helioseismic inversion [1], but in our opinion, it has to be appreciated as occasional at the moment.

We must note that the ionization degree for H and He reaches its maximum in the convection zone; for C it occurs in the core only, whereas for other chemical elements it does not reach the maxima even in the centre of the sun. It points to a significant role of bound states of atoms and ions in the solar plasma and knowledge of their energy level structure as an adequate description of contribution to thermodynamic functions and equation of state.

4. Conclusions

In this work, we have proposed calculations of the solar plasma by the thermodynamic model SAHA-S. To isolate discrepancies in Γ_1 between the theoretical data and the data of the helioseismic inversion, the contribution of various plasma effects has been analysed. The most important factors which affect the behaviour of the adiabatic exponent in the convection zone are the Coulomb correlations and the bound states of atoms and ions. In the region of

the solar radiation zone and core, the relativistic and radiation effects are of great importance. Extending the set of heavy elements with Fe and Si leads to the removal of additional peaks of the adiabatic exponent because of the ionization of Ne inner shells.

Acknowledgments

This work was supported by the Program for Scientific Research in Thermal Physics and Mechanics of Extreme States of Matter of the Presidium of the Russian Academy of Sciences and President of Russian Federation Grant-1257.2003.2.

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