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Line formation of neutral aluminium in the Sun

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Abstract. We investigate the formation of neutral aluminium lines in the solar photosphere using an atomic model containing 58 levels plus the ground state of Al II connected via radiative and collisional interaction. Synthetic line flux and intensity profiles are compared with the solar spectrum to study the relevant kinetic processes and their influence on level populations and line profiles. For neutral aluminium with its extremely large ground state photoionization cross-section near 2071 Å the reduction of the ultraviolet radiation field due to metallic line absorption has to be taken into account using Kurucz' (1992) ODF opacities. In the photosphere of a cool star excitation and ionization due to collisions with neutral hydrogen can outweight electronic collisions. The influence of different types of collisional interactions with electrons and neutral hydrogen is therefore examined.

As expected, the non-LTE effects in most of the solar Al I lines are small, irrespective of the details of the atomic model. The cores and innermost parts of the wings of the resonance lines at 3944 and 3961 Å are affected by only small deviations from the observed profiles, part of which is due to the uncertainty connected with the proper choice of the continuum flux in the region of the Ca II H+K lines. Since the first excited state, $4s\,^2S$, is slightly overpopulated with respect to both the $3p\,^2P^\circ$ ground state and to $4p\,^2P^\circ$ the strongest evidence for non-thermal excitation is found in the infrared lines at 1.3 and particularly at 12 μm. Empirical evidence for the necessity to include neutral particle collisions in the kinetic equilibrium of aluminium arises from comparison of these lines with observations. General agreement with solar line profiles in the infrared and in the visible is found for an atomic model with both electronic collisions and a strongly reduced amount of neutral particle collisions. The solar model will serve as a reference for the investigation of cool metal-poor stars in which both the reduced electronic collision rates and the enhanced UV intensities lead us to expect more pronounced deviations from LTE.

Key words: Atomic processes – Line: formation – Sun: abundances – Sun: photosphere – Stars: abundances

1. Introduction

Understanding the line formation of light metals in cool stars is essential for learning more about nucleosynthesis and stellar masses during Galactic evolution. Here, aluminium plays an important role since the abundance ratio of aluminium to magnesium (or iron) is particularly sensitive to the formation process and the available constituents. Nucleosynthesis of the neutron-rich isotope ^{27}Al requires the presence of free neutrons during carbon burning. One of the possible scenarios is explosive nucleosynthesis as first proposed by Arnett (1969, see also Arnett 1971, Truran and Arnett 1971), in which the available neutrons are parametrized by a *neutron excess* $\eta = (N_n - N_p)/(N_n + N_p)$. This excess is provided by any neutron-rich nuclei such as e.g. ^{18}O having survived the preceding He-burning phases. In typical population II stars these nuclei are deficient or even absent, and it is therefore that supernovae with low initial metal abundance should have a reduced neutron excess (Arnett 1969, Woosley 1986). The natural consequence would be an underabundance of odd neutron-rich nuclei such as ^{27}Al or ^{23}Na compared with ^{24}Mg in unevolved stars of the Galactic halo. Another production site for Al is the *hydrostatic* carbon burning phase. Stars of intermediate mass can produce a neutron excess due to the $^{12}C\,(^{12}C\,,n)^{23}Mg(e^+\nu)^{23}Na$ reaction which yields a lower limit for η even in extremely metal-poor stars. This allows also the immediate production of other neutron rich elements, which for stars of lower mass are returned to the interstellar medium via stellar winds (Fujimoto 1984) or for more massive stars via type II supernovae. In this case either no overdeficiency of Al is expected or the underabundance of Al is restricted by a minimum value around [Al/Mg] ≈ -1 (cf. the footnote in Bessell and Norris 1984).

The spectroscopic determination of aluminium abundances in metal-poor stars can help to decide which processes and sites are important. Peterson (1981) analyzed the Al resonance lines and found an overdeficiency of Al with respect to iron in metal-poor stars, however, this is not confirmed in the analyses of Spite and Spite (1978,1980). The analyses of Gratton and Sneden (1987, 1988) and Magain (1989) result in an overdeficiency of aluminium for metal-poor stars, but due to the scatter found in the abundances this effect is not very pronounced. Arpigny and Magain (1983) could show, that one of the resonance lines (3944 Å) is blended by CH, especially affecting the abundance determination in giants. Using higher excited lines François (1984, 1986) again could *not* find this overdeficiency. Note, that in extremely metal-poor subdwarfs only the resonance lines are useful for an abundance determination since all subordinate lines become increasingly weaker whith decreasing overall metal abundance.

There exist indications for non-LTE effects, found in cool giants by Begley and Cottrell (1983), and such effects could

Send offprint requests to: D.Baumüller also influence the abundance determination in halo dwarfs. Therefore, Steenbock calculated the statistical equilibrium of aluminium in the solar photosphere. (Gehren et al. 1991, Steenbock 1991). Exposing a 26 level atomic model with 27 radiative transitions to the atmosphere of Holweger and Müller (1974) he found only small deviations from LTE, in particular those affecting the shapes of the resonance lines. Most interestingly he found a relatively strong deviation of the *departure coefficients* of the resonance line levels, $3p\,^2P^o$ and $4s\,^2S$, from LTE in regions of optical depth ($\tau_c \approx 1$) that are normally known to follow LTE excitation. His explanation was that the ground state of aluminium has a very large photoionization cross-section, and that the rate coefficient was an order of magnitude higher than the corresponding *bb* radiative and collision rates. The ionization edge is, however, in the near ultraviolet region (2071 Å) where the metal line blocking is an extremely important source of background opacity, an influence that must be investigated carefully since it affects the UV mean intensities particularly at large optical depths. An additional benefit of UV line blocking is that for metal-poor stars the reduced opacity may provide even larger photoionization rates thus possibly increasing the deviation from LTE. It has been argued repeatedly (Athay and Canfield 1969, Gehren 1975, Steenbock and Holweger 1984) that kinetic equilibria are affected by electronic collisions as much as by neutral hydrogen collisions. In fact, taken at face value, in cool and metal-poor stars the hydrogen collisions could even outweight their electronic counterparts. Unfortunately, the proper calculation of the collision rates is restricted by very simple approximations of the collision cross-sections. It is therefore hard to specify the influence of the different types of collisions from basic principles without reference to observed line profiles.

To make the derivation of aluminium abundances more reliable we investigate the statistical equilibrium of aluminium and, in particular, determine the influence of radiation field and collisions under conditions found in cool stellar photospheres. In this paper we present results of our calculations for the Sun as a reference star, using excellent observed spectra that enable us to study the influences of all model parameters and methods. The results will create a standard model for further use in the analyses of metal-poor stars. The section to follow is related to the atomic model and the various approximations used for interaction cross-sections. It also gives a short introduction to the atmospheric models employed, and it accounts for the details of the statistical equilibrium calculations. Sect. 3 includes the results, both for departure coefficients and line profiles. The last section then is meant to discuss the present evidence for non-thermal excitation and ionization of aluminium in the Sun and its possible variation with decreasing metal abundance.

2. The model

The model atom contains 51 Al I terms describing the complete doublet system with principal quantum numbers n $\leq$ 10 and angular quantum numbers $L \leq$ n-1. All levels are below the ionization potential (Fig. 1). Also included is the quartet term $3p^2\,^4P$, coupled to the doublet system by collisional interaction only. The atomic model is completed with the Al II ground state. Fine structure splitting of the levels is neglected with the exception of the Al I $3p\,^2P^o$ ground state. This is equivalent to assuming thermal excitation among the levels of a common term. The system of Al I levels is extended to include terms of common principal quantum number between n = 11 and 15 thus reaching an energy of 0.06 eV below the ionization limit. For levels above n = 15 upper state sums are included up to n = 20 to account for number conservation. The necessary quantum defect data is from Butler (1993). Energy levels are taken from Kaufman and Martin (1991) if available there. For levels up to n = 10 and L = 5 the data from Butler (1993) is used. For levels higher in principal or angular quantum number hydrogenic energy values are assumed.

Fig. 1. Energy level diagram of the Al I model atom (doublets only) including linearized radiative bound-bound transitions considered. For better visualization fine structure splitting is enlarged and levels with n > 10 and L > 5 are not plotted

2.1. Radiative data

The transition probabilities for allowed radiative transitions between levels with n $\leq$ 10 and L $\leq$ 5 are again taken from Butler, for the other transitions we use the hydrogenic approximation given by Green (1957). The Ca H+K line f-values are taken from the compilation of Morton (1991). In our model we do not include transitions to autoionization states; the rates are negligible in the solar photosphere. The accuracy of the transition probabilities is estimated to be quite high, with errors less than $\approx 10\%$. The photoionization cross-sections have been computed by Dr. K. Butler. As observed in the solar spectrum the photoionization coefficient of the aluminium ground state is quite high. The photoionization cross-sections show a number of strong resonance peaks due to autoionization. (Fig. 2). To account for this we include the cross-sections explicitly for the levels 3p to 5p and 4s to 6s and 3d to 4d. For all other levels we use a simple asymptotic approximation to the cross-sections. However, as mentioned above, it turns out that the influence of the autoionization peaks on the statistical equilibrium is relatively small. Only the cross section of the $4p\,^2P^o$ level, showing quite a high level over a broad wavelength region has some influence on the population of the lower levels. The autoionization peaks are mostly situated at wavelengths below 2000 Å where the intensity is no longer high enough to create significant ionization rates.

Fig. 2. Photoionisation cross-section for $3p\,^2P^o$ (top), $4s\,^2S$ (middle) and $4p\,^2P^o$ (bottom) levels as calculated by Butler (1993)

2.2. Collisional data

In a cool star like the Sun the ratio of electrons to hydrogen atoms leads to an estimate of the importance of either type of collisions. If the Coulomb interaction between electrons and aluminium atoms is to be replaced by less efficient neutral hydrogen collisions it is obvious that a large overdensity of hydrogen atoms with respect to electrons is required. Drawin (1968) has published a simple approximation for hydrogen collisions that has been widely used, and the formula suggests that collisional thermalization in plasmas as cool as the solar atmosphere is determined not only by electronic but also by hydrogenic collisions. We note here, that for both types of collisions accurate data are not available. Due to the lack of better data for electronic collisions causing optically allowed transitions we adopt the formula of van Regemorter (1962). For forbidden transitions the semi-empirical formula of Allen (1973) is applied. The *scaling parameter* is set equal to 1 except for the transition between the fine structure levels for which we take a value of 100 to ensure thermalization between the two levels in the photosphere.

Collisions with neutral hydrogen atoms are described with Drawin's formula in the generalized form of Steenbock and Holweger (1984) for allowed transitions. For forbidden transitions we use the formula proposed by Takeda (1992). More recent calculations of Kaulakys (1985, 1986) tend to result in significantly lower rates. Investigating the statistical equilibrium of alkali elements Caccin et al. (1993) have found evidence that Drawin's formula leads to neutral hydrogen collisional rates approximately a factor of 1000 higher than those of Kaulakys. Since we cannot decide *a priori* which calculation is more appropriate, we will compare different atomic models including and excluding hydrogenic collisions in order to derive upper and lower limits from their influence on aluminium line profiles. Furthermore, we will investigate the behaviour of models in which the collision cross-sections are scaled by various factors.

2.3. Model atmospheres

The statistical equilibrium calculations are based on horizontally homogeneous LTE model atmospheres in hydrostatic equilibrium. We account for metallic UV line absorption using Kurucz' (1992) opacity distribution functions interpolated for the proper solar mix of abundances. The solar abundances are adopted from Holweger (1979) with minor modifications for carbon (Stürenberg and Holweger 1990) and iron (Holweger et al. 1994). For Fe and Al we use values of 7.51 and 6.43, respectively. For comparison two solar temperature stratifications are explored; the first is a flux-conserving model with parametric account of convection applying a mixing-length of 0.5 pressure scale heights (Fuhrmann et al. 1993) and line blanketing included with Kurucz' ODFs. This is our *standard* solar model although it does not reproduce the center-to-limb variation of the solar intensities very well. The reason for rating this model as a standard is that we can easily use the model as a differential *stellar* atmosphere with full physics included. This does not hold for the second type of solar model which is the semi-empirical model of Holweger and Müller (1974). As was shown by Fuhrmann et al. (1993, 1994) scaled semi-empirical temperature stratifications should not be used for stars with parameters very different from the Sun; this is particularly important for metal-poor stars. Experience with the two solar temperature stratifications shows that they are both able to reproduce most of the line flux spectra provided that abundances and damping constants are thoroughly adjusted.

No attempt has been undertaken to model the solar chromospheric temperature rise that undoubtedly has an important influence on the strongest lines such as the resonance line doublet. There are essentially two reasons why we do not think this is necessary; only the very cores of the extremely strong resonance lines are formed in chromospheric layers. Their source function depends on the *ratio* of the corresponding population densities, and this does not seem to depend much on temperature stratification (cf. Gehren 1975). The resonance line cores are, however, influenced by non-thermal and depth-dependent velocity fields that are not part of our solar models. Instead the turbulence has been assumed constant with depth where the most probable non-thermal velocities are 1.0 km/s for flux profiles and 1.3 km/s for intensity profiles at the solar center.

2.4. Statistical equilibrium calculations

The statistical equilibrium is calculated using the code DETAIL (Giddings 1981, Butler and Giddings 1985) which is based on the method of complete linearization as described by Auer and Heasley (1976). The linearization includes 103 radiative line transitions, which are represented by Doppler profiles. The resonance lines are treated with full radiative and van der Waals damping. The bound-free transitions of the 11 lower levels are linearized, too.

2.5. Background opacities

In a star like the Sun the flux in the ultraviolet spectral region is determined to a large part by opacities due to metal line absorption. Especially in the case of aluminium with its strong ionization edge in the UV these opacities must be taken into account. Again we use the opacity distribution functions of Kurucz (1992). In these ODF data single line opacities in small frequency intervals are represented by superlines; consequently, the ODF opacity is not identical to that required at a certain position in frequency space. For the calculation of a model atmosphere this simplification is a sufficient approximation, but for non-LTE line formation the actual radiation field across a line transition or an ionization continuum is important for the determination of the statistical equilibrium of an atom. For bound-free transitions the exact position of the absorbing lines is less important, and the use of the ODFs seems to be reliable, provided the intervals are small enough in the frequency region near the ionization edge. For a bound-bound transition with its narrow line width it can be important, on what part of the broad synthetic ODF line it is formed. In our case it turns out that the statistical equilibrium of aluminium is mostly determined by bound-free transitions from the lower levels and infrared line transitions. Thus we include the additional ODF opacity in the UV up to a wavelength of 2100 and between 3100 and 4400 Å to allow for a realistic behaviour of the ionization from the ground state and the first excited level without affecting the line transitions. In this region only few aluminium lines are found allowing us to omit additional line opacities as most of the line transitions in this wavelength region are of minor importance for the statistical equilibrium. The additional line opacity introduced by the Ca II H and K lines is taken into account by explicitly including it in the calculation to provide a realistic background for the resonance lines.

3. Results

The statistical equilibrium of aluminium is subject to influences from a number of different effects. To understand the physics behind these mechanisms we compare four different models:

(A) LTE model
(B) NLTE model including electronic collisions only

Fig. 3. Departure coefficients vs. depth for non-LTE models (B), (C), and (D) (from top to bottom). The bottom panel shows an enlarged portion of model (B) demonstrating the importance of the ground-state photoionization

(C) NLTE model including electronic and hydrogen collisions
(D) NLTE model including electronic collisions; hydrogenic collision coefficients *reduced* by a factor of 500

3.1. Departure coefficients

In Fig. 3 we compare the departure coefficients of the lower Al levels for the different models calculated for an ODF-blanketed solar model atmosphere. As usual we have plotted the departure coefficients, $b_i = n_i^{\rm NLTE}/n_i^{\rm LTE}$ as a function of continuum optical depth τ_c , where n_i is the population of level i and the optical depth refers to $\lambda = 5000$ Å. We present only those levels necessary for subsequent line profile synthesis, only one of the ground state departure coefficients is shown as they are equal. (For the relative departure coefficients of levels $7h\,^2H^o$ and $6g\,^2G$ see Fig. 11).

We start our discussion with model (B) demonstrating some of the more important features: one of the most striking details found in Fig. 3 is the underpopulation of the $3p\,^2P^o$ levels far inside the atmosphere at optical depths around $\tau_c = 1$. The reason for this outstanding non-LTE effect is the photoionization cross-section of the ground state of neutral aluminium which is known to be exceptionally large. Experimental measurements give 65.0 ± 6.0 Mb (Kohl and Parkinson 1973). Quantum mechanical calculations of the cross-section (Butler 1993) result in a threshold value of 49 Mb and a number of resonance peaks due to autoionization transitions. The excited states have much smaller treshold values (0.1 Mb for $4s\,^2S$, but again with autoionization peaks, cf. Fig. 2). In the region *outside* $\log \tau_c = 0$ the angle-averaged ultraviolet intensity J_ν begins to exceed the Planck function $B_\nu(T_e)$, and simultaneously the efficiency of electronic collisions decreases thus amplifying the depopulation of the ground state. Higher in the photosphere the $3p\,^2P^o$ overionization disappears again, the population starts to be influenced by line transitions as explained below. The depopulation effect is also evident — at least to a smaller extent — for levels $4s\,^2S$, $3d\,^2D$ and $4p\,^2P^o$ as they are strongly coupled to the ground state via line transitions and collisions.

Another surprising result is the overpopulation of the $4s\,^2S$ level outside $\log \tau_c = -2$. The levels $3d\,^2D$ and $4p\,^2P^o$ show a similar but less pronounced peak deeper in the atmosphere. The ground state departure from LTE population is negligible around $\log \tau_c = -2$ with the b_i again decreasing at smaller optical depths. These features are the result of a number of processes interacting in a very complicated manner. The $4s\,^2S$ level is connected with the photoionization-dominated ground state by the strong resonance lines. The ground state overionization seen deeper in the photosphere is no longer present in this depth region since the ionization rate becomes smaller and can no longer compete with bound-bound transitions. The departure coefficients of $3p\,^2P^o$ and $4s\,^2S$ start to diverge at a depth of $\tau_c \approx 1$, where the optical depth of the resonance lines is still very large. Yet there is a small but non-negligible net radiative absorption leading to the divergence, which has its maximum near $\log \tau_c = -3$. At this depth the overpopulation of $4s\,^2S$ is also triggered by another process, the 'photon sucction' as described in more detail by Bruls et al. (1992). The $4s\,^2S$ population is filled up from the $4p\,^2P^o$ level via the infrared line transition around 1.3 μm. There exists an effective cascade of infrared transitions with high transition probabilities including levels 6h-5g-4d-4p-4s which is connecting the $4s\,^2S$ level efficiently to the highly excited levels and the continuum. The energy loss due to escaping line photons results in a subthermal radiation field outward $\log \tau_c = -2.5$ leading to a flow of recombining electrons from the continuum down to $4s\,^2S$ and to a lesser extent to the $3d\,^2D$ level which is part of a similar but less efficient chain connecting the levels 6h-5g-4f-3d-3p. In the UV region where most of the $4s\,^2S$ ionizing photons come from, the radiation field is superthermal in this depth but the relatively small photoionization cross sections of $4s\,^2S$ and $3d\,^2D$ result in quite small rates which are not able to compensate the downward flow. The departure of the $3d\,^2D$ level is connected to $4p\,^2P^o$ over a wide depth range. While the line transition between these levels is not very effective, they are strongly coupled by collisional interactions because of similar level energies.

The above argumentation is verified by a number of test runs with different adjustments to the atomic model. The dependence of the $4s\,^2S$ overpopulation on the resonance line scattering can be shown by excluding the resonance line from the linearization scheme: the overpopulation disappears.

Finally, the strong underpopulation of *all* levels starting in the lower chromosphere is a result of the inefficient recombination due to the low temperatures of our atmospheric model. Adding a *chromospheric temperature rise* is expected to provide for a significant overpopulation instead.

3.1.1. Influence of collisions

The influence of collisional interaction on the departure coefficients is easy to detect. In the calculation (C) including collisions with neutral hydrogen atoms (mid panel in Fig. 3) the underpopulation of the ground state near $\tau_c = 1$ is considerably reduced, and the overpopulation of $4s\,^2S$ is enhanced and shifted farther out in the atmosphere. The same holds for the ground state. Levels $3d\,^2D$ and $4p\,^2P^o$ are coupled even more tightly having lost most of their overpopulation. In model (D) the decrease of the hydrogenic collision cross-sections results in a behaviour deep in the atmosphere quite similar to model (B). In higher atmospheric regions the electronic collisions are less effective, even the reduced collisions with hydrogen in model (D) increase the interaction of the lower levels with the continuum, and the $3p\,^2P^o$ population is enhanced. The highly excited levels $5f\,^2F^o$ and $6f\,^2F^o$ are also populated more efficiently in this depth region.

A realistic estimate of the respective fractional contributions of the different collisional interaction processes is very important for the following reason: while the two collision processes may replace each other in the Sun due to the similar interaction *rates* this would not be possible in metal-poor stars. Since at $T_{\rm eff} \leq 6500$ K the free electrons originate from metals with low ionization potentials, the electron density and with it the electronic collision rates will decrease in proportion to the metal abundance. At the same time, the neutral hydrogen density does *not* suffer from the low metal abundance, and the hydrogen collision rates would be similar to those in the Sun. The situation would be even more complicated in evolved metal-poor subgiants or giants where also the neutral hydrogen densities would decrease. Thus in order to be able to determine non-LTE populations of aluminium in metal-poor stars it is necessary to evaluate by comparison with observed line profiles whether hydrogen collisions are important at all.

3.2. Line profiles

Fig. 4. Synthetic LTE flux profile for the Ca II H+K line region (dots) compared with the observed solar spectrum (continuous line).

Table 1. Data used for line synthesis

	λ [Å]	E_{low} [eV]	$\log gf$	$\log C_6$
Al I	3961.53	0.00	0.345	–31.20
	6696.02	3.14	–1.510	–30.00
	6698.67	3.14	–1.870	–30.00
	7835.31	4.02	–0.680	–29.10
	7836.13	4.02	–0.500	–29.10
	7836.13	4.02	–1.842	–29.10
	8772.87	4.02	–0.190	–30.00
	8773.90	4.02	–0.020	–30.00
	8773.90	4.02	–1.500	–30.00
	13123.28	3.14	–0.210	–32.30
	16763.29	3.14	–0.492	–31.40
	119251.00	5.60	1.152	–28.00
	122565.00	5.61	1.160	–28.00
Ca II	3968.47	0.00	–0.201	–32.30*
	3933.66	0.00	0.104	–32.30

* The Ca II resonance lines were computed with $\log C_4 = -12.90$

Fig. 5. Synthetic flux profiles of the Al I resonance line at 3961 Å compared with the observed solar spectrum (continuous line). The profiles refer to models (A) (LTE: dashes), (B) (electronic collisions only: dot-dashed), (C) (electronic plus hydrogen collisions: dash-three dots), and (D) (scaled hydrogenic collisions: dots)

The synthetic line profiles shown in this section have been calculated on the basis of the standard $gf\varepsilon$ data set as used for the determination of statistical equilibrium. The lines are compared with solar flux observations taken from the Kitt Peak Atlas (Kurucz et al. 1984) and with solar center intensity profiles from the infrared data of Hall (1970) and Brault (1995). The synthetic flux profiles have been convolved with a profile that combines a small damping contribution with a depth-independent Gaussian macroturbulence distribution of Ξ = 1.4 km/s and a rotation velocity of $v \sin i$ = 2 km/s. This profile is derived from a series of fits to faint solar lines. A corresponding pseudo-instrumental profile for synthetic center intensity profiles in the IR includes a Gaussian width of 3.8 km/s for 1.3 and 1.7 μm lines. At 12 μm we use 1.6 km/s for μ=0.5 and 2.0 km/s for μ=0.2.

The C_6 values are evaluated from the solar line fits, too. C_4 damping due to the quadratic Stark effect has been included for the Ca II profiles only to produce a better fit to the core region.

3.2.1. Resonance lines

As expected the analysis of the resonance lines turns out to be complicated. The local continuum is poorly determined in the observed solar spectrum and the lines are placed on the wings of the Ca II H+K resonance lines. Since a CH blend strongly disturbs the 3944 Å line profile we restrict our investigation to the 3961 Å line. The continuum is adjusted as to give a reasonable fit to the synthetic calcium line wings since *they* define the local reference continuum for the Al line (Fig. 4). In Fig. 5 the synthetic resonance line profiles representing the different atomic models are compared with the Kitt Peak solar flux atlas. The line assuming LTE reproduces the observed line depth, but the line wings and the core itself are too broad. A reduction of the microturbulence from 1.1 to a value of 0.5 km/s yields a narrower core, but it cannot reproduce the rest of the line shape. In the region of the shoulder between core and wing the LTE line always remains deeper than the observed profile.

Fig. 6. Synthetic flux profiles of subordinate lines around 6696 Å compared with the observed solar spectrum. On this wavelength scale model (A) (LTE: dashes) is nearly indistinguishable from model (B) (dot-dashed)

Fig. 8. Synthetic flux profiles of the doublet near 7836 Å compared with the observed solar spectrum. Line patterns are the same as in Fig. 6

Fig. 7. Synthetic flux profiles of the doublet near 8773 Å compared with the observed solar spectrum. Line patterns are the same as in Fig. 6

For all non-LTE models the core of the resonance line is too deep by $\approx 2\%$ of the continuum flux; it is formed mostly outward of log τ_c = -4, where the atmospheric stratification of the solar model is not realistic. As mentioned above it does neither account for the chromospheric temperature rise nor for complicated gradients of the non-thermal velocity field. Thus the upper line core is narrower for all non-LTE lines, which accounts for a reasonable fit in the core-wing transition area. The different models (B to D) result in rather similar shapes irrespective of the treatment of the collisions, which does not play an important role in the lower chromosphere. Except for the very line core deviations from LTE in the solar atmosphere do not seem to affect the resonance line profile very much.

3.2.2. Excited lines

The red lines connecting excited levels show a surprisingly small influence of non-LTE population. In Fig. 6 we show the solar flux profiles of the 4s ^{2}S - 5p ^{2}P° transition near 6696 Å compared with the synthetic LTE and the non-LTE line profiles for model (B) only, since here the effects are strongest. The contributions to the faint doublet profiles come from inside log τ_c = -1, thus there is few difference between LTE and non-LTE. However, in order to arrive at a reasonable fit we would have to increase the Al abundance by ≈ 0.01 dex.

Another series of red doublets connects the 3d ^{2}D level with different f levels. As documented in Fig. 3 the lower level deviates from LTE in the region log $\tau_c \leq -1$ and therefore medium strong lines could be affected. For the multiplet connecting 3d ^{2}D with 5f ^{2}F° (8773 Å, Fig. 7) the LTE profile is weaker than that found assuming non-LTE indicating a better fit to the non-LTE profile. A reasonable LTE fit would require an increase of the Al abundance of 0.05 and 0.1 dex for 8772.9 and 8773.9 Å , respectively. For the transition 3d ^{2}D to 6f ^{2}F° (7836 Å, Fig. 8) the non-LTE effect is almost not visible in the line profiles; both lines are slightly too weak to give an excellent fit. Due to the faintness of the lines the non-LTE effects in the doublets (Figs. 8 and 7) are quite small, with their contribution functions all peaking at log $\tau_c \geq -1$.

As already discussed above the overpopulation of the first excited state, 4s ^{2}S , around log $\tau_c = -3$ is triggered by a downward cascade of electrons via infrared lines with relatively high transition probabilities. Thus the 4s-4p (13123 Å) and the 4s-5p (6696 Å) transitions differ in their transition probabilities by a factor of 40. Correspondingly, one would expect distinct deviations from LTE in the 1.3 μm line. For the Sun this part of the spectrum has been published in the infrared intensity atlas of Hall (1970). In Fig. 9 we compare the observed line profile at 1.3123 μm connecting levels 4s ^{2}S and 4p ^{2}P° with synthetic spectra computed for models (A) to (D). This is the first of the subordinate lines showing a relatively strong difference between LTE and non-LTE profiles that cannot be compensated by minor adjustments of abundances, f-values or damping constants. In Fig. 3 the levels 4s ^{2}S and 4p ^{2}P° show diverging departure coefficients outside log τ_c = -1 that lead to the enhancement of the non-LTE line. The non-LTE models (B) and (D) excluding or reducing hydrogen collisions result in the strongest lines reproducing the measured line, the profiles calculated with model (C) as well as the LTE line profile are weaker. Unfortunately the line is strongly blended, a best fit cannot be found. The line near 1.67 μm connecting levels $4p\,^2P^o$ and $4d\,^2D$ is hardly affected by non-LTE effects. The LTE profile is marginally deeper in the inner core, however, this is not visible in Fig. 10. This line is weaker than the 1.3 μm line, it is formed deeper in the atmosphere where the relative population divergences are small.

To demonstrate the influence of atmospheric models with their different temperature stratifications we compare both lines at 1.3 and 1.7 μm with LTE profiles calculated using the Holweger-Müller atmosphere (1974), (continuous line in Figs. 9 and 10). Obviously the HM profiles are much weaker than those computed for our atmosphere. A reliable fit is not possible; it would require a change of either f values or abundance by +0.2 dex. Whereas the first alternative of a 60% error of both f values is possible but very unlikely, any abundance change would affect all the rest of the Al lines and must therefore be ruled out.

Fig. 9. Calculated line intensity profile of the $4s\,^2S$ - $4p\,^2P^o$ transition at 1.3 μm compared with the spectrum observed at the solar disk center (Hall 1970) (crosses). The continuous profile was calculated assuming LTE with the Holweger-Müller atmosphere. Other line patterns are the same as in Fig. 5

Fig. 10. Calculated line intensity profiles of the $4p^2P^o$ - $4d\ ^2D$ transition at 1.7 μm compared with the spectrum observed at solar disk center (Hall 1970) (crosses); (LTE: dashes; non-LTE model (B): dot-dashed); The continuous profile was calculated assuming LTE with the Holweger-Müller atmosphere

3.2.3. Emission lines near 12 μm

In the solar spectrum around 12 μm some emission features have been detected and identified as transitions between highly excited levels of Mg and Al (Chang and Noyes 1983). Carlsson et al. (1992) carried out non-LTE calculations for Mg I, and they were able to reproduce the emission lines. As was pointed out also by Lemke and Holweger (1992) these lines are formed in the *photosphere*; therefore modelling the chromospheric temperature rise is not required. Even small deviations from LTE of the corresponding level populations create a relative population inversion that produces an outward increase of the line source function sufficient to form an emission profile. The reason lies in the increasing importance of stimulated emission in this wavelength region. For aluminium we can expect similar results as for magnesium. The strongest infrared Al line near 12.26 μm is due to a transition between levels $6g\,^2G$ and $7h\,^2H^o$, another weaker line at 11.93 μm results from a $6f\,^2F^o$ – $7g\,^2G$ transition. There is a faint emission *observed* at the solar disk center, but towards the limb we find marginal evidence for an emission line core. In Fig. 11 the ratio of departure coefficients for the relevant levels is plotted for the different atomic models. The relative overpopulation of the upper level in the region of line formation around log τ_c = -2.5 is small, but yet is strong enough to produce remarkable non-LTE effects in the line profiles both at disk center and at the solar limb. As shown in Fig. 12 we compute weak emission line profiles for the standard model (B) at the solar center, but a better fit is found for model (D). On the other hand, the LTE model (A) and model (C) including enhanced collisional interactions cannot offer a fit since both are too deep in absorption.

At the solar limb we observe emission as indicated in Fig. 12. Again, LTE does not fit, and the full amount of hydrogen collisions nearly thermalizes the populations. The best accordance for center *and* disk is found for model (D) including some reduced amount of hydrogenic collisions. A similar fit seems possible by increasing the electronic collision cross sections by a factor of ten. However, this type of collision is more effective deeper in the atmosphere, and other levels near the ground state are then forced to an LTE population over a wide range of optical depths. Thus all the line profiles in shorter wavelength regions become nearly identical to those computed from LTE.

As these far IR lines are extremely sensitive to the model constellation, they also can serve to recover the influence of the completeness of the atomic model. Test calculations with a number of different models either not including the highly excited levels or representing only levels with $L \leq 5$ have been compared. Both variations destroy the efficiency of the electronic cascading process since in the first case the coupling to the continuum is reduced and in the second case the line transitions with $\Delta n = 0$ or $+1$ can no longer contribute to the level populations. The departure coefficient remains mostly unaffected in deeper regions, but the overpopulations outside log τ_c = -3 are reduced for such incomplete models. As a consequence the limb emission features at 12 μ are weaker.

4. Discussion

The non-LTE calculations shown in Fig. 3 confirm that deviations from LTE of the population of neutral aluminium are

Fig. 11. Ratio of $7g\,^2G$ to $6f\,^2F^o$ (top) and $7h^2H^o$ to $6g^2G$ (bottom) departures vs. depth for the different NLTE models (model (B): dash-dots; model (C): dash-three dots; model (D): dots

quite small in the Sun. The resulting effects on line formation are almost negligible in the visible solar spectrum. Except for the very cores of the resonance lines which are, however, affected by chromospheric properties we have found that only lines in the infrared show a significant non-LTE effect. The lines at 12 μm allow the strongest discrimination between the models, and it seems that they cannot be fitted without some additional collisions using model (D). In fact, a small amount of hydrogen collisions obtained by applying a cross-section significantly reduced with respect to Drawin's (1968) formula produces the most realistic profile centers. Due to the different behaviour of solar disk and center profile shapes a slight change of line $gf\varepsilon$ value cannot improve the result. These lines show the importance of treating a sufficiently complete model atom to reproduce a realistic interaction of the lower levels with the continuum. The influence of the strong ground state ionization of Al I on the populations of even the most highly excited levels is evident from comparing the profiles resulting from a series of more and more complete atomic models. Thus our present conclusions are drawn from a *converged* solution.

Though not quite as significant, the 1.3 μm line provides another basis for discrimination of the types of collisional interaction. Although the differences in central line intensities between the standard LTE and non-LTE models are only between 5 and 10%, such differences cannot simply be compensated by accepting different f-values, since such a manipulation would also affect the line halfwidth. For this reason at least the LTE profile should be discarded. The standard model (B) profile fits without further adjustment, and this holds also for model (D). The profile obtained from model (C) shows too weak a line core though it could be adjusted by a change of the line's f-value.

The atypical deviation from LTE populations found in the models (B) and (D) around $\tau_c = 1$ is the result of strong photoionization from the ground state which is equivalent to the conspicious Al I absorption edge seen in the solar spectrum at 2071 Å. This region of significant underpopulation would be removed whenever hydrogen collisions were to become the dominant source of thermalization. In the Sun, the remaining differences of the flux profiles in the visible are around 1%, and they can be compensated by a small adjustment of either abundance or f-value.

Fig. 12. *Top*: Calculated line intensity profiles of the $6f\,^2F^o$ – $7g\,^2G$ transition at 11.93 μm compared with the spectrum observed for the solar disk center and limb (from top to bottom: $\mu = 1.0, 0.5, 0.2$, limb profiles are vertically shifted)(Brault 1995); *bottom*: Same for the $6g\,^2G$ – $7h\,^2H^o$ transition at 12.26 μm.

Having used the solar atmosphere as a laboratory plasma we can try to estimate the reliability of our present results. (a) With a number of test calculations including more levels of both Al I and Al II we have found that in order to use infrared lines from highly excited levels as diagnostic tools it is indispensible to represent many more interaction channels than normally required to model visible lines from weakly-excited levels. Such interaction can be well described by hydrogenic cross sections. (b) Radiative interaction cross-sections of simple ions can now routinely be calculated allowing for configuration interaction. The corresponding interaction due to collisions is by far less well determined. Formulae such as those described in Sect. 2.2 and used for our atomic model are at best order-of-magnitude estimates. (c) To deal with such amounts of uncertainty it is necessary to take on a step-by-step approach. A first improvement can be obtained by using *scaling factors* for the predicted cross-sections. Thus, a factor of 0.002 applied to the Drawin formula has led to significantly homogenized fits to *all* solar Al I lines investigated. But model (B) excluding hydrogenic collisions also can reproduce the emission features to some extent. As the maximal amount of emissivity accounts for a scaling factor lying between those of models (B) and (D), the latter defines an upper limit for collisional interactions between high-lying levels. Lemke and Holweger (1992) conclude that e.g. fitting the similar Mg I infrared emission line may require hydrogen collision cross sections that depend on the excitation energy of the lower level. This is in accordance with our results for Al, since — with the possible exception of the 1.3 μm line — all other lines of Al I are only marginally affected by hydrogen collisions. A model with unscaled cross-sections for transitions between low-lying and reduced ones for those between upper levels results in line profiles similar to those found for model (D). The notion of hydrogen collision cross-sections decreasing systematically with excitation energy would also be in rough agreement with Kaulakys (1985,1986). Similar results are found for Mg (Zhao 1995).

Since the present investigation will serve as a basis for further analyses of the statistical equilibrium in metal-poor stars, it is interesting to speculate about the changes expected with a reduced metallicity. With the density of free electrons decreasing in proportion to the star's metal abundance we expect considerably reduced collisional interaction. This could lead to stronger deviations from LTE at optical depths log τ_c between -3 and 0, if the reduced electronic interaction is not compensated by hydrogen collisions. This will affect the *wings* of the resonance lines. Simultaneously, the reduced UV opacity will substantially increase the ground state photoionization rate thus enhancing the 4s-4p decoupling. Corresponding calculations will be presented in a forthcoming paper.

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