THE CENTER-TO-LIMB BEHAVIOR OF Ca I $\lambda$6573
AND [Ca II] $\lambda$7324

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Abstract. Center-to-limb measurements of the Ca I $\lambda$6573 intercombination line and the Ca II $\lambda$7324 forbidden line are compared with synthetic profiles based on a simple representation of the non-LTE Ca–Ca$^+$ ionization equilibrium. The effects of photoionizations from low lying excited states of neutral calcium are found to reduce the sensitivity of the $\lambda$6573 center-to-limb behavior as a thermal structure diagnostic. The synthetic center-to-limb behavior is also sensitive to uncertainties in the nonthermal broadening. Nevertheless, the measured center-to-limb behavior of $\lambda$6573 favors a ‘cool’ photospheric model similar to the Vernazza, Avrett, and Loeser model M over hotter models based on the Ca II K wings. The non-LTE calcium abundance obtained from the disk center equivalent widths of $\lambda$6573 and $\lambda$7324 using the best fit model is $A_{Ca} = 2.1 \pm 0.2 \times 10^{-6}$ (by number relative to hydrogen). Applications of these lines as diagnostics of the Ca–Ca$^+$ ionization equilibrium in other stars are briefly discussed.

1. Introduction

The $\lambda$6573 intercombination line of Ca I (4s$^2$1$S_o$–4s 4p $^3P_1$) and the forbidden $\lambda$7324 electric quadrupole transition of Ca II (4s$^2$2$S_{1/2}$–3d$^2$2$D_{3/2}$) have been used in a variety of recent studies of the solar photosphere and the atmospheres of several late-type stars. Schorn et al. (1975) have estimated the solar calcium abundance based on a flux-average equivalent width of the [Ca II] $\lambda$7324 line, which they separated from an overlapping terrestrial water vapor blend using the Doppler shifted solar reflection spectrum of Venus. Ayres (1977a, b) has applied LTE analyses of the Ca I and [Ca II] line shapes, obtained from disk-center tracings in the KPNO solar atlas (Brault and Testerman, 1972), to study the model dependence of calcium abundance estimates, and to determine the radial component of nonthermal broadening in the deeper layers of the solar photosphere. Ramsey (1977) has measured $\lambda$7324/$\lambda$6573 line ratios in five late-type giant stars to investigate possible departures from LTE ionization equilibrium.

As Ramsey has shown, the $\lambda$6573 and $\lambda$7324 features are useful probes of the Ca–Ca$^+$ ionization balance for two reasons: (1) each transition arises from the most populous level of the particular ionization stage (i.e. the ground states); and (2) the

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$\equiv 10^3$ times smaller $gf$-value of the Ca II forbidden line partially compensates for the ionization equilibrium, which favors Ca$^+$ over Ca by roughly that factor at typical photospheric temperatures and densities. Therefore, the $\lambda 6573$ and $\lambda 7324$ lines should have similar strengths and contribution functions. Furthermore, these features are relatively weak, at least in the solar spectrum, and the interpretation of the profile shapes and equivalent widths should be less ambiguous than analyses of stronger, more saturated transitions.

The Ca--Ca$^+$ ionization equilibrium in the solar photosphere should be sensitive to temperature because of the low ionization potential of neutral calcium (I.P. $\sim 6.1$ eV). In fact, initial LTE calculations suggested that the center-to-limb behavior of $\lambda 6573$ equivalent widths would be a useful probe of thermal conditions in the upper photosphere ($10^{-3.0} \leq \tau_{5000} \leq 10^{-1.5}$) and might indicate whether these layers are relatively cool (e.g. the Vernazza et al. (1976) model $M$) or hot (e.g. the Linsky and Ayres (1978) Ca II $K$ wing model).

To test this premise, we have obtained high-quality center-to-limb spectral measurements of $\lambda 6573$ using the main image and vertical spectrograph of the McMath Solar telescope at Kitt Peak. In addition, we have assessed the diagnostic value of $\lambda 6573$ allowing for departures from LTE in the Ca--Ca$^+$ ionization equilibrium.

2. The Observed Profiles

2.1. Photoelectric Profile Measurements

High resolution ($\lambda / \Delta \lambda \sim 4.5 \times 10^5$) photoelectric profiles of Ca I $\lambda 6573$ were obtained at four heliocentric angles ($\mu = 1.0$, 0.50, 0.25, and 0.20) on September 28 and 29, 1976. The photoelectric scanner used has been described by Brault et al. (1971). The spectrograph was operated in the 4th order, double pass mode, with a slit corresponding to 50″ by 0.25″ on the solar disk. The combined seeing and image motion was of order 2–3″ on both days.

Observations were restricted to regions of minimal activity on the solar disk. A selected region, identified by means of Fe I $\lambda 8688$ and He I $\lambda 10830$ magnetograms, was positioned over the entrance slit of the predisperser and stabilized by limb guiders. To obtain high signal-to-noise and to average over an integral number of 300 s oscillations, a 3 Å interval centered on the line was scanned for an integration time of 30 min. No corrections of the image position were made to allow for solar rotation during the observations.

A numerical filter was applied and the instrumental profile was removed by the technique described by Brault and White (1971). The data were normalized to the continuum level and set to the wavelength scale of the Kitt Peak solar atlas, preliminary edition (Brault and Testerman, 1972).

We were unable to observe the Ca II $\lambda 7324$ line under conditions as dry as the atlas data. We therefore have adopted the atlas profiles ($\mu = 1.0$ and 0.20) for this work.
Disk center and limb profiles of \( \lambda 6573 \) and \( \lambda 7324 \) are illustrated in Figure 1. The depressed background level in the vicinity of \( \lambda 6573 \) at disk center is caused by the Stark-broadened long wavelength wing of H\( \alpha \).

Fig. 1. Disk center and limb profiles of Ca I \( \lambda 6573 \) and [Ca II] \( \lambda 7324 \) (KPNO Solar Atlas). The feature designated @ is a terrestrial water vapor line.

2.2. Gaussian widths and equivalent widths

Aside from a weak blend in the long wavelength wing of \( \lambda 6573 \), the Ca I profiles are very nearly gaussian at all limb positions. Therefore, we describe the center-to-limb behavior of \( \lambda 6573 \) in terms of line shape parameters obtained by fitting gaussians to the measured profiles. In the fitting procedure, the H\( \alpha \) wing was treated as a linearly sloping background. Only very small, and probably insignificant, variations were found in the gaussian widths and equivalent widths of \( \lambda 6573 \) in the several independent profile measurements at each heliocentric angle. The mean line shape parameters are listed in Table I. Widths and equivalent widths were estimated for the
TABLE I

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>$\Delta \lambda_0$ (mÅ)</th>
<th>$W_\lambda$ (mÅ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00</td>
<td>Ca I</td>
<td>51.4 ± 0.6</td>
</tr>
<tr>
<td></td>
<td>[Ca II]</td>
<td>58 ± 6</td>
</tr>
<tr>
<td>0.50</td>
<td>Ca I</td>
<td>69.3 ± 0.6</td>
</tr>
<tr>
<td>0.25</td>
<td>Ca I</td>
<td>74.9 ± 2.3</td>
</tr>
<tr>
<td>0.20</td>
<td>Ca I</td>
<td>75.9 ± 0.8</td>
</tr>
<tr>
<td></td>
<td>[Ca II]</td>
<td>82 ± 8</td>
</tr>
</tbody>
</table>

* $\frac{1}{2}$ full 1/e width of fitted gaussian.

KPNO solar atlas profiles of $\lambda 7324$ by fitting overlapping gaussians to the [Ca II]-water vapor blend. The values obtained for $\lambda 7324$ at $\mu = 0.20$ are much more uncertain than the disk center parameters, owing to the greater distortion of the [Ca II] profile by water vapor absorption in the atlas limb tracings.

3. Model Calculations

3.1. Non-LTE Ca–Ca$^+$ Model

Both the $\lambda 6573$ and $\lambda 7324$ line source functions should be close to LTE (i.e. $S_i = B$) owing to the small radiative decay rates of the upper levels. However, departures from LTE caused by photoionizations are likely to be important in the Ca–Ca$^+$ ionization equilibrium. In particular, neutral calcium has low-lying excited states with absorption edges in the optical and near ultraviolet regions of the spectrum where solar radiation fields are substantial (cf., Ramsey, 1977). Furthermore, neutral calcium is the minority species at photospheric temperatures and densities.

We assessed possible non-LTE effects in the Ca–Ca$^+$ ionization equilibrium using a neutral calcium model consisting of four bound levels plus the continuum (Ca$^+$). The atomic model includes the ground state (4s$^2$ 1S$_0$) and the upper levels of the Ca I $\lambda 4227$ resonance line (4s 4p $^1P^0_1$) and the $\lambda 6573$ intercombination line (4s 4p $^3P^0_1$). Both of these line transitions are treated explicitly in the transfer solution. The fourth level is intended to represent the low-lying metastable $^1D$ and $^3D$ states. All four levels in the model atom are coupled by collisions to each other and to the continuum. Rate coefficients for collisional excitation and ionization of neutral calcium by electrons were kindly provided by A. Zachary and E. H. Avrett. Photoionizations are treated by means of prescribed fixed rates, using the radiation temperature scheme of Auver et al. (1972). Depth-dependent photoionization rates, from which radiation temperatures were derived, were kindly provided by E. H. Avrett. Theses rates were obtained by numerically folding the detailed frequency dependence of each photoionization cross section into depth-dependent solar radiation fields simulated using the PANDORA model atmospheres code (Vernazza...
et al., 1973). The relevant atomic data for the neutral calcium model are summarized in Table II.

Although our atomic model is relatively simple, it does include what we feel are the important physical processes which control the Ca–Ca\(^+\) ionization equilibrium in the solar photosphere. In fact, Ca\(^+\) ground state departure coefficients based on the four-level Ca atom compare favorably with a much more elaborate eight-level plus continuum simulation of neutral calcium (Avrett, 1977a). In addition, the eight-level calculations suggested that autoionization played only a minor role in the ionization equilibrium under solar conditions, so we omitted autoionization transitions from our simplified atomic model.

### TABLE IIA

<table>
<thead>
<tr>
<th>l</th>
<th>g(_l)</th>
<th>(E_l) (cm(^{-1}))</th>
<th>(CE_{l\nu}) (^*)</th>
<th>(\alpha_{l\nu}) (^{(cm^2)})</th>
<th>(T_{rad}(K))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) ((^1S_0))</td>
<td>1</td>
<td>0</td>
<td>(8(-8)) (^a)</td>
<td>1.3((-18)) (^c)</td>
<td>4800</td>
</tr>
<tr>
<td>(2) ((^2P_1^0))</td>
<td>3</td>
<td>15210</td>
<td>(9(-8)) (^b)</td>
<td>6((-18)) (^d)</td>
<td>4550</td>
</tr>
<tr>
<td>(3) ((^1D + ^3D))</td>
<td>20</td>
<td>20730</td>
<td>(1.3(-7)) (^b)</td>
<td>5((-18)) (^d)</td>
<td>4550</td>
</tr>
<tr>
<td>(4) ((^1P_2^0))</td>
<td>3</td>
<td>23652</td>
<td>(1.6(-7)) (^b)</td>
<td>8((-18)) (^e)</td>
<td>4775</td>
</tr>
</tbody>
</table>

\(E_{ion} = 49304.8\) cm\(^{-1}\)

\(CE_{l\nu} = n_\nu CE_{l\nu}(T/5000)^{0.5} e^{-(E_{ion}-E_l)/kT}\)

\(\alpha_{l\nu} = 7.54 \times 10^{11} (E_{ion} - E_l)^3 \alpha_{l\nu} F[1.4388(E_{ion} - E_l)/T_{rad}]\), where \(F(x)\) is given by Auer et al. (1972; p. 19).

\(^a\) Okuno (1971).

\(^b\) House (1964).

\(^c\) Carter et al. (1971).

\(^d\) Kelm and Schlüter (1962).

\(^e\) Travis and Matsushima (1968).

### TABLE IIB

Collision rate coefficients

<table>
<thead>
<tr>
<th>(l - u)</th>
<th>(CE_{l\nu}) (^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>1 ((-8)) (^a)</td>
</tr>
<tr>
<td>1-3</td>
<td>1 ((-9)) (^a)</td>
</tr>
<tr>
<td>1-4</td>
<td>1.07((-7)) (^b)</td>
</tr>
<tr>
<td>2-3</td>
<td>5 ((-9)) (^a)</td>
</tr>
<tr>
<td>2-4</td>
<td>1 ((-9)) (^a)</td>
</tr>
<tr>
<td>3-4</td>
<td>1 ((-8)) (^a)</td>
</tr>
</tbody>
</table>

\(CE_{l\nu} = n_\nu CE_{l\nu}(T/5000)^{0.5} e^{-hv_{l\nu}/kT}\)

\(^a\) Based on approximation formulae (van Regemorter, 1962).

\(^b\) Crandall et al. (1974).
3.2. Spectrum synthesis

The combined statistical equilibrium and radiative transfer equations for the model Ca atom were solved using a modification of the complete linearization method of Auer et al. (1972). The λ 4227 resonance line was treated with a partial redistribution formalism (e.g. Milkey, 1976), while the λ 6573 intercombination line was assumed to be formed by complete redistribution. \( R^\| \) redistribution weights for λ 4227 were computed using Kneer's (1975) approximation.

The derived departure coefficients for neutral calcium were introduced into a separate spectrum synthesis code which incorporated more detailed opacities (including the Hα wing) than the generalized non-LTE code and which allowed modeling of the center-to-limb behavior of λ 6573 taking into account variations in microturbulence models and the calcium abundance. Variations in the latter quantities should produce only second-order effects on the departure coefficients. The spectrum synthesis code incorporates Auer’s (1976) Hermitian differencing scheme. A ten-point-per-decade optical depth spacing was used.

3.3. Model atmospheres

Two representative models of the solar photosphere (see e.g. Avrett, 1977b) are illustrated in Figure 2. The thermal structures of these models differ primarily in the upper photosphere layers above \( \tau_{5000} \equiv 10^{-1.5} \). The \( T(\tau) \) relation below \( \tau_{5000} \equiv 10^{-1.2} \) corresponds to the Vernazza et al. (1976) model M scaled slightly in temperature (see Ayres, 1978a). The deep photosphere of the modified VAL model M accurately reproduces the center-to-limb behavior and absolute intensity of the background continuum at λ 6573 and λ 7324.

The upper photosphere of Model 1 represents the thermal structure proposed by Linsky and Ayres (1978) to fit calibrated integrated sunlight profiles of the cores and inner wings of the Ca II K λ 3934 resonance line (see also Ayres, 1977a). Model 1 has a minimum temperature of 4400 K near \( \tau_{5000} = 10^{-4} \) and, more important, generally hotter upper photosphere temperatures than the VAL model M. Model 2 represents the upper photosphere of the VAL Model M, with a slightly hotter minimum temperature \( T_{\text{min}} = 4200 \) K. Both models include chromospheric temperature rises consistent with that of the VAL Model M.
Fig. 2. Adopted thermal structure models of the solar photosphere. VAL 1.015 is a version of the VAL model M scaled slightly in temperature to produce a better fit to absolute continuum intensities.

Pressures and densities for each model were computed assuming planar geometry, hydrostatic equilibrium, and an equation of state based on LTE for the important electron donor metals and non-LTE for hydrogen and $\text{H}^-$. The chemical abundances of Withbroe (1977) were adopted with the exception of helium which is taken to be 0.088 by number relative to hydrogen. Opacities used in the $\tau \rightarrow P$ conversion are described by Ayres (1978a). A possible turbulent contribution to the atmospheric pressures (Vernazza et al., 1973) is unimportant in the photosphere and was ignored.

4. Results and Conclusions

4.1. LTE vs non-LTE

Figure 3a compares the LTE and non-LTE center-to-limb behavior of Ca I $\lambda$ 6573 predicted with the adopted atomic model, the two photospheric thermal structures and a depth-independent, isotropic microturbulent velocity of 1.5 km s$^{-1}$. (Here, nonthermal velocities and Doppler widths are defined in terms of the 'most probable speed'.) It is clear that the temperature sensitivity of the $\lambda$ 6573 center-to-limb behavior is substantially reduced by non-LTE effects on the ionization equilibrium. In particular, photoionizations from the low-lying excited states of neutral calcium –
Fig. 3a–c. Synthetic center-to-limb behavior of λ6573 and λ7324 computed using atmospheric models of Figure 2 with LTE and non-LTE ionization equilibrium (Figure 3a), and range of microturbulence models (Figures 3b, c). The notation in Figure 3b is ($\xi_{\mu} = 1$, $\xi_{\mu} < 1$).

described by the same radiation temperatures for Models 1 and 2 – tend to compensate for the thermal differences between the outer layers of the two model photospheres.

The non-LTE ionization equilibrium also affects the calcium abundances required to fit the measured disk center equivalent widths of λ6573: the calcium abundance determined with Model 1 ($A_{\text{Ca}} = 2.40 \times 10^{-6}$) decreases by about 3% from LTE to non-LTE ionization ($A_{\text{Ca}} = 2.34 \times 10^{-6}$), while the abundance obtained with Model 2 increases by nearly 20% ($1.81 \times 10^{-6}$ to $2.13 \times 10^{-6}$). The corresponding abundances determined from [Ca II] λ7324, which is insensitive to non-LTE effects on the ionization equilibrium since Ca$^{+}$ is the dominant ionization stage in the solar photosphere, are $2.12 \times 10^{-6}$ and $2.03 \times 10^{-6}$ for models 1 and 2, respectively.

4.2. EFFECTS OF MICROTURBULENT VELOCITIES

The potential usefulness of λ6573 as a thermal structure diagnostic is compromised not only by non-LTE effects, but also by the uncertain nonthermal broadening for this line. Figure 3b illustrates the center-to-limb behavior of λ6573 equivalent widths predicted with two ‘extreme’ possibilities for microturbulent velocity distributions which are consistent with the observed line shapes. The solid curves in Figure 3b are based on a depth-independent but anisotropic microturbulent velocity which reproduces the entire observed line widths ($\xi \equiv 1.5$ km s$^{-1}$ for $\mu = 1$; $\xi \equiv$...
2.5 km s\(^{-1}\) for \(\mu < 1\)). The dashed curves in Figure 3b are for a much smaller angle-and-depth-independent microturbulent velocity of 0.5 km s\(^{-1}\). The residual broadening in excess of the 0.5 km s\(^{-1}\) microturbulent component would be attributed to ‘macroturbulent’ motions, which do not alter the equivalent width. Figure 3b suggests that the center-to-limb behavior of \(\lambda 6573\) is dominated by rather large anisotropic microturbulent velocities (cf. Evans and Testerman, 1975).

4.3. Which thermal model fits the observations best?

The uncertainty in the nonthermal broadening as well as the uncertainty in the measured center-to-limb behavior of [Ca II] \(\lambda 7324\) (e.g., Figure 3c), are such that we cannot distinguish unambiguously between the two much different upper photosphere structures of Models 1 and 2, on the basis of our observations alone. In fact, the uncertainty in the synthetic center-to-limb behavior of \(\lambda 6573\) based on the extremes of possible microturbulent velocity models is much larger than the difference between LTE and non-LTE.

However, we could adopt a microturbulent velocity model based on independent observations. For example, a depth-independent anisotropic velocity model with a disk-center component of \(\xi = 1.0\) km s\(^{-1}\) and a limb component of \(\xi = 1.5\) km s\(^{-1}\) reproduces the measured center-to-limb behavior of partially saturated first overtone vibration-rotation transitions of carbon monoxide (Ayres, 1978b). \(\lambda 6573\) center-to-limb curves based on such a model would be somewhat steeper than the 1.5 km s\(^{-1}\) isotropic calculations illustrated in Figure 3a. The observed limb darkening of \(\lambda 6573\) would then clearly favor thermal Model 2. (The CO spectrum also favors Model 2 (e.g., Ayres, 1978b).)

The fact that the Ca I line (and CO) apparently favors the cooler photosphere model rather than the hotter model indicated by the Ca II K wings may be a consequence of the different temperature sensitivities of these diagnostics. The thermal emission in the Ca II wings tends to weight exponentially \((I_\nu \sim e^{-hc/\lambda kT})\) towards hotter components in averaging over solar inhomogeneities, whereas the Ca–Ca\(^+\) ionization equilibrium (and the dissociative equilibrium of CO) accentuates cooler components \((n_{Ca}/n_{Ca}^+ \sim e^{+E_{ion}/kT})\). In this sense, the picture of the solar photosphere given by analyses of spatially-averaged measurements of thermal diagnostics based on single-component models may be somewhat misleading. This problem must be resolved before reliable estimates of the upper photosphere energy balance can be derived from radiative cooling models (e.g., Ulmschneider, 1974). In particular, the sum of individual net cooling rates in a distribution of thermal components may be substantially different from the total net cooling estimated by modeling the ‘mean’ atmosphere. However, in certain applications, for example abundance estimates, single-component models may be entirely adequate.

4.4. The solar calcium abundance

We find a non-LTE calcium abundance of \(A_{Ca} = 2.1 \times 10^{-6}\) based on the disk center \(\lambda 6573\) and \(\lambda 7324\) equivalent widths and Model 2. The uncertainty in \(A_{Ca}\) attribut-
able to the photospheric models and nonthermal broadening (i.e. $\approx \pm 5\%$) is smaller than that attributable to the theoretical and measured oscillator strengths ($\approx \pm 10\%$). This value of $A_{\text{Ca}}$ is consistent with those obtained in previous studies based primarily on permitted transitions of Ca I (Ayres, 1977a; references therein).

4.5. Application of the $\lambda 6573$ and $\lambda 7324$ diagnostics to other stars

Based on the abundances obtained by fitting disk center equivalent widths of $\lambda 6573$ and $\lambda 7324$, we find an effective ‘over-ionization’ of calcium relative to LTE of about 20% for Model 2, but an under-ionization of a few percent for the hotter Model 1. These values should be compared with the factors of 3–5 over-ionization obtained by Ramsey (1977) in his study of late-type giants. In such stars, both the collisional ionization and photoionization rates for the excited levels of Ca I are greatly reduced from the solar values, hence over-ionizations relative to LTE of the cited magnitude are certainly possible. Nevertheless, the fact that the Ca I and [Ca II] features are heavily saturated in such stars argues against using these lines to diagnose relatively small departures from LTE ionization equilibrium when, for example, angle-dependent nonthermal broadening can produce significant effects compared to the angle-independent case that might be misinterpreted as departures from ionization equilibrium. A better place to look for large departures from ionization balance may be in F- and G-type subgiants and giants. In such stars the Ca I photoionizing radiation fields are comparable or larger than for the solar case, but the collision rates are reduced owing to the much smaller photospheric electron pressures. In addition, the stellar $\lambda 6573$ line should be of comparable strength to the solar feature, since the LTE Ca I opacity scales the same way with surface gravity as the H$^-$ background continuum. Therefore $\lambda 6573$ should be as relatively unsaturated in the ‘hot’ giants as it is in the solar case. The $\lambda 7324$ line will be stronger in the giants since the Ca II opacity increases relative to H$^-$ with decreasing surface gravity ($\sim g^{-1/2}$). Nevertheless, the $\lambda 7324$ line is initially very weak in the Sun and a factor of $\approx 50$ decrease in surface gravity would be required to cause appreciable saturation of this feature.

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