

# NON-EQUILIBRIUM SPECTRUM FORMATION AFFECTING SOLAR IRRADIANCE

Rob Rutten

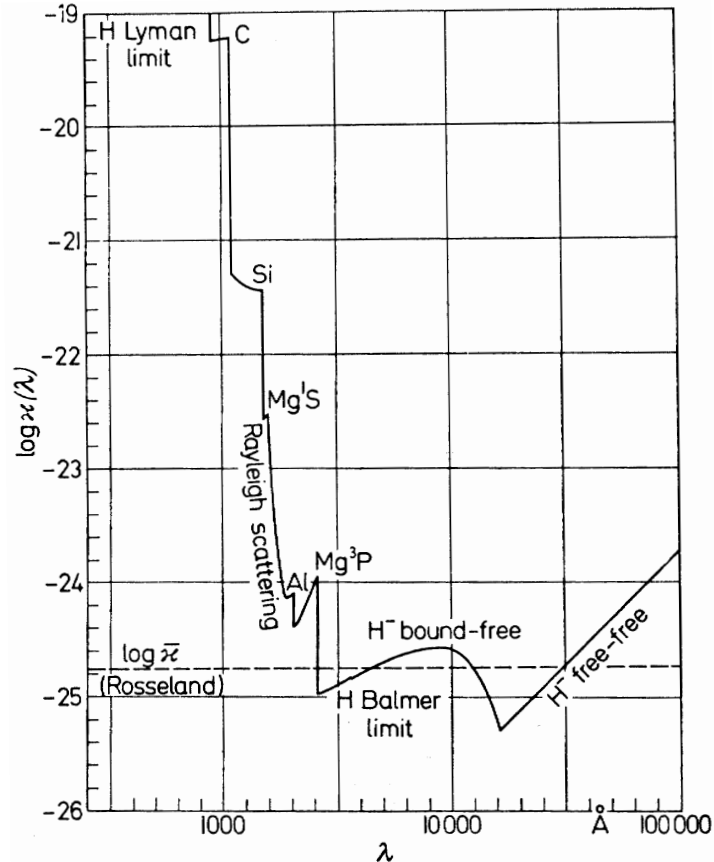
Lingezicht Astrophysics Deil & Institutt for Teoretisk Astrofysikk Oslo

lecture displays <http://www.staff.science.uu.nl/~rutte101>

- *microcourse “solar spectrum formation”*
  - photonic processes
  - NLTE lines and continua
  - NSE
- *modeling “haze” lines*
  - methods
  - demo: FTS versus RH
- *modeling network/plage “fluxtubes”*
  - methods
  - demo: 1600 Å versus 1700 Å
- *to do for spectral irradiance modeling*
  - haze: define tractable recipe
  - fluxtubes: 3D(t) MHD with NLTE synthesis
  - caveat: hydrogen NSE

# SOLAR ATMOSPHERE RADIATIVE PROCESSES

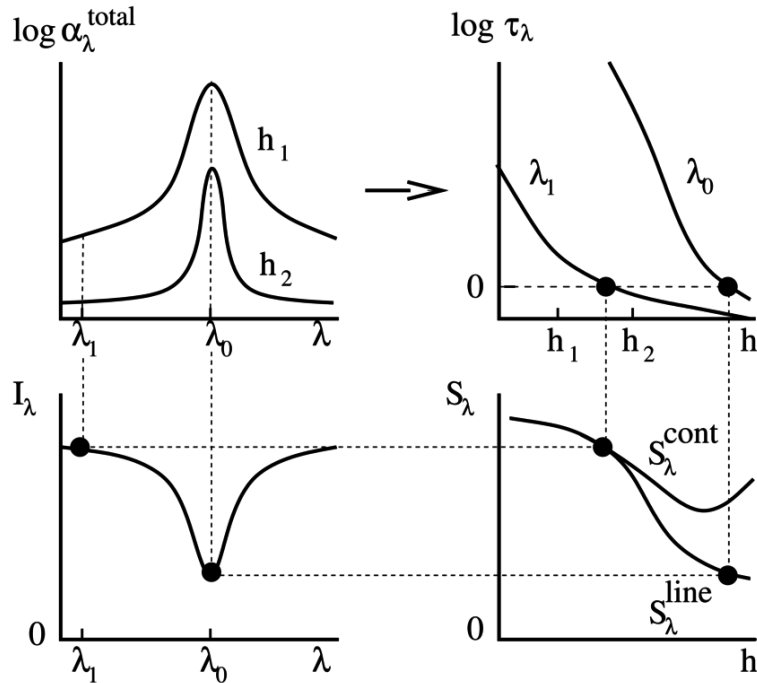
- *bound-bound* –  $\kappa_\nu, S_\nu$ : CE, LTE, NLTE, PRD, NSE?
  - neutral atom transitions
  - ion transitions
  - molecule transitions
- *bound-free* – same except always CRD
  - H<sup>-</sup> optical, near-infrared
  - H I Balmer, Lyman; He I, He II
  - Fe I, Si I, Mg I, Al I = electron donors
- *free-free* –  $S_\nu = B_\nu$ 
  - H<sup>-</sup> infrared, sub-mm
  - H I mm, radio
- *electron scattering* –  $S_\nu = J_\nu$ 
  - Thomson scattering
  - Rayleigh scattering
- *collective* – p.m.
  - cyclotron, synchrotron radiation
  - plasma radiation



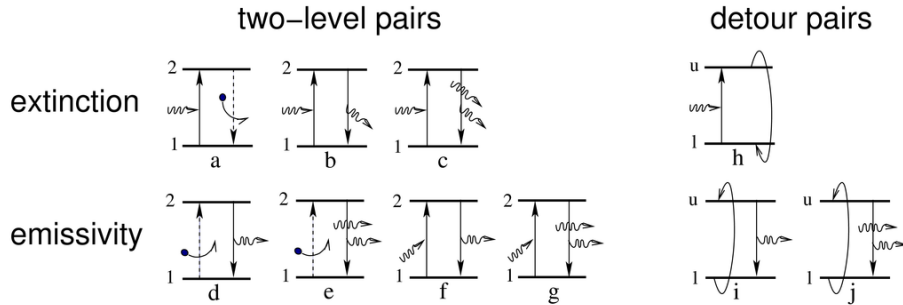
E. Böhm-Vitense

# SCHEMATIC THICK SOLAR LINE FORMATION

- extinction: symmetric bb peak in  $\alpha_\lambda$  becomes lower and narrower with height
- optical depth:  $\tau_\lambda \equiv -\int(\alpha_\lambda^l + \alpha_\lambda^c) dh$  increases roughly log-linear with geometrical depth
- source function: split line (bb) and continuum (bf, ff, electron scattering) processes
- intensity: Eddington-Barbier  $I_\lambda \approx S_\lambda(\tau_\lambda = 1)$  for  $S_\lambda^{\text{total}} = (\alpha_\lambda^c S_\lambda^c + \alpha_\lambda^l S_\lambda^l)/(\alpha_\lambda^c + \alpha_\lambda^l)$



# LINE FORMATION AS SEEN BY THE ATOM



- *pair combinations*
  - beam of interest to the right
  - $a / d + e =$  collisional destruction / creation of beam photons
  - $b + h / f + i + j$  scattering & detour photons out / into beam (c, g cancel)
- *equilibria*
  - LTE:  $a + d + e$  dominate;  $bb$  Boltzmann  $f(T)$ ,  $bf$  Saha  $f(T, N_e)$
  - CE:  $d$  only;  $bb$   $f(T, N_e)$ ,  $bf$   $f(T)$
  - NLTE, NSE: scattering and/or detours important;  $bb$  and  $bf$   $f(T, N_e, \bar{J}_{ul}, \bar{J}_{ij}, \bar{J}_{ic}) [t]$
- *line extinction and line source function*
  - $\alpha^l = \alpha^a + \alpha^s + \alpha^d$  absorption + scattering + detour extinction
  - $\varepsilon \equiv \alpha^a / \alpha^l$  destruction probability       $\eta \equiv \alpha^d / \alpha^l$  detour probability
  - $S^l = (1 - \varepsilon - \eta) \bar{J} + \varepsilon B(T) + \eta S^d$        $\bar{J}$ : mean mean intensity       $S^d$ : all detours

# KEY LINE FORMATION EQUATIONS

population departure coefficients

$$b_l = n_l/n_l^{\text{LTE}} \qquad b_u = n_u/n_u^{\text{LTE}}$$

Zwaan:  $n^{\text{LTE}} =$  Saha-Boltzmann fraction of  $N_{\text{el}}$       Harvard:  $n/n_c$  (main stages  $\approx 1/b_c$ )

general line extinction and line source function

$$\alpha_\lambda^l = \frac{\pi e^2}{m_e c} \frac{\lambda^2}{c} b_l \frac{n_l^{\text{LTE}}}{N_{\text{el}}} N_{\text{H}} A_{\text{el}} f_{lu} \varphi \left[ 1 - \frac{b_u}{b_l} \frac{\chi}{\varphi} e^{-hc/\lambda kT} \right] \qquad S_\lambda^l = \frac{2hc^2}{\lambda^5} \frac{\psi/\varphi}{\frac{b_l}{b_u} e^{hc/\lambda kT} - \frac{\chi}{\varphi}}$$

CRD approximation:  $\psi = \chi = \varphi$

Wien approximation: neglect stimulated parts

$$\alpha^l \approx b_l \alpha^{\text{LTE}}$$

$$S^l \approx (b_u/b_l) B(T)$$

PRD: Ly $\alpha$ , Mg II h & k, Ca II H & K, strong UV

Wien: up to H $\alpha$  ( $\lambda T = hc/k$  at 21 900 K)

probabilities per extinction of collisional photon destruction and of detour photon conversion

$$\varepsilon \equiv \frac{\alpha^a}{\alpha^s + \alpha^a + \alpha^d}$$

$$\eta \equiv \frac{\alpha^d}{\alpha^s + \alpha^a + \alpha^d}$$

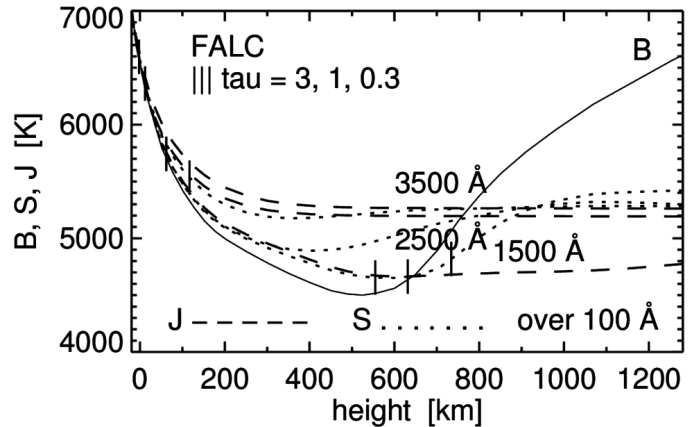
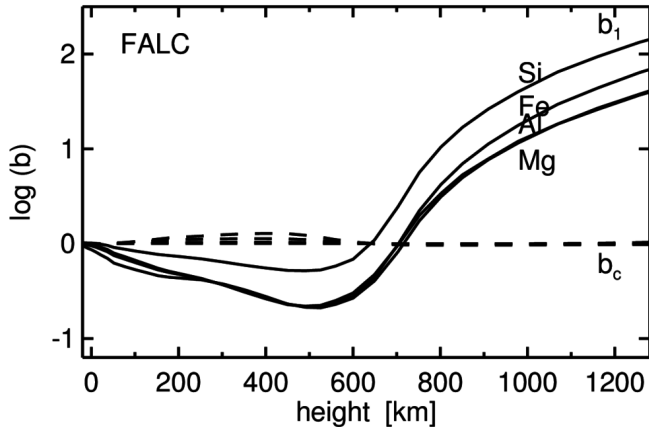
line source function (for CRD, monofrequent for PRD)

$$S^l = (1 - \varepsilon - \eta) \bar{J} + \varepsilon B(T) + \eta S^d$$

“source” = local addition of new photons into beam per local extinction in terms of energy

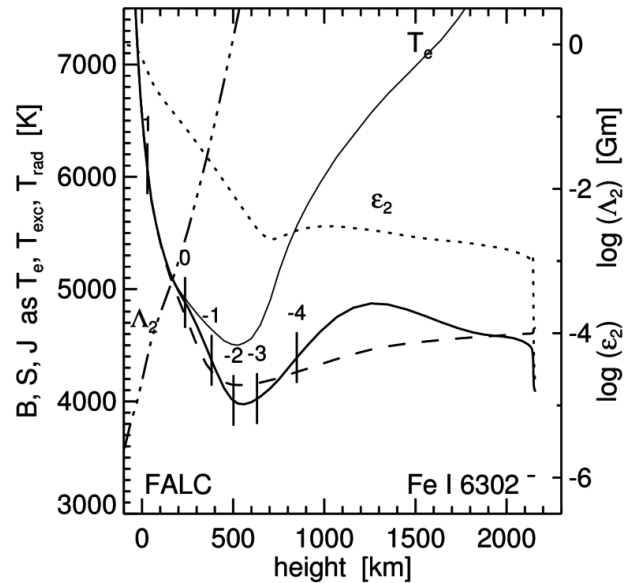
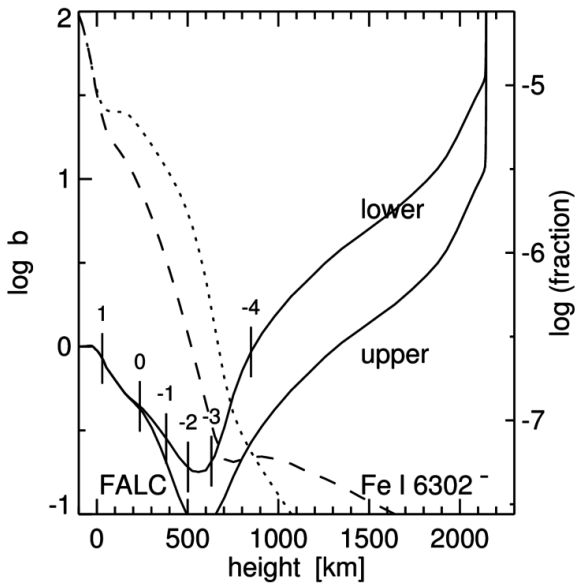
$\bar{J} \equiv (1/4\pi) \iint I \varphi \, d\Omega \, d\lambda$  reservoir       $\varepsilon B$  thermal creation       $\eta S^d$  detour production

## NLTE IN ULTRAVIOLET CONTINUA

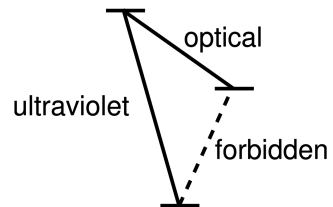


- ultraviolet bound-free edges produce scattering continua with  $S \approx J > B$  from:
  - upper-photosphere  $T(h)$  gradient defined by radiative equilibrium for the bulk  $\approx$  optical (all quiet 1D models  $\approx$  RE model, e.g., Kurucz)
  - deep thermalization depth; above it  $S \approx (1 - \alpha)\bar{J} + \alpha B$  as in two-level scattering
  - $\Lambda$  operator (wide averager of  $S$  into  $J$ ) produces larger  $J > S$  excess for steeper  $S(\tau)$
  - $B(h)$  steeper at depth following  $T(h)$  and in ultraviolet from Wien nonlinearity
- corresponding  $b_1/b_c$  ratios for main edge providers (Mg I, Fe I, Si I, Al I) show increasing neutral-stage population depletion across photosphere and steep boost in chromosphere because  $b_c \approx 1$  (ions contain most of  $A_{ei}$ )
- lines of Mg I, Fe I, Si I, Al I tend to have:
  - outward increasing NLTE extinction deficits in photospheric temperature declines
  - outward increasing NLTE extinction excesses in chromospheric temperature rises worse for steeper deep temperature gradients (e.g., granule centers)

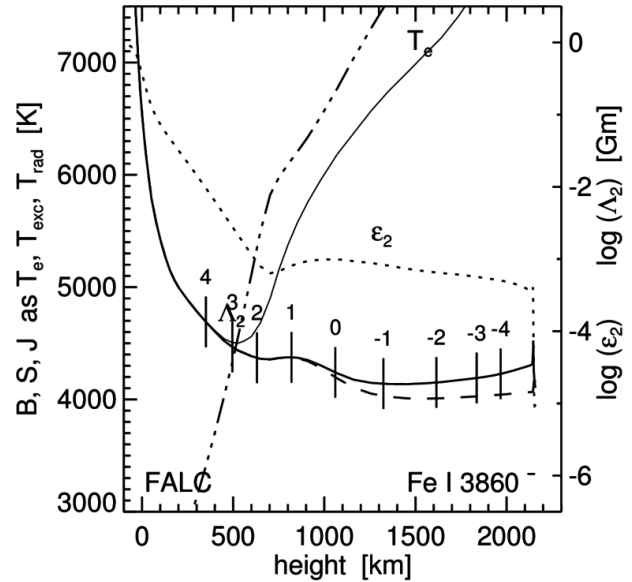
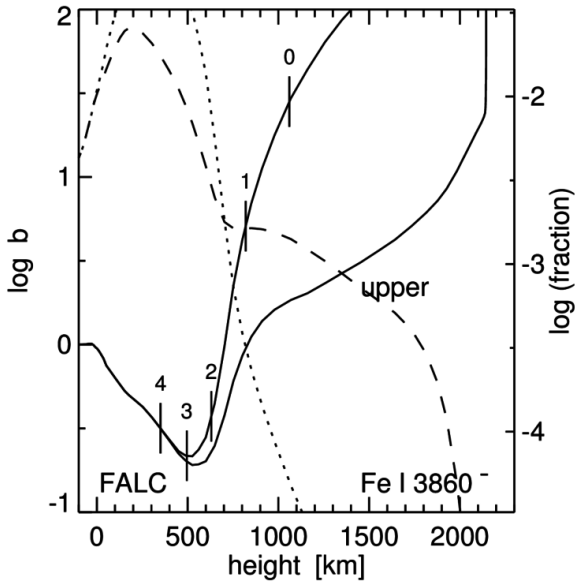
# NLTE IN WEAK Fe I LINE (6301.5 Å, multiplet 816)



- left:  $b_l$  opacity decline from photospheric  $J_{UV} > B_{UV}$  compresses  $\tau$  scale around  $\tau=1$
- right:  $S \approx B$  at  $\tau=1$  because  $b_u < b_l \approx S < B$  split starts higher up
- source function: in two-level description this line scatters with deeper  $S < B$ , but Fe I has very rich term structure in which most optical Fe I lines are subordinate and forced to  $b_u \approx b_l$  through upper-level sharing with stronger, more opaque UV lines



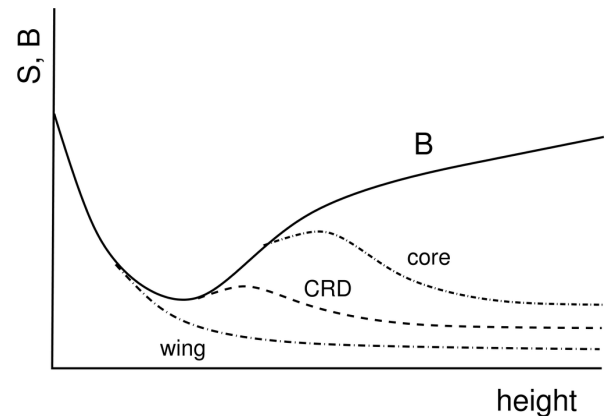
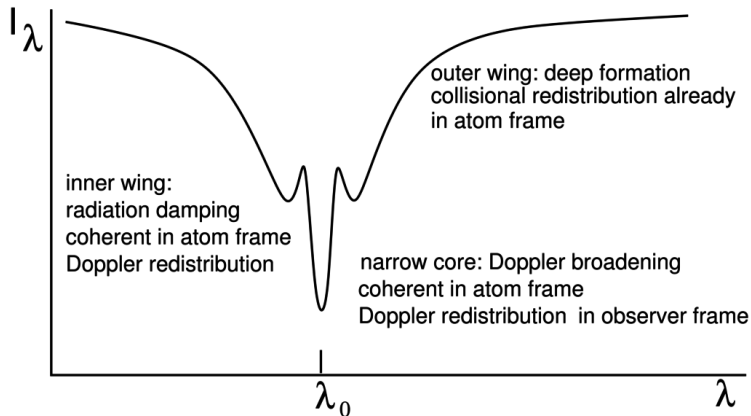
## NLTE IN STRONG Fe I LINE (3859.9 Å, multiplet 4)



- left:  $b_l$  opacity increase from chromospheric  $J_{\text{UV}} < B_{\text{UV}}$  extends  $\tau$  scale around  $\tau=1$
- right:  $S < B$  around  $\tau=1$  because  $b_u < b_l \approx S < B$  split starts from deep thermalization
- two-level description works well, no multi-level detour interlocking
- such strong lines force  $b_u \approx b_l$  across the photosphere for weaker upper-level sharers

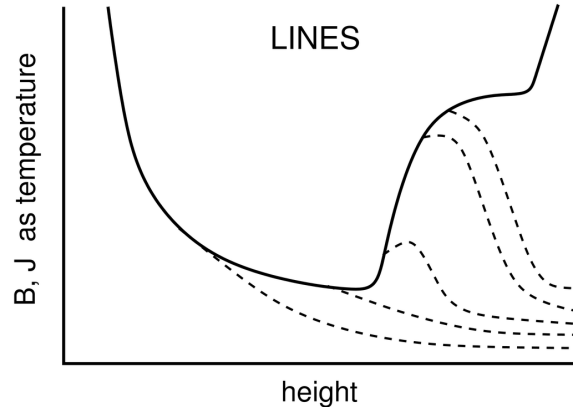
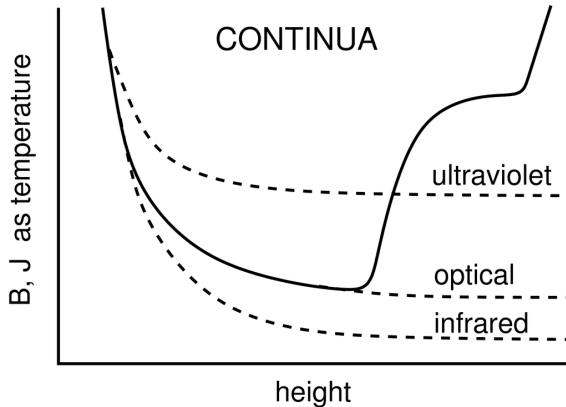


# PARTIAL REDISTRIBUTION ( $\text{Ly}\alpha$ , Mg II h & k, Ca I HK, strong UV lines)



- Doppler core: monofrequent (“coherent”) scattering per atom in its moving frame; Doppler redistribution over parcel Doppler width for observer (snag: microturbulence?)
- inner damping wing: Heisenberg  $\Rightarrow$  coherent scattering with Doppler redistribution
- outer damping wing: collisional damping at high density  $\Rightarrow$  complete redistribution
- if the line is so strong that radiation damping dominates in the inner wings (high formation at low collider density) then the inner-wing photons are independent Doppler-wide ensembles with their own line source functions
- inner-wing line source functions decouple deeper from the Planck function than the core source function due to smaller opacity: they represent weaker lines
- the PRD core source function decouples further out than for complete redistribution because core photons cannot escape from deeper layers via occasional wing sampling

# SUMMARY 1D SCATTERING SOURCE FUNCTIONS



- *continua*

- optical:  $J \approx B$  for radiative equilibrium
- ultraviolet:  $S \approx J > B \rightarrow$  overionization of minority neutrals
- infrared:  $J < B$  but  $J$  doesn't matter since  $H_{\text{ff}}^-$  and  $H_{\text{ff}}$  have  $S = B$

- *lines*

- $dB/d\tau = dB/d(\tau^c + \tau^l)$  much less steep, so closer to isothermal  $S \approx \sqrt{\epsilon} B$
- for stronger lines  $S$  sees more of the model chromosphere
- PRD lines have frequency-dependent core-to-wing  $S \approx J$  curves like these

# NON STATISTICAL EQUILIBRIUM (AKA “DYNAMIC IONIZATION”)

- *nature*

- SE (statistical equilibrium): population equations (rate equations) sum to zero = all populations and radiation defined instantly; NSE: non-zero sums = memories
- bound-bound relaxation time = equilibrium settling time to new temperature: at small net radiative bracket (large radiative rates that nearly balance) Boltzmann sensitivity from  $C_{lu} = C_{ul}(g_l/g_u) \exp(-E_{ul}/kT)$ : slowest for strongest EUV lines at low T

- *hydrogen*

- Ly $\alpha$  closely in detailed radiative balance due to enormous opacity; collisional balancing to reach SE takes minutes in gas cooling below 8 000 K
- hydrogen ionization/recombination occurs predominantly in a faster Balmer loop from  $n = 2$  and follows Ly $\alpha$  settling: Ly $\alpha$  is the NSE culprit ( $\Rightarrow$  “NSE Ly $\alpha$  balancing”)
- key hydrogen NSE demonstrations:
  - 1D RADYN HD shocks: Carlsson & Stein [2002ApJ...572..626C](#)
  - 2D Stagger MHD shocks: Leenaarts et al. [2007A&A...473..625L](#)
  - 3D MHD+GOL spicules-II: tbd = Bifrost? MURaM? Mancha?
- other elements:
  - He: He I 584 Å candidate but competition from downward irradiation; others: tbd

- *effects on spectral irradiance*

- optical: don’t bother, too deep = too dense
- ultraviolet: electron density boost at partial hydrogen ionization ( $10^3$  at 10%) is highly NSE-sensitive to dynamic cooling (RRC: only NSE dynamism explains H $\alpha$ )
- submm and mm: idem, affecting H I ff extinction (RRC: ALMA will show H $\alpha$ -like)

# MODELING THE LINE HAZE FOR SPECTRAL IRRADIANCE

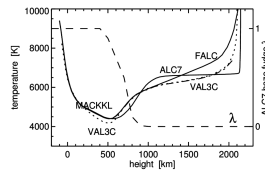
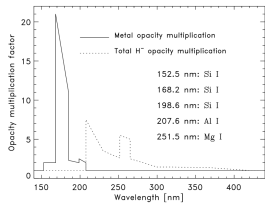
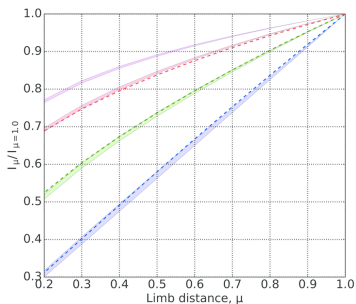
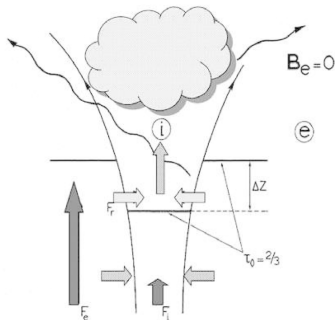
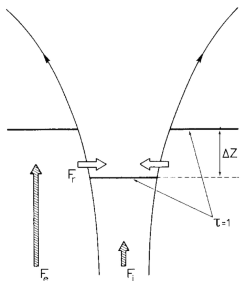


Table 2  
Atom/Ion Solved by Full Non-LTE Radiative Transfer Calculations, the Number of Levels and Sublevels Included for Each of them, and the Elemental Abundance ( $\log \epsilon_{\odot}/\mu$ )

Ion	Levels/ Sublevels	Ion	Levels/ Sublevels	Ion	Levels/ Sublevels	Abundance
H I	20/20	...	...	...	...	1.0
He I	20/32	He II	15/25	...	...	0.1
C I	45/87	C II	27/50	...	...	2.4e-4
N I	26/61	N II	33/61	...	...	1.0e-4
O I	23/51	O II	31/68	...	...	3.5e-4
Ne I	80/80	Ne II	57/57	...	...	6.92e-5
Na I	23/29	Na II	14/25	Na III	2/2	3.0e-6
Mg I	26/44	Mg II	14/23	Mg III	54/93	3.39e-5
Al I	18/31	Al II	20/34	Al III	33/42	4.4e-6
Si I	33/65	Si II	14/25	Si III	40/108	3.24e-5
S I	20/30	S II	30/65	...	...	6.92e-6
Ar I	44/48	Ar II	57/57	...	...	1.52e-6
K I	10/16	...	...	...	...	2.5e-7
Ca I	22/38	Ca II	24/35	Ca III	34/65	1.04e-6
Ti I	116/296	Ti II	79/244	Ti III	43/83	7.94e-8
V I	120/342	V II	41/111	V III	40/99	1.0e-8
Cr I	103/238	Cr II	34/85	Cr III	20/50	4.3e-7
Mn I	85/261	Mn II	28/74	Mn III	40/112	2.45e-7
Fe I	119/377	Fe II	120/344	Fe III	90/235	2.82e-5
Co I	60/167	Co II	38/77	Co III	50/143	8.32e-8
Ni I	61/136	Ni II	28/68	Ni III	40/102	1.70e-6

- *Bruls opacity fudge* 1992A&A...265..237B
  - fit MULTI output VALIIC to VALII data
  - multipliers to bound-free metal and H<sup>-</sup> opacities
- *Avrett grosso-modo scattering trick* 2008ApJS..175..229A
  - post-VALIII models less steep photosphere from Kurucz lines
  - no Kurucz reversals from imposed  $S = (1 - \lambda) J + \lambda B$
- *Uitenbroek RH options*
  - Bruls / Kurucz lines LTE / Kurucz lines 2-level
  - FTS versus RH
- *Fontenla brute-force solution* 2015ApJ...809..157F
  - very many lines in detail
  - good result but only doable for 1D model
- *suggestions for massive spectral synthesis (RH 1.5D?)*
  - distill Bruls-like fudge from Fontenla et al. results
  - impose strong-line *b* departures from schematic Fe-like model atom

# MODELING NETWORK / PLAGE MAGNETISM FOR SPECTRAL IRRADIANCE



- *golden age of fluxtube modeling = hole in surface*
  - Zwaan – Spruit: **idealized** magnetostatic fluxtubes
  - Stenflo – Solanki – Keller: unresolved FTS polarimetry
  - Steiner – Keller – **Carlsson**: realistic MHD simulations
- *bright-point enhancements = hole deepening*
  - CH G-band, CN 3883 band: dissociation
  - Fe I line gaps: ionization
  - Balmer line wings: small collision broadening
  - Mn I line cores: large hyperfine broadening
- *dark age of 1D irradiance modeling = down the rabbit hole*
  - “chromospheric cloud”  $\Rightarrow$  “photosphere heating”
  - **FALP** > **FALC fudge**  $\Rightarrow$  SATIRE (ADS N39 H13)
  - **1600 Å – 1700 Å** [SST/CHROMIS Ca II K wing scans]
- *coming age of simulation irradiance modeling  $\Rightarrow$  of age  $\sim$  1D  $\Rightarrow$  3D abundances (“pre/post Asplund”)*
  - **first step: MURaM with LTE**
  - to do: 3D(t) MHD with NLTE, line haze, H NSE?

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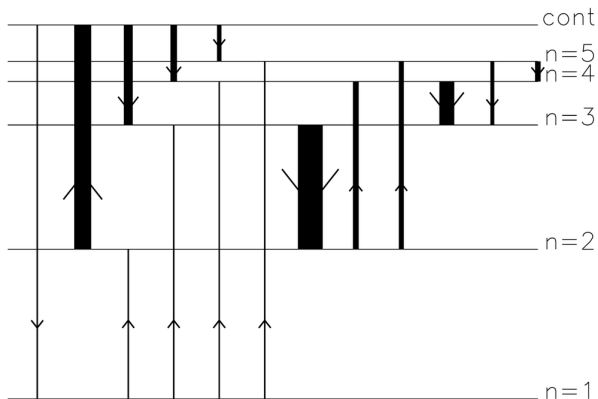
Lingezicht Astrophysics Deil & Institutt for Teoretisk Astrofysikk Oslo

lecture displays <http://www.staff.science.uu.nl/~rutte101>

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# NON-EQUILIBRIUM HYDROGEN IONIZATION IN 1D SHOCKS

Carlsson & Stein 2002ApJ...572..626C



atom top  $\sim 3.4$  eV alkali: NLTE-SE ionization loop

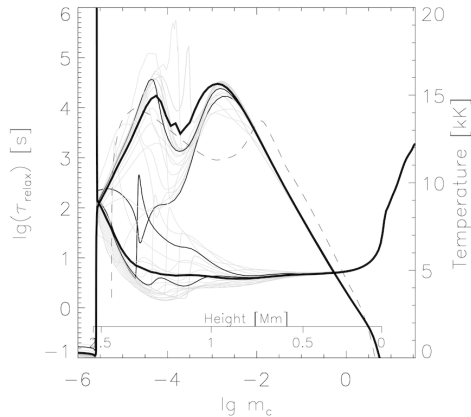
- driven by photon pumping Balmer continuum, scattering from deep,  $\approx 5300$  K, smooth
- closure by photon losses in  $n_\alpha$  lines

atom bottom actually up to 10 eV: non-E Ly $\alpha$

- tremendous scattering from small  $\varepsilon$
- tremendous opacity from huge H abundance
- small structures already detailed radiative balance
- non-E: fast settling at high T, slow at low T

- RADYN code: 1D(t) hydrodynamics, time-dependent, NLTE radiation, simple PRD
- observed subphotosphere piston drives acoustic waves up that shock near  $h=1000$  km
- Ly $\alpha$  scatters in radiative balance and controls  $n=2$ . Within shocks  $S \approx J$  saturates to  $B$  from radiation lock-in (increased  $\varepsilon$  from partial hydrogen ionization) so that  $b_2 \approx 1$
- collisional Ly $\alpha$  balancing has Boltzmann temperature sensitivity: fast (seconds) in hot gas, slow (minutes) in cool gas, resulting in retardation: post-shock cooling gas maintains the high  $n_2$  shock value at increasing  $b_2$  during minutes, up to huge overpopulation ( $b_2 \approx 10^{10}$ )
- ionization from  $n=2$ : instantaneous statistical-equilibrium balance driven by Balmer continuum  $J \neq B$  and closed by cascade recombination, with  $b_{\text{cont}}/b_2 \approx 10^{-1}$  in hot and  $\approx 10^{+3}$  in cool gas, the latter adding to much larger retarded  $b_2$
- between shocks hydrogen remains hugely overionized versus SE and LTE predictions

## DETAILED BALANCING



*Hydrogen ionization/recombination relaxation timescale throughout the solar-like shocked RAdyn atmosphere. The timescale for settling to equilibrium at the local temperature is very long, 15–150 min, in the chromosphere but much shorter, only seconds, in shocks in which hydrogen partially ionizes.*

*Carlsson & Stein 2002ApJ...572..626C*

net radiative and collisional downward rates (Wien approximation)

$$n_u R_{ul} - n_l R_{lu} \approx \frac{4\pi}{h\nu_0} n_l^{\text{LTE}} b_u \sigma_{\nu_0}^l \left( B_{\nu_0} - \frac{b_l}{b_u} \bar{J}_{\nu_0} \right) \quad \text{zero for } S = \bar{J}, \text{ no heating/cooling}$$

$$n_u C_{ul} - n_l C_{lu} = n_l C_{lu} \left( \frac{b_u}{b_l} - 1 \right) = b_u n_l^{\text{LTE}} C_{lu} \left( 1 - \frac{b_l}{b_u} \right) \quad \text{zero for } b_u = b_l, \text{ LTE } S^l$$

dipole approximation for atom collisions with electrons (Van Regemorter 1962)

$$C_{ul} \approx 2.16 \left( \frac{E_{ul}}{kT} \right)^{-1.68} T^{-3/2} \frac{g_l}{g_u} N_e f$$

Einstein relation

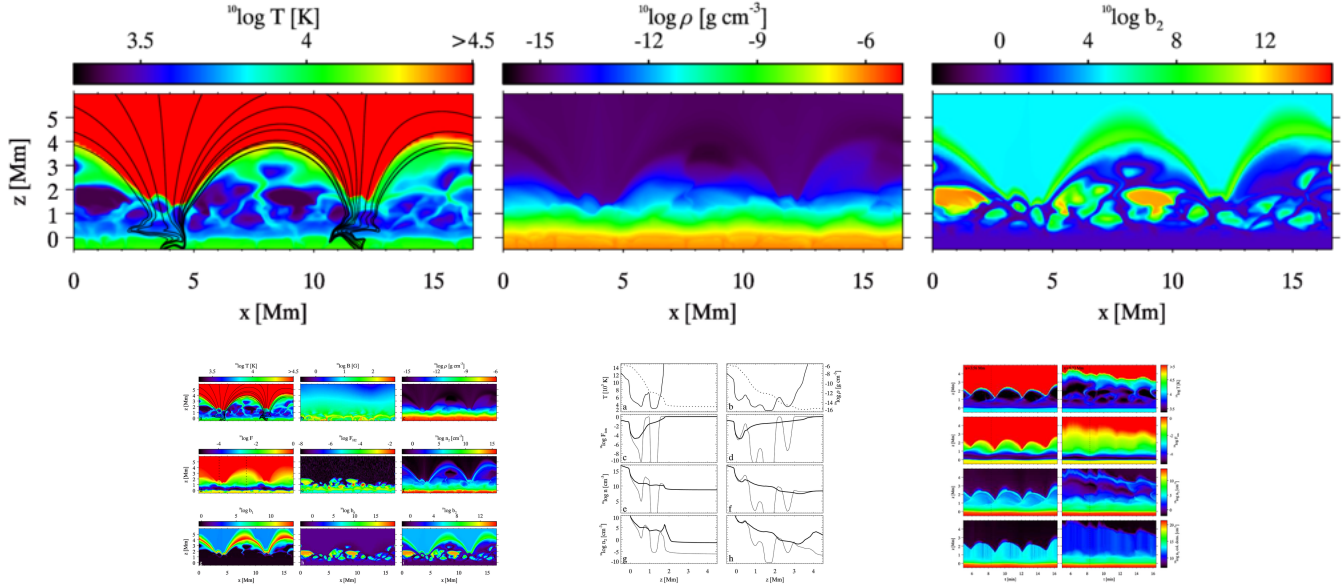
$$C_{lu} = C_{ul} \frac{g_l}{g_u} e^{-E_{ul}/kT}$$

$C_{ul}$  is not very temperature sensitive (any collider will do);  $C_{lu}$  has Boltzmann sensitivity



# NON-E HYDROGEN IONIZATION IN 2D MHD SHOCKS

Leenaarts et al. 2007A&A...473..625L

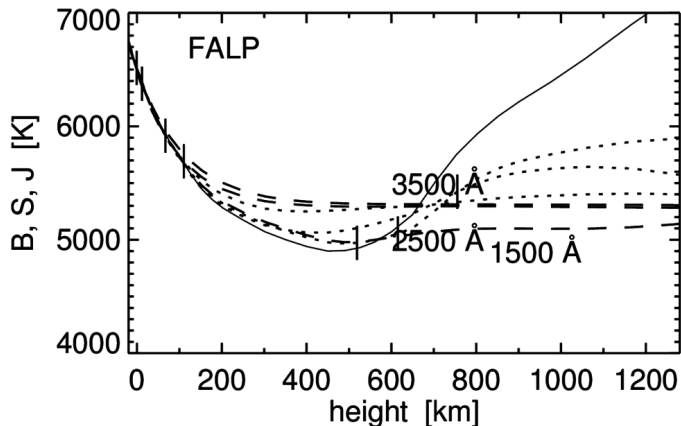
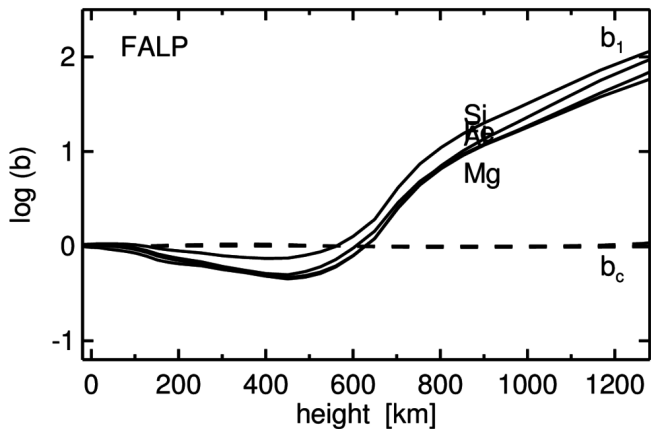
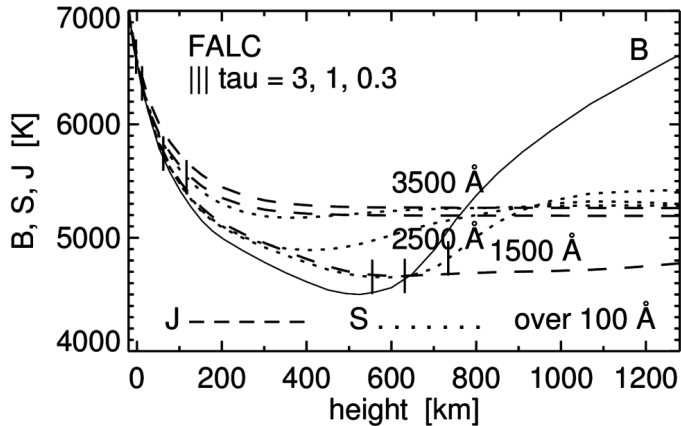
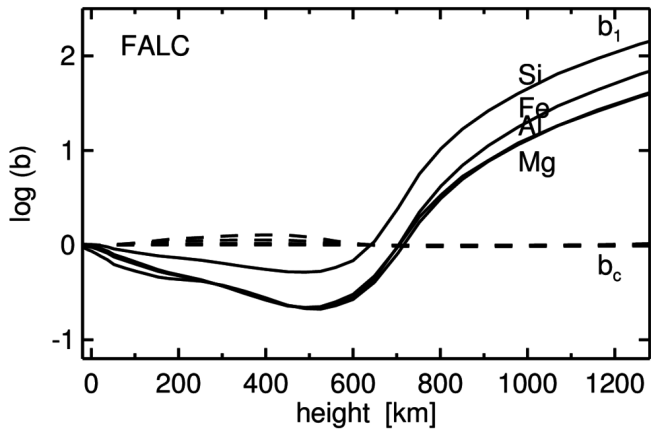


- in shocks  $\text{Ly}\alpha$  has  $S \approx B$  from high  $T$  (fast balancing) and  $N_e$  (10% H ionization)
- retarded collisional balancing in  $\text{Ly}\alpha$ :  $n_2$  hangs near high shock value  $n_2 \approx n_2^{\text{LTE}}$
- gigantic post-shock  $n=2$  overpopulations versus LTE (“S-B underestimates”)
- yet larger post-shock overionization from hydrogen-top Balmer balancing
- no Lyman RT: green arches artifacts, no lateral  $N_e$  boost from  $\text{Ly}\alpha$  scattering

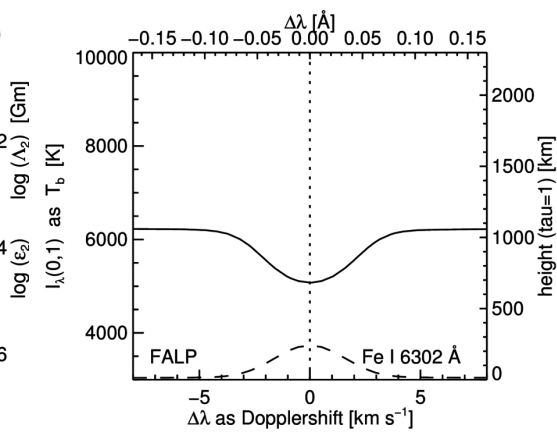
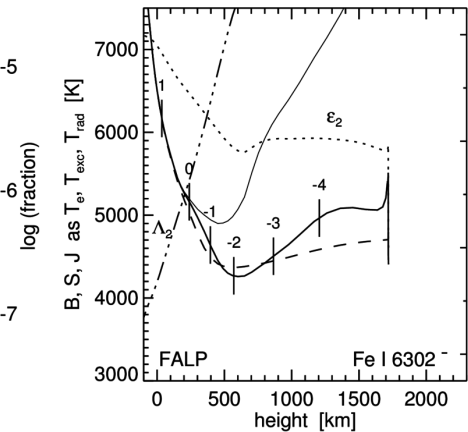
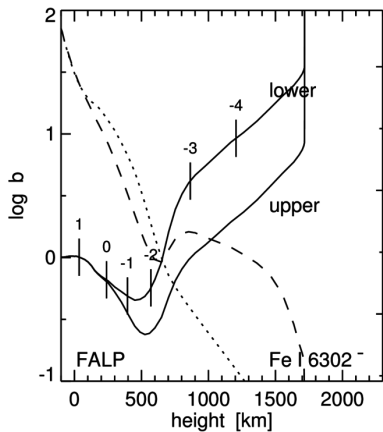
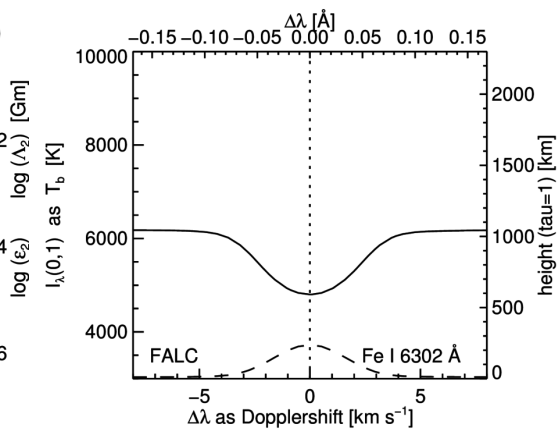
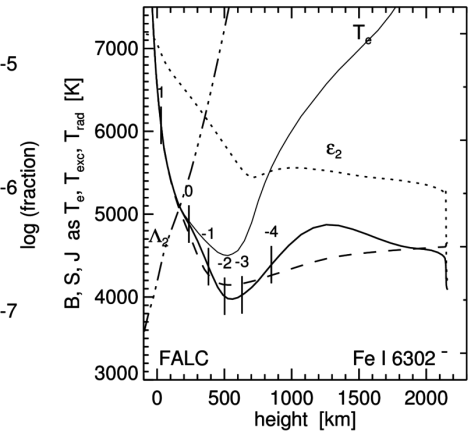
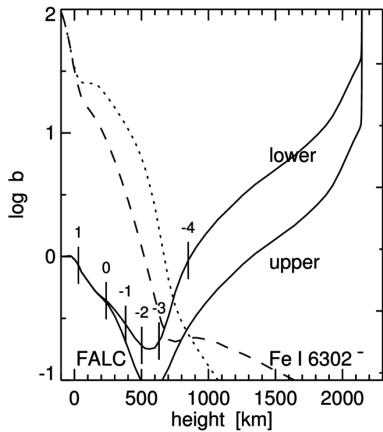
# RECENT DEVELOPMENTS IN PRD LINE SYNTHESIS

- *RH code: Uitenbroek 2001ApJ...557..389U*
  - Rybicky & Hummer: not  $\Lambda(S)$  but  $\Psi(j)$  iteration; preconditioning
  - overlapping lines
  - 1D, 2D, 3D, spherical versions
- *RH 1.5D: Pereira & Uitenbroek 2015A&A...574A...3P*
  - 1.5D = column-by-column
  - massively parallel
  - also molecular lines (but Kurucz lines in LTE)
- *angle-dependent redistribution: Leenaarts et al. 2012A&A...543A.109L*
  - good summary PRD theory and equations
  - non-stationary atmosphere requires angle-dependent PRD
  - hybrid approximation: transform to gas parcel frame, assume angle-averaged PRD ( $\approx$  angle dependent from deep isotropy), transform back
- *towards Bifrost PRD: Sukhorukov & Leenaarts 2017A&A...597A..46S*
  - hybrid approximation for small memory
  - linear frequency interpolation for speed
  - $252 \times 252 \times 496$  grid, 1024 CPUs: 2 days for Mg II k  $\approx$  doable
- *next: 3D PRD with multigrid (Björge & Leenaarts 2017A&A...599A.118B)*

# ULTRAVIOLET CONTINUA IN FALC AND FALP

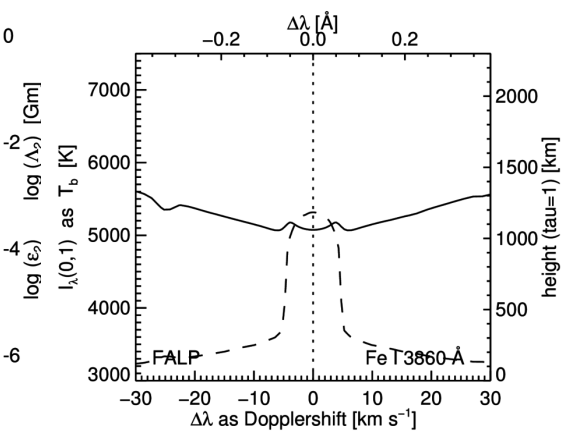
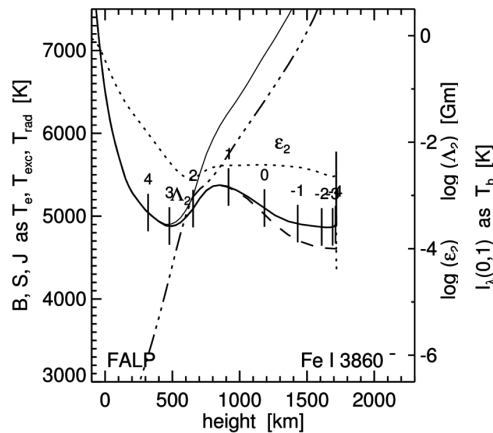
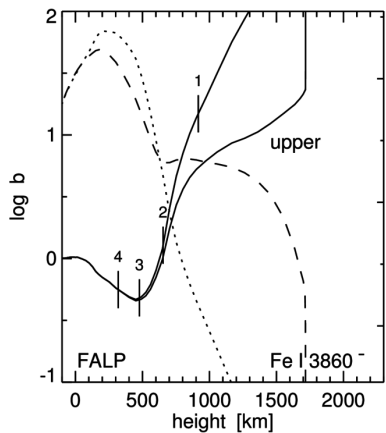
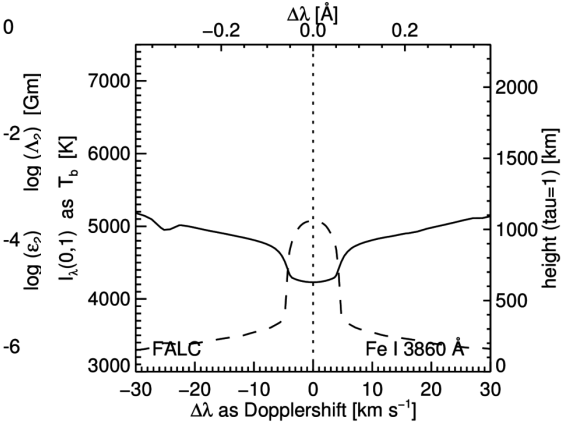
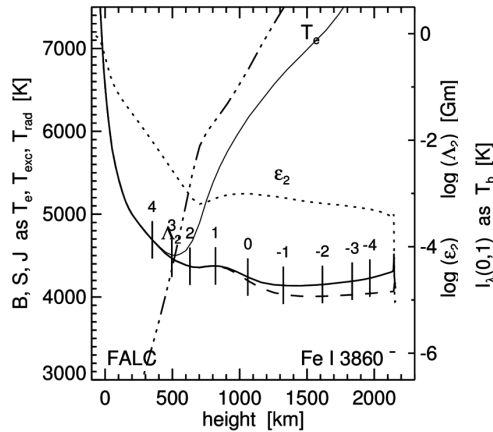
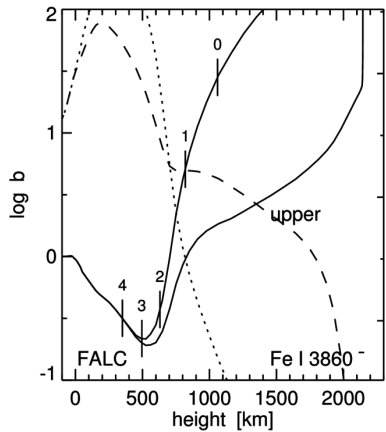


# Fe I 6301.5 Å IN FALC AND FALP



*standard polarimetry line*

# Fe I 3859.9 Å IN FALC AND FALP



*strong ground-state Fe I line*

### NON-EQUILIBRIUM SPECTRUM FORMATION AFFECTING SOLAR IRRADIANCE

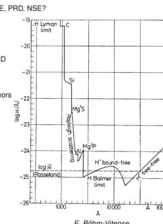
Rob Rutten  
 Lingzhi Astrophysics Del. & Institut for Teoretisk Astrofysikk Oslo  
 lecture displays <http://www.nslf.science.uio.no/~rutten201>

- microsource "solar spectrum formation"
  - photos. process
  - NLTE lines and continua
  - NSE
- modeling "haze" lines
  - methods
  - demo: FTS versus RH
- modeling network/ "plage flutubest"
  - methods
  - demo: 1600 Å versus 1700 Å
- to do for spectral irradiance modeling
  - hazes: define trampoline recipe
  - flutubest: 3000 MHz with NLTE synthesis
  - caveat: hydrogen NSE

1

### SOLAR ATMOSPHERE RADIATIVE PROCESSES

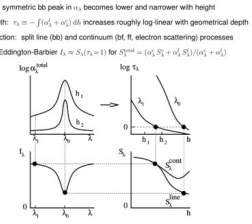
- bound-bound  $\rightarrow$   $\dots$ ,  $S_{\nu}$ , CE, LTE, NLTE, PRD, NSE?
  - neutral atom transitions
  - ion transitions
  - molecule transitions
- bound-free - same except always CRD
  - H<sup>+</sup> optical, near-infrared
  - H I Balmer, Lyman; He I, He II
  - Fe I, Si I, Mg I, Al I = electron donors
- free-free  $\rightarrow$   $S_{\nu} = B_{\nu}$ 
  - H<sup>+</sup> infrared, sub-mm
  - H mm, radio
- electron scattering  $\rightarrow$   $S_{\nu} = J_{\nu}$ 
  - Thomson scattering
  - Rayleigh scattering
  - cyclotron, synchrotron radiation
  - plasma radiation



2

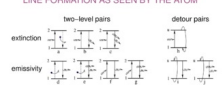
### SCHEMATIC THICK SOLAR LINE FORMATION

- extinction: symmetric lb peak in  $\kappa_{\nu}$  becomes lower and narrower with height
- optical depth:  $\tau_{\nu} = \int \kappa_{\nu}(z) dz$  increases roughly log-linear with geometrical depth
- source function: split line (bb) and continuum (ff, if electron scattering) processes
- intensity: Eddington-Barbier rule  $I_{\nu} \approx S_{\nu}(\tau_{\nu} = 1)$  for  $S_{\nu}^{cont} = (e^{-\tau_{\nu}} S_{\nu}^{line} + \tau_{\nu}^{-1} S_{\nu}^{cont}) / (1 + e^{-\tau_{\nu}})$



3

### LINE EXTINCTION AS SEEN BY THE ATOM



- pair combinations
  - beam of interest to the right
  - $a \rightarrow b + e$ : collisional destruction / creation of beam photons
  - $b \rightarrow a + \gamma$ : scattering & detour photons out / into beam (e.g. canal)
- equilibria
  - LTE:  $a \rightarrow e$  dominate; detour photons (ff), bf Saha ( $T_e, N_e$ )
  - CE:  $d$  only; bb ( $T_e, N_e$ ), bf ( $T_e$ )
  - NLTE, NSE: scattering and detours important; bb and bf ( $T_e, N_e, T_e, T_e, J$ )
- line extinction and line source function
  - $a \rightarrow e = a^* + e^*$ : absorption + scattering + detour extinction
  - $a \rightarrow a^*$ : destruction probability  $g = a^*/a$ ; detour probability  $\delta = (1 - a - \delta) J + B(T) + g S^*$ ;  $J$ : mean mean intensity  $S^*$ : all detours

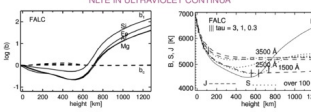
4

### KEY LINE FORMATION EQUATIONS

population departure coefficients  $k_a = n_a/n_a^{LTE}$ ,  $k_b = n_b/n_b^{LTE}$  (main stages  $= 1/k_a$ )  
 Zwaan:  $n_a^{LTE} =$  Saha Boltzmann fraction of  $N_{\nu}$  Harvard:  $n_a/n_b =$  (main stages  $= 1/k_a$ )  
 general line extinction and line source function  
 $a^*_a = \frac{a^*}{a} \frac{g_a}{g_a} \frac{N_a}{N_a} k_a k_b \nu_{ab} \left[ \frac{1}{2} (1 - \delta) + \delta \tau_{ab} \right]$   
 $S^*_a = \frac{J_{\nu}}{4\pi} \frac{g_a}{g_a} \frac{N_a}{N_a} k_a k_b \nu_{ab} \left[ \frac{1}{2} (1 - \delta) + \delta \tau_{ab} \right]$   
 CRD approximation:  $\psi = \chi = \psi^*$  Wien approximation: neglect stimulated parts  
 $a^*_a = n_a/n_a^{LTE}$ ,  $b^*_b = n_b/n_b^{LTE}$   
 PRD: Ly $\alpha$ , Mg II h, Ca I H&K, strong UV. Warn:  $u \rightarrow$  up to  $(1 - \delta) k_a k_b$  at 21 900K  
 probabilities are extinction of collisional photon destruction and of detour photon conversion  
 $\delta = \frac{a^*}{a} \frac{g_a}{g_a} \frac{N_a}{N_a} k_a k_b \nu_{ab} \left[ \frac{1}{2} (1 - \delta) + \delta \tau_{ab} \right]$   
 $\psi = \frac{a^*}{a} \frac{g_a}{g_a} \frac{N_a}{N_a} k_a k_b \nu_{ab} \left[ \frac{1}{2} (1 - \delta) + \delta \tau_{ab} \right]$   
 line source function (for CRD, monoquant for PRD)  
 $S^*_a = (1 - \delta) J_{\nu} + B(T) + g S^*$   
 "source" = local addition of new photons into beam per local extinction in terms of energy  
 $J = \frac{1}{4\pi} \int J_{\nu} d\Omega$ ;  $B(T)$ : thermal emission;  $g S^*$ : detour production

5

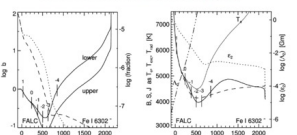
### NLTE IN ULTRAVIOLET CONTINUA



- ultraviolet bound-free edge produce scattering continua with  $S_{\nu} = J_{\nu} + B_{\nu}$  from:
  - upper-photosphere ( $J_{\nu}$ ) gradient defined by radiative equilibrium for the bulk  $\approx$  optical (all quiet ID models = RE model, e.g. Kurucz)
  - deep thermalization depth; above  $S_{\nu} = (1 - \delta) J_{\nu} + B_{\nu}$  as two-level scattering
  - $\delta$  operator (wide average of  $\delta$  into  $J_{\nu}$ ) produces larger  $J_{\nu}$  excess for steeper  $S(\tau) = B_{\nu}$  steeper at depth following  $T(z)$  and in ultraviolet from Wien nonlinearity
- corresponding  $k_a, k_b$  ratios for main edge providers (Mg I, Fe I, Si I, Al I) show increasing neutral-state population depletion across photosphere and steep boost in chromosphere because  $k_a \approx 1$  (cons constant of  $k_a$ )
- lines of Mg I, Fe I, Si I, Al I tend to have:
  - outward increasing NLTE extinction deficits in photospheric temperature declines
  - outward increasing NLTE extinction excesses in chromospheric temperature rises worse for steeper deep temperature gradients (e.g., granule centers)

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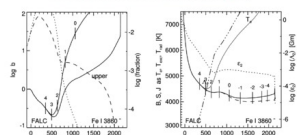
### NLTE IN WEAK Fe I LINE (6301.5 Å, multiplet 816)



- left:  $k_a$  opacity decline from photospheric  $k_a \approx k_b$  compresses  $\rightarrow$  scale around  $-1$
- right:  $\delta \approx B(T) + g S^*$  because  $k_a, k_b \approx S$  split starts higher up
- source function: two-level description fits line scatterers with deeper  $S_{\nu}$ , but Fe I has very rich term structure in which most optical Fe I lines are subordinate and forested,  $\tau_{\nu} \approx 1$  through upper-level sharing with stronger, more opaque UV lines

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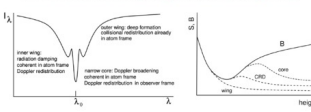
### NLTE IN STRONG Fe I LINE (3859.9 Å, multiplet 4)



- left:  $k_a$  opacity increase from chromospheric  $k_a \approx k_b$  expands  $\rightarrow$  scale around  $-1$
- right:  $\delta \approx B(T) + g S^*$  because  $k_a, k_b \approx S$  split starts from deep thermalization
- two-level description works well, no multi-level detour interlinking
- such strong lines force  $k_a, k_b$  across the photosphere for weaker upper-level shares

8

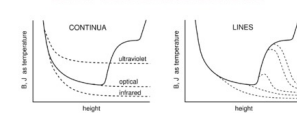
### PARTIAL REDISTRIBUTION (Ly $\alpha$ , Mg II h, Ca I H&K, strong UV lines)



- Doppler core: monoquant (coherent) scattering per atom in its moving frame; Doppler redistribution over parcel Doppler width for observer (narrow, microturbulence?)
- inner damping wing: Heisenberg  $\rightarrow$  coherent scattering with Doppler redistribution
- outer damping wing: collisional damping at high density  $\rightarrow$  complete redistribution
- if the line is so strong that radiation damping dominates in the inner wings (high formation at low collisional density) then the inner-wing photons are independent Doppler-wide ensembles with their own line source functions
- inner-wing line source functions decouple deeper from the Planck function than the core source function does (to smaller opacity, they represent weaker lines)
- the PRD core source function decouples further out than for complete redistribution because core photons cannot escape from deeper layers via occasional wing sampling

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### SUMMARY 1D SCATTERING SOURCE FUNCTIONS



- continua
  - optical:  $J = B$  for radiative equilibrium
  - ultraviolet:  $S > B$   $\rightarrow$  overionization of minority neutrals
  - infrared:  $J < B$  but  $J$  doesn't matter since  $H_2$  and  $H_2^+$  have  $S = B$
- lines
  - $\delta B(T) = \delta B(T + \delta)$  much less steep, to closer to isothermal  $S = g S^* B$
  - for stronger lines  $S$  sees more of the model chromosphere
  - PRD lines have frequency-dependent core-to-wing  $S \approx J$  curves like these

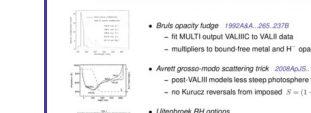
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### NON STATISTICAL EQUILIBRIUM (AKA "DYNAMIC IONIZATION")

- nature
  - SE (statistical equilibrium): population equations (rate equations) sum to zero = all populations and radiation defined instantly; NSE: non-zero sums = memories
  - bound-bound relaxation time = equilibrium settling time to new temperature; at small net radiative lagrange (large radiative rates that nearly balance) Boltzmann sensitivity from  $(n_a - C_a) / (n_a - n_a^{LTE}) \sim \tau_{ab} / T$ ; slowest for strongest EUV lines low T
- hydrogen
  - Ly $\alpha$  closely in detailed radiative balance due to enormous opacity; collisional balancing to reach SE takes minutes in gas cooling below 8000K
  - hydrogen ionization/recombination occurs predominantly in a faster Balmer loop from  $n = 2$  and follows Ly $\alpha$  settling; Ly $\alpha$  is the NSE output ("NSE Ly $\alpha$  balancing")
  - key hydrogen NSE demonstrations:
    - 1D RADYN HD shocks: Carlsson & Stein 2002ApJ...572...626C
    - 2D Stagger MHD shocks: Leemann et al. 2007ApJ...673...429L
    - 3D MHD-QOOL spicules II: Iod - Bilofit? MURM@? Mancha? - other elements
  - He: He I 854 Å candidate but competition from downward irradiation; others: ID?
- effects on spectral irradiance
  - optical: don't bother; too deep  $\rightarrow$  too dense
  - ultraviolet: electron density boost at partial hydrogen ionization ( $10^9$  at  $10^8$ ) is highly NSE sensitive to dynamic cooling (PRD: only NSE dynamism explains  $H_{\nu}$ )
  - sub-mm and mm: idem, affecting H II emission (RRR: ALMA show  $H_{\nu}$ -like)

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### MODELING THE LINE HAZE FOR SPECTRAL IRRADIANCE



- Bruls opacity fudge 1990A&A...285...278B
  - H I N&T1 output MUMC2 to MUMI data
  - multipliers to bound-free metal and H<sup>+</sup> opacities
- Avrett porous-media scattering trick 2010ApJ...715...228A
  - post-MUMI models less steep photosphere from Kurucz lines
  - no Kurucz reversals from imposed  $S = (1 - \delta) J + B$
- Uitenbroek RH opacities
  - Bruls / Kurucz lines LTE / Kurucz lines 4-level
  - FTS versus RH
- FontanaI brute-force solution 2015ApJ...809...157F
  - very many lines in detail
  - good result but only done for 1D model
- suggestions for massive spectral synthesis (RH / S2?)
  - distl Bruls-like fudge from FontanaI et al. results
  - impose strong-line  $\delta$  departures from schematic Fe-like model atom

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MODELING NETWORK / PLAGE MAGNETISM FOR SPECTRAL IRRADIANCE

- golden age of fluxtube modeling = hole in solar irradiance
  - Zwaan - Spruit: idealized magnetostatic fluxtubes
  - Stenflo - Solanki - Keller: unresolved FTS polarimetry
  - Balmer - Keller - Carlsson: realistic MHD simulations
- bright point enhancements = hole deepening
  - Chi Q-band, CN 3883 band: dissociation
  - Fe I line gaps: ionization
  - Balmer line wings: small collision broadening
  - Mn I line cores: large hyperfine broadening
- dark age of 1D irradiance modeling = down the rabbit hole
  - "chromospheric cloud" => "photosphere heating"
  - FALP - FALC tubes => SATIRE (ADS NSR HIC)
  - 1600 Å - 1700 Å (SSTICROMS Ca II wing scans)
- coming age of simulation irradiance modeling = of age
  - 1D => 3D abundances (pre-post Asplund)
  - first step: MURaM with LTE
  - to do: 3D(MHD) with NLTE, line haze, HNSE?



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NON-EQUILIBRIUM SPECTRUM FORMATION AFFECTING SOLAR IRRADIANCE

- Rolf Rutten  
 Lingöström Astrophysical Observatory & Institut för Teoretisk Astrofysik Oav  
 lecture displays <http://www.staff.lth.se/~rolfr/rutten1>
- microturbulence "solar spectrum formation"
    - photonic processes
    - NLTE lines and continua
    - NSE
  - modeling "hazy" lines
    - methods
    - demo: FTS versus RH
  - modeling network / "plage fluxtubes"
    - methods
    - demo: 1600 Å versus 1700 Å
  - to do for spectral irradiance modeling
    - haze: define radiative recipe
    - fluxtubes: 3D(M) MHD with NLTE synthesis
    - causet: hydrogen NSE

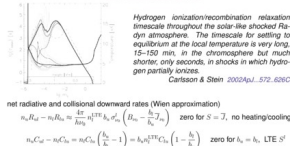
14

NON-EQUILIBRIUM HYDROGEN IONIZATION IN 1D SHOCKS

- Carlsson & Stein 2002ApJ...572..626C
- 
- The bar chart shows ionization fractions for Lyman series lines. The y-axis is labeled 'ionization fraction' and ranges from 0 to 1. The x-axis lists Lyman lines from Ly-1 to Ly-10. Ly-1 is at 1.0, Ly-2 is at ~0.9, Ly-3 is at ~0.8, Ly-4 is at ~0.7, Ly-5 is at ~0.6, Ly-6 is at ~0.5, Ly-7 is at ~0.4, Ly-8 is at ~0.3, Ly-9 is at ~0.2, and Ly-10 is at ~0.1.
- RADYN code: 1D(1) hydrodynamics, time-dependent, NLTE radiation, simple PRD
  - observed subphotospheric piston drives acoustic waves up that shock near  $z = 1000$  km
  - Ly $\alpha$  scatters in radiative balance and controls  $n = 2$ . Within shocks  $S = J$  saturates to  $I$  from radiation locks in (increased  $I$  from partial hydrogen ionization) so that  $n = 1$
  - collisional Ly $\alpha$  balancing has Boltzmann temperature sensitivity; (seconds) in hot gas, slow (minutes) in cool gas, resulting in retardation: post shock cooling gas maintains the high  $n$  shock value as (increasing  $J$ ) during minutes, up to huge overpopulation ( $n = 10^7$ )
  - ionization from  $n = 2$ : instantaneous statistical-equilibrium balance driven by Balmer continuum  $J$  &  $I$  and cooled by cascade recombination, with  $k_{10,9} = 10^{-11}$  in hot and  $10^{-10}$  in cool gas, the latter adding to much larger retarded  $k_{10,9}$
  - between shocks hydrogen remains hugely overionized versus SE and LTE predictions

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DETAILED BALANCING



net radiative and collisional downward rates (Wien approximation)

$$n_e n_p - n_e n_H = \frac{dJ}{dt} - n_e n_H \left( \frac{dJ}{dt} \right)_{\text{coll}}$$

zero for  $S = 2$ ,  $\rightarrow$  no heating/cooling

$$n_e n_H - n_e n_p = n_e n_H \left( \frac{dJ}{dt} - 1 \right) = k_{10,9} n_H \left( 1 - \frac{J}{I} \right)$$

zero for  $n = 1$ ,  $n = 10^7$

dipole approximation for atom collisions with electrons (Van Regemorter 1962)

$$C_{10} = 2.16 \left( \frac{R_{\infty}}{T} \right)^2 T^{-1/2} N_e f$$

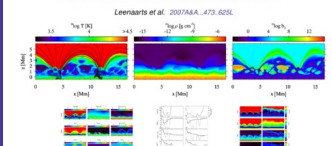
Einstein relation

$$C_{10} = C_{01} \frac{g_0}{g_1} e^{-E_{10}/kT}$$

$C_{10}$  is not very temperature sensitive (any collider will do);  $C_{10}$  has Boltzmann sensitivity

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NON-E HYDROGEN IONIZATION IN 2D MHD SHOCKS



- in shocks Ly $\alpha$  has  $S=I$  from high  $T$  (fast balancing) and  $N_e$  (10% H ionization)
- retarded collisional balancing in Ly $\alpha$ :  $n_2$  hangs near high shock value  $n_2 = n_1^{1/2}$
- gigantic post shock  $\rightarrow$  overpopulations versus LTE ('S-B underestimates')
- yet larger post shock overionization from hydrogen log Balmer balancing
- no Lyman RT: green arches artifacts, no lateral  $N_e$  boost from Ly $\alpha$  scattering

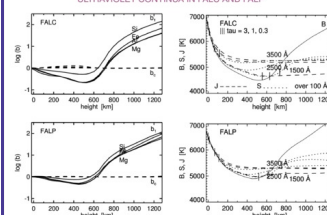
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RECENT DEVELOPMENTS IN PRO LINE SYNTHESIS

- RH code: Ultenbroek 2004ApJ...657..388U
  - Rybicki & Hummer: not A(S) but  $\Psi(I)$  iteration: preconditioning
  - overlapping lines
  - 1D, 2D, 3D, spherical versions
- RH V.1.5D: Pereira & Ultenbroek 2015A&A...574A...3P
  - 1.5D = column-by-column
  - massively parallel
  - also molecular lines (but Kurucz lines in LTE)
- single-dependent redistribution: Leenarts et al. 2017A&A...544A..109L
  - good summary PRD theory and equations
  - non-stationary atmosphere requires angle-dependent PRD
  - hybrid approximation: transform to gas parcel frame, assume angle-averaged PRD (no angle dependent from deep isotropy), transform back
- towards *Bifrost* PRD: Sahnoune & Leenarts 2017A&A...587A..453
  - hybrid approximation for small memory
  - linear frequency interpolation for speed
  - 252-252-496 grid, 1024 CPUs: 2 days for Mg II  $k$ : double
- next: 3D PRD with *multiGrid* (Bergien & Leenarts 2017A&A...319A..118B)

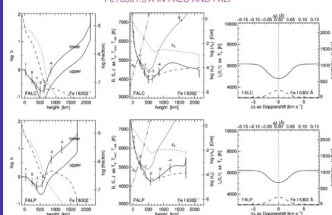
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ULTRAVIOLET CONTINUA IN FALC AND FALP



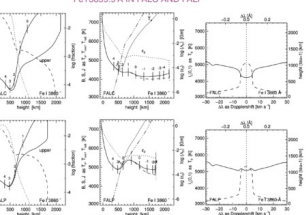
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Fe I 6301.5 Å IN FALC AND FALP



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Fe I 3859.9 Å IN FALC AND FALP



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