Uncertainties in atomic data and how they propagate in STELLAR chemical abundances:

Li & Na

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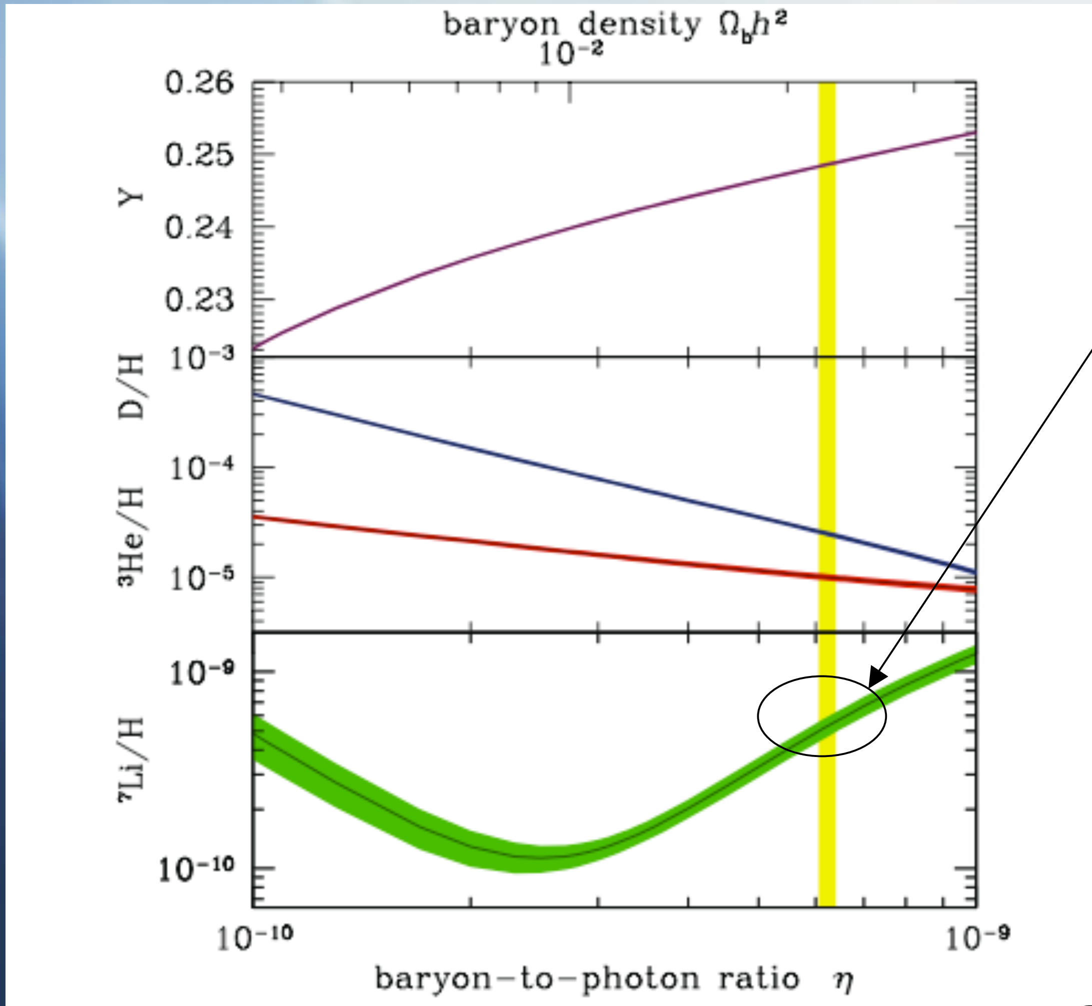
Astrophysical motivation: Li

- Complex chemical evolution:
  - Big Bang nucleosynthesis
  - Cosmic ray spallation
  - Stellar nucleosynthesis -- destruction AND production in stars.
  - Surface evolution a sensitive probe of internal stellar structure -- convection, turbulence, rotation, gravity waves, microscopic diffusion… Li used for age determination.

The cosmological Li problem



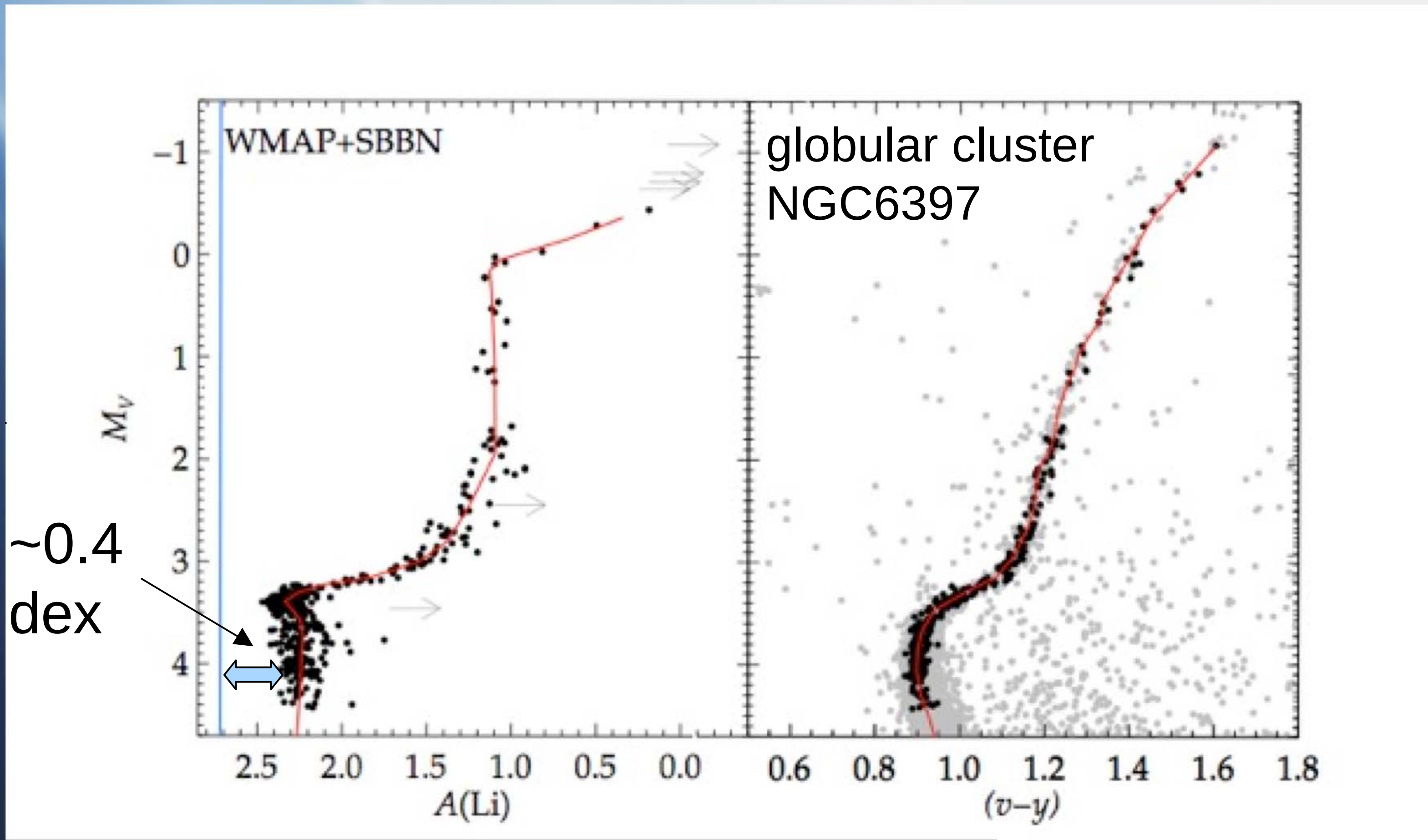
SBBN + WMAP

$$A(Li) = \log\left(\frac{N(Li)}{N(H)}\right) + 12$$

$$= 2.72 \pm 0.06$$

Cyburt et al 2008

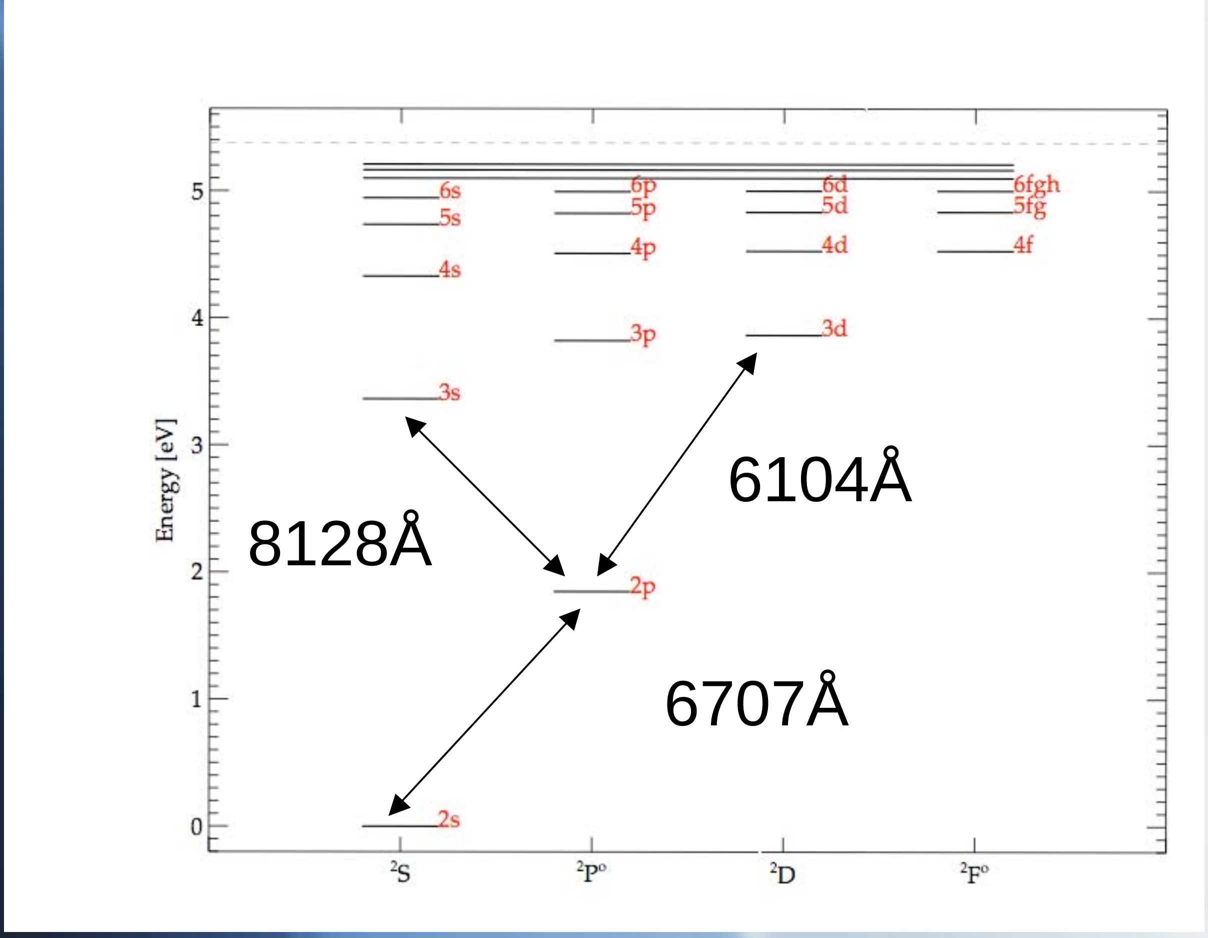
The cosmological Li problem



Lind et al (2009b)

Li model atom

- 21 energy levels
- 113 optically allowed bound-bound transitions
- ~200 bound-bound collisional transitions (e & HI)



Lind et al 2009a

Atomic data: energies and radiative transitions for l<=3

	Experiments	Calculations
Energy levels	Plenty	TOP base Peach et al (1988)
Oscillator strengths, lifetimes	Gaupp et al (1982) Hansen et al (1983)	TOP base Yan et al (1998)
Photoionisation cross-sections	Baig, Amin, Hussain, Saleem, 2006-2007	TOP base

Atomic data: energies and radiative transitions for l<=3

Yan et al. 1995

TABLE II. Comparison of lithium $2\,^2S$-$2\,^2P$ oscillator strength. The numbers next to the authors' names are dates, i.e., (1973), etc.

Author	Method	Reference	f (length)	f (velocity)
	Theory			
Ahlenius and Larsson (73)	Hylleraas	[13]	0.748	0.758
Sims *et al.* (76)	CI-Hylleraas	[14]	0.747 59	
Lindgård and Nielsen (77)	Coulomb approx.	[15]	0.741 2	
Cheng *et al.* (79)	MCDF	[16]	0.765 6	
Fischer (88)	MCHF	[17]	0.747 97	0.748 71
Peach *et al.* (88)	Opacity project	[18]	0.747 5	
Blundell *et al.* (89)	MBPT	[19]	0.746 7	0.747 1
Mårtensson-Pendrill and Ynnerman (90)	Coupled-cluster	[20]	0.747 1	
Theodosiou and Curtis (91)	Coulomb approx.	[21]	0.741 45	
Weiss (92)	CI	[22]	0.747 8	0.749 8
Pipin and Bishop (92)	CI-Hylleraas	[23]	0.747 0	
Tong *et al.* (93)	MCHF	[24]	0.747 2	0.747 0
Chung (93)	FCPC	[25]	0.747 04	0.747 04
Ponomarenko and Shestakov (93)	Green function	[26]	0.754	
Brage and Fischer (94)	MCHF-CCP	[27]	0.747 2	
Barnett *et al.* (95)	QMC	[28]	0.743 1(6)	
This work ($M=\infty$)			0.746 957 2(10)	0.746 957 1(54)
This work (finite M)[a]			0.746 787 1(10)	0.746 789 2(54)
	Experiment			
Gaupp *et al.* (82)	Laser excitation	[2]	0.741 6(12)	
Carlsson and Sturesson (89)	Delayed coincidence	[3]	0.743 9(55)	
McAlexander *et al.* (95)	Photoassociation	[4]	0.750 2(44)	

[a]Result for ^{7}Li with $m/M=7.820\,814\,7\times10^{-5}$.

Atomic data: energies and radiative transitions for l<=3

Qi, Yue-Ying et al 2009

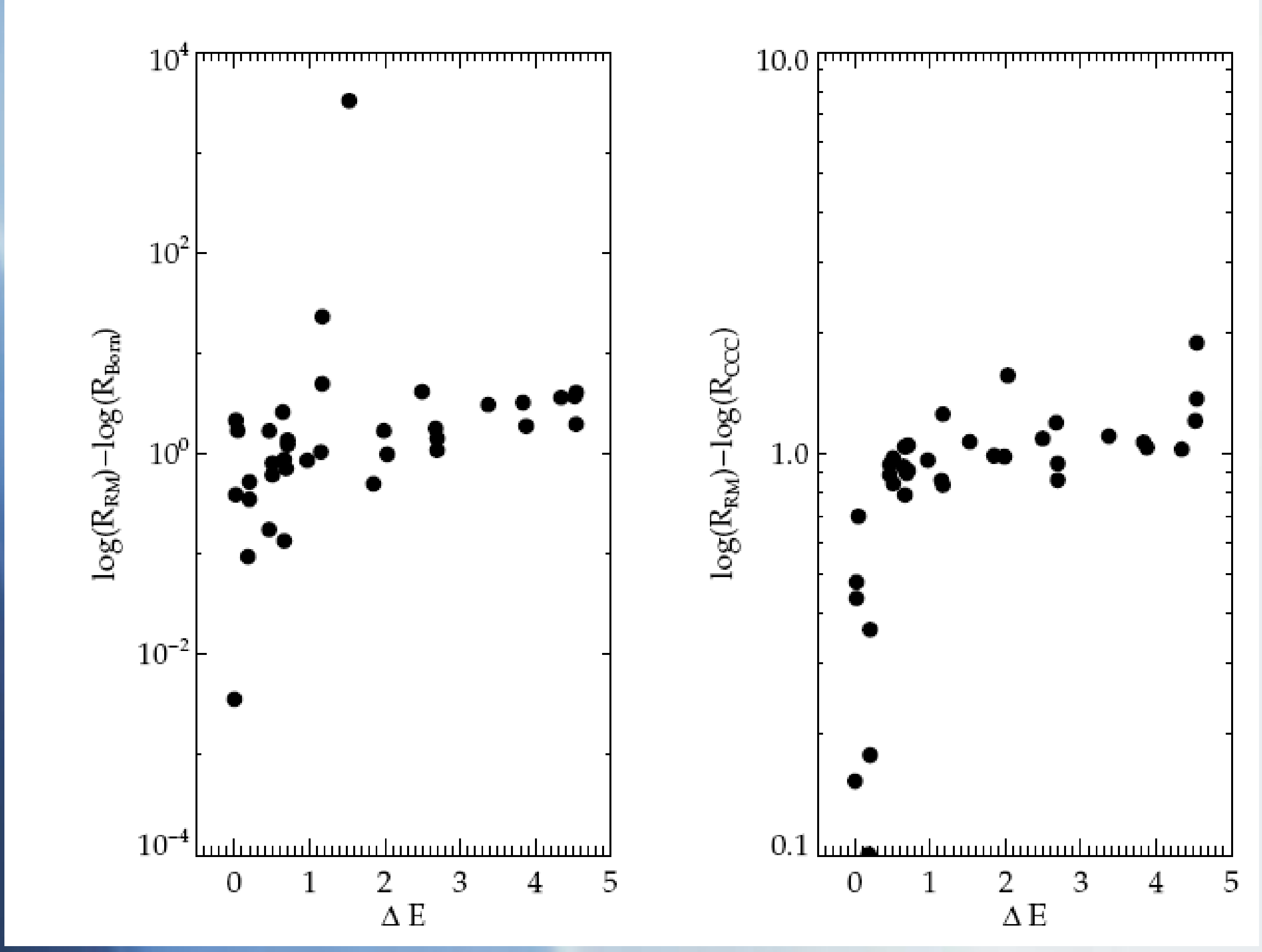
Table 1. Photo-ionization cross sections at or close to the thresholds of ground state and excited states of lithium atoms and the photo energies are given in units of wavelength nm.

State	Wavelength (nm)	Photo-ionization cross section (Mb)		
		Present work	Previous theoretical results	Experimental results
$2s$	229.95(threshold)	1.43	1.4,[6] 1.50[7]	1.54 ± 0.23 [5]
$2p$	350.67(threshold)	15.75		
	349.8	15.65	15.2[8]	14.8 ± 2.6[1]
$3s$	613.15(threshold)	1.32		1.32 ± 0.24[4]
$3p$	796.55(threshold)	28.73		
	760	25.79		28.5 ± 4.3[3]
$3d$	819.88(threshold)	18.29		
	819.4	18.29	17.5,[9] 18.2[10]	
	780	15.89		16.9 ± 3.0[1]
$4s$	1178.05(threshold)	1.22		
	1064	1.30		1.15 ± 0.21[2]
$4p$	1425.32(threshold)	41.94	41.70[10]	
	1064	22.48		23.9 ± 4.3[2]
$4d$	1457.54(threshold)	36.01		
	1456.9	36.01	36.20[10]	
	1064	15.08		18.7 ± 3.4[2]
$4f$	1458.03(threshold)	18.73		
$5s$	1925.02(threshold)	1.12		
$5p$	2236.57(threshold)	55.76		
$5d$	2277.49(threshold)	53.44		
$5f$	2278.17(threshold)	39.83		
$5g$	2278.18(threshold)	16.77		

Atomic data:
electron impact excitation and ionisation

- R-matrix (Osorio et al 2010)
- CCC (Schweinzer et al 1999)
- General recipes
  - When more rigorous calculations are missing, simple semi-empirical formulae are applied
  - Corrections to Born approximation at low impact parameters (Park 1971, Seaton 1962 (IPA), Van Regemorter 1962).

Atomic data:
electron impact excitation and ionisation



Rate coefficients at T=6000K

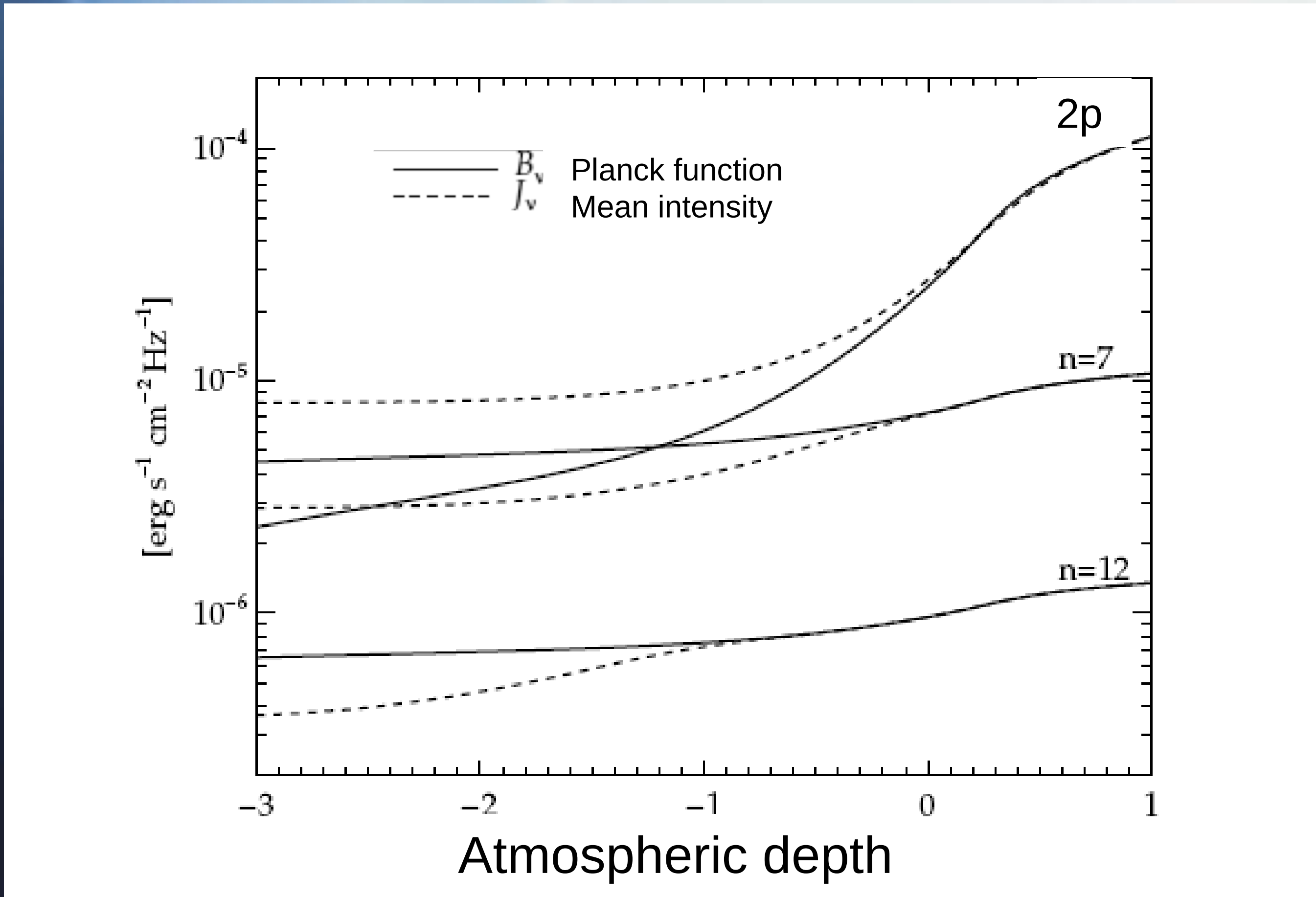
Atomic data: hydrogen impact excitation and charge exchange reactions

- Belyaev & Barklem (2003), Croft et al (1998):
  - rate coefficients for hydrogen impact excitation:

    1-6 orders of magnitude lower than Drawin (1968) recipe
  - Li + HI <--> Li^+ + H^- (Charge exchange)

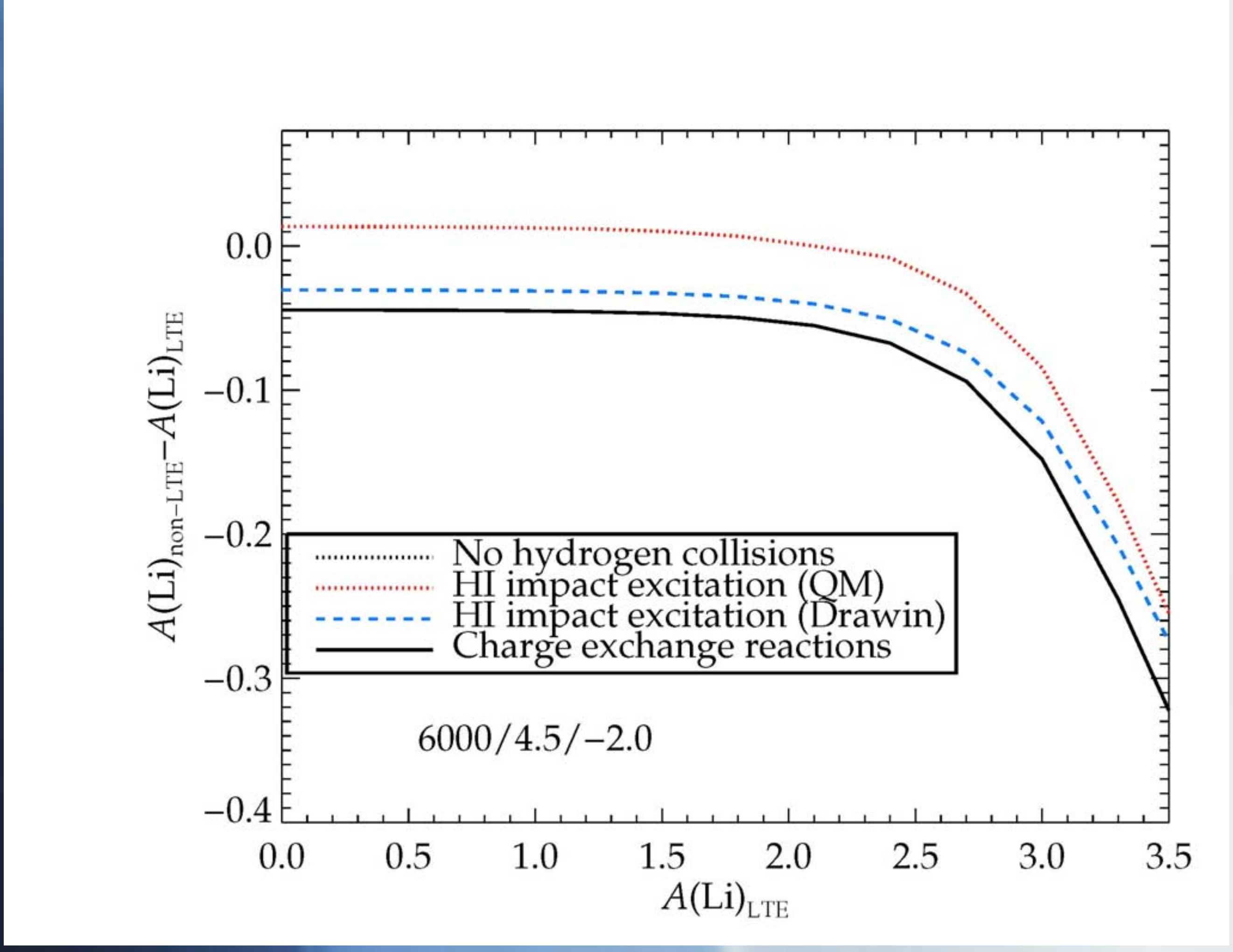
    Previously neglected completely.

Departures from LTE



The superthermal ultra-violet radiation field 'overionise' LiI

The impact of hydrogen collisions



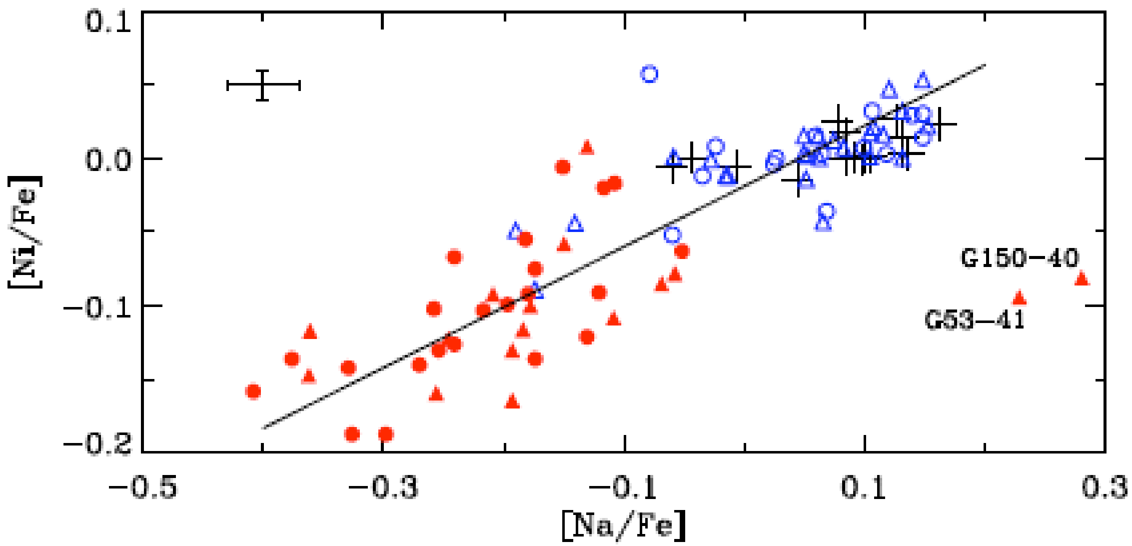
Collisional excitation by H has small impact on Li abundances using proper QM calculations

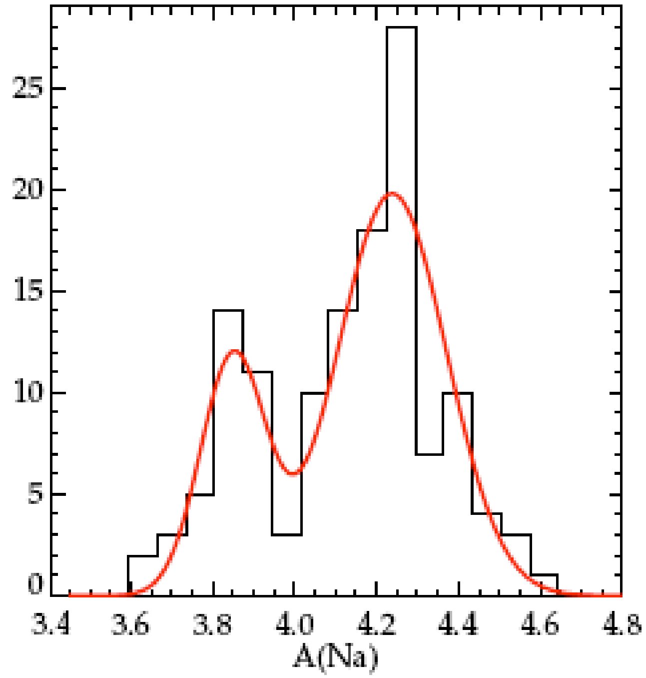
Charge exchange much more influential

Lind et al (2009a)

Na as population discriminator

Nissen & Schuster (2010)
Halo field stars

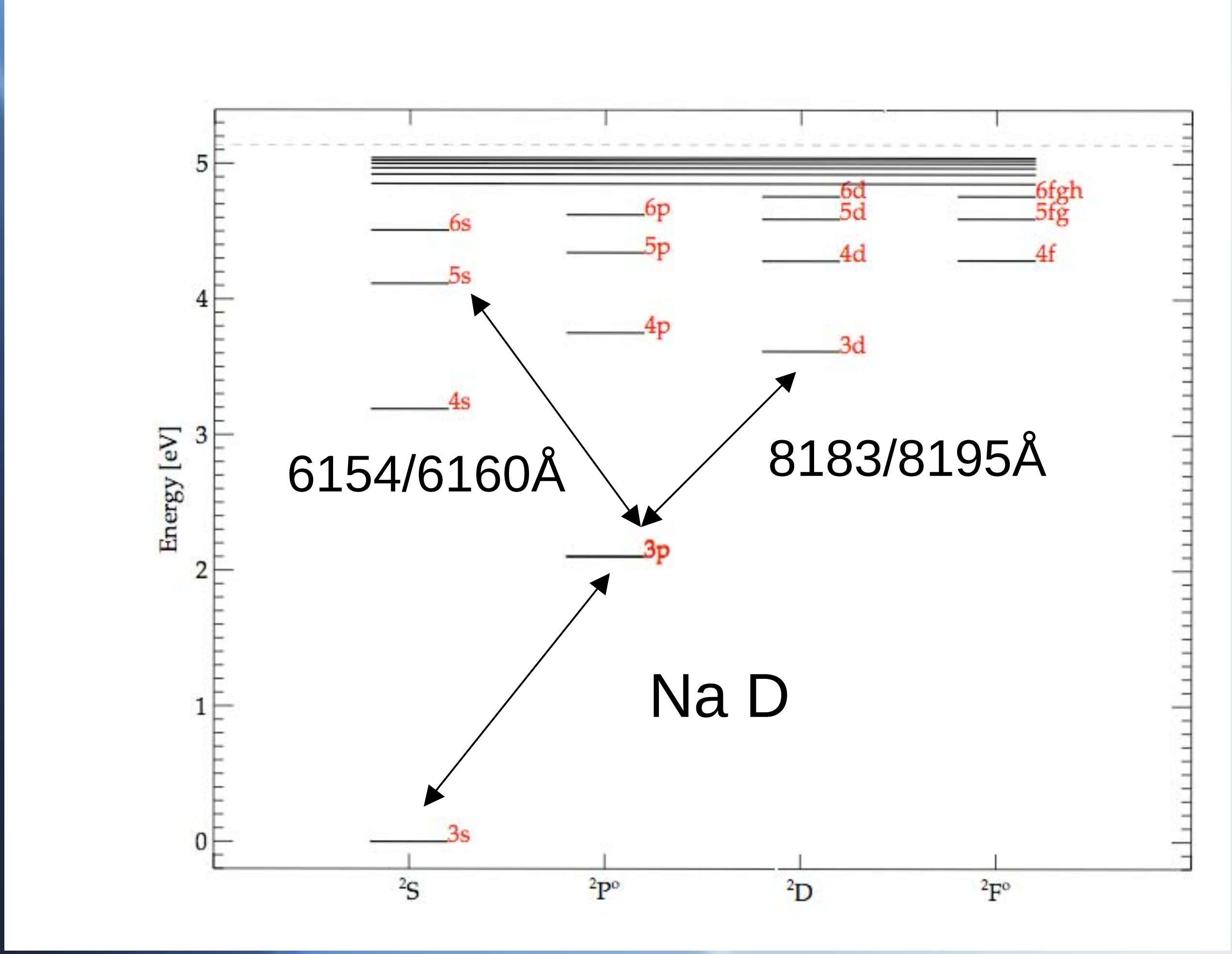




Lind et al (2010a)
Globular cluster
NGC6397

Multiple production channels, thereby useful to separate stellar generations

Na model atom



- 23 energy levels
- 166 allowed bound-bound transitions
- ~220 bound- bound collisional transitions

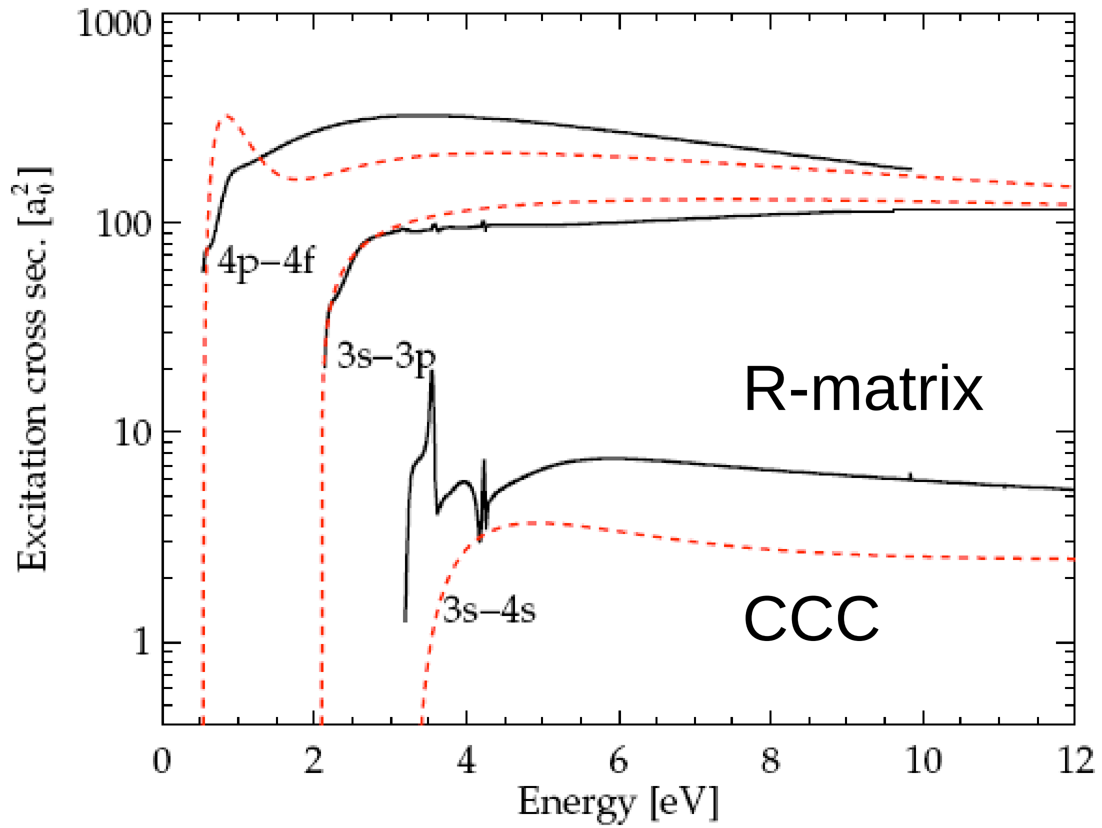
  (e & HI)

Lind et al 2010b

Atomic data: energies and radiative transitions for l<=3

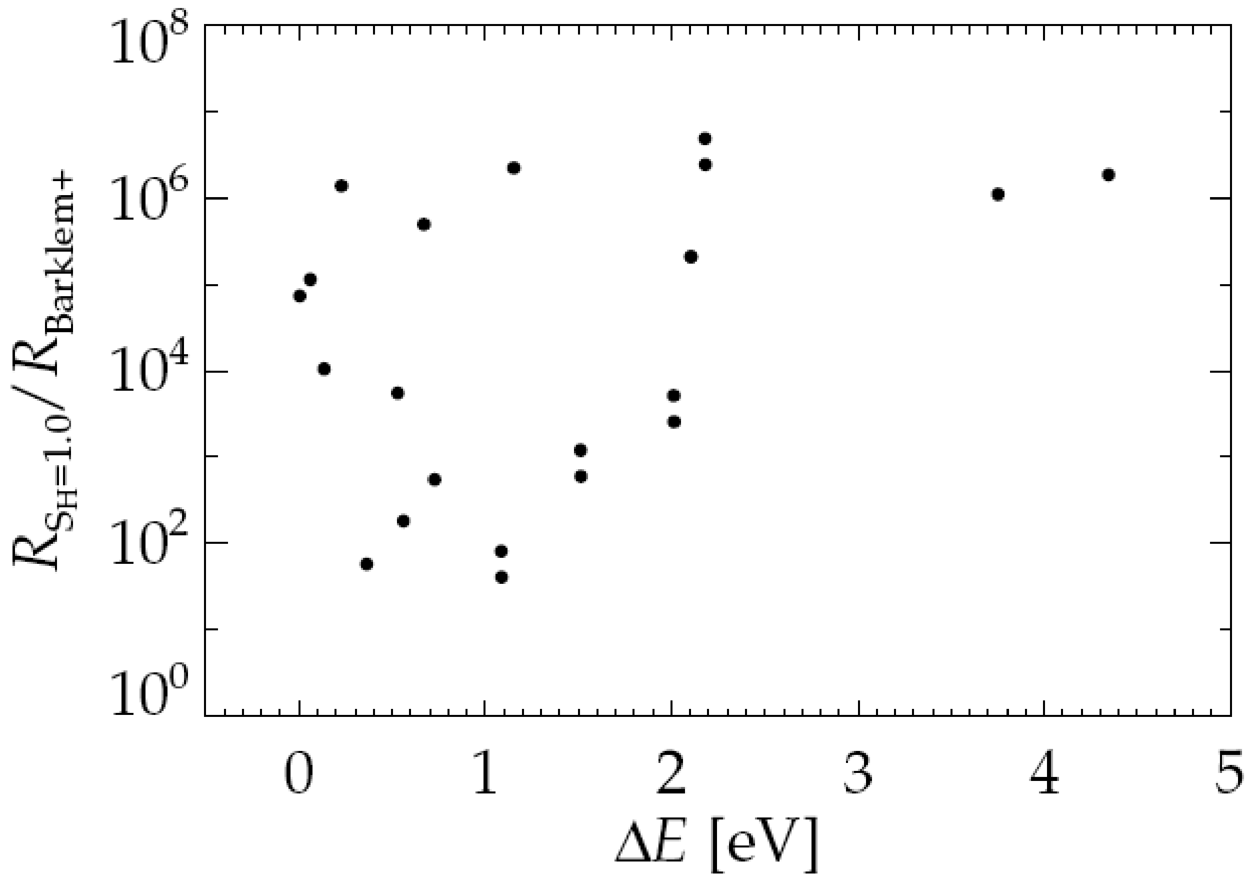
	Experiments	Calculations
Energy levels	see refs in Sansonetti 2008	TOP base K.T. Taylor
Oscillator strengths, lifetimes	see refs in Sansonetti 2008	TOP base C. Froese Fischer
Photoionisation cross-sections	Wippel et al 2001 Amin et al 2006	TOP base

Atomic data: collisional transitions



Na+e cross-sections Gao et al, Feautrier et al, Igenbergs et al

Atomic data: collisional transitions

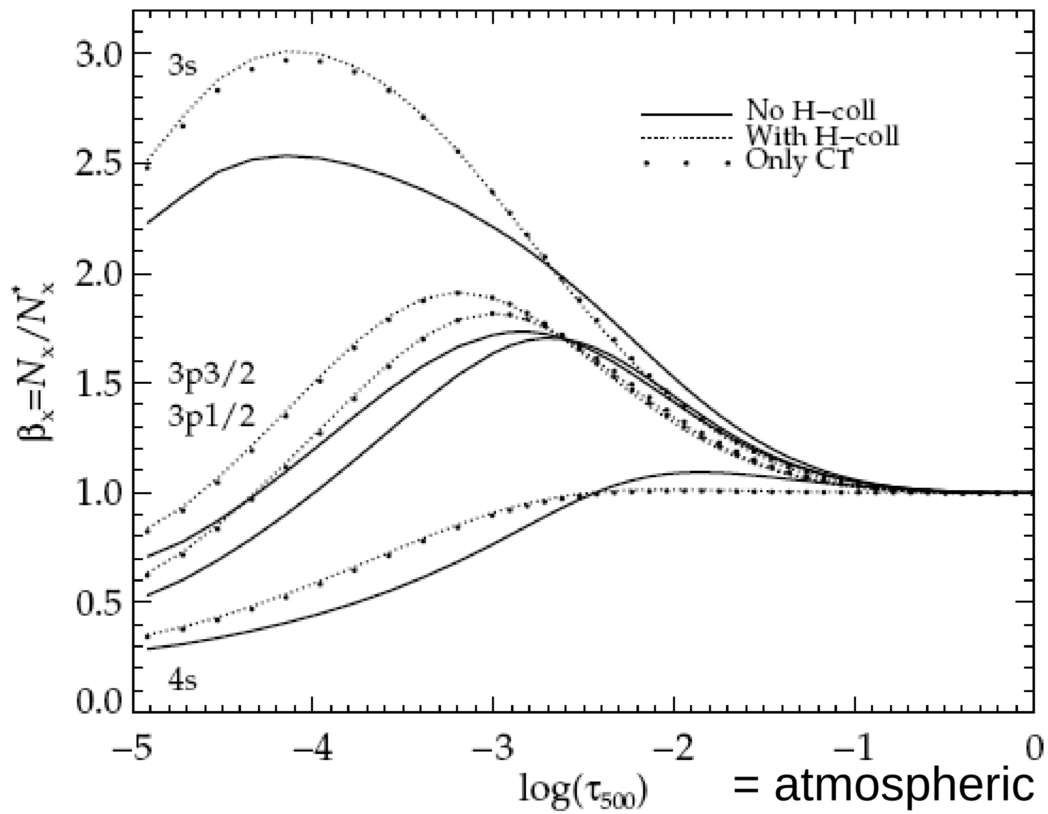


Na+H rate coefficients

Belyaev et al 2003

The impact of hydrogen collisions (Sun)

Non-LTE/LTE number density

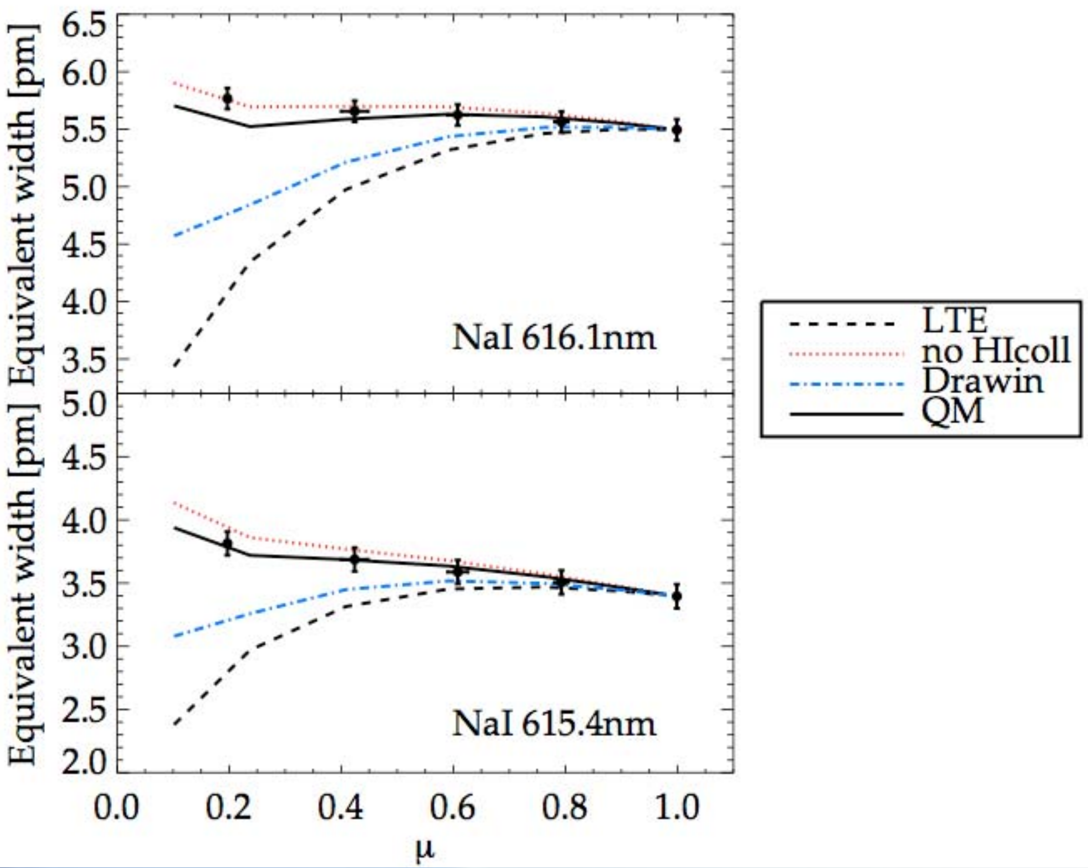


= atmospheric optical depth

Collisional excitation by H has small impact on Na abundances using proper QM calculations

Charge exchange much more influential

Centre-to-limb variation as test of model atom (and atmosphere)



Line strength variation of solar Na lines as function of viewing angle

Conclusions

- Li and Na are highly interesting elements to trace Galactic chemical evolution, Big Bang nucleosynthesis, star formation, stellar evolution, stellar ages etc.
- High accuracy abundances clearly require non-LTE analysis.
- The non-LTE abundances appear very robust with respect to estimated uncertainties in radiative and collisional data for these simple atoms. This is certainly not true for all elements.

Wish list

- An extension of TOPbase to more neutral atoms and singly ionised species such as P & K, iron-peak (Sc, Ti, V, Cr, Mn, Co, Ni, Zn) and neutron capture elements (Sr, Y, Zr, Ba, Eu).
- Quantum mechanical calculations for HI collisions are needed for MANY more elements, or at least a rigorous investigation into the expected impact of such collisions for different species. We have Li+H, Na+H. We need Mg+H, O+H, Ca+H, Fe+H…

References

Amin, N, Mahmood, S., Anwar-Ul-Haq, M.; Baig, M. A. 2006. Journal of Quant. Spectr. and Rad. Transfer, 102, 269
Amin, N.; Mahmood, S.; Saleem, M.; Kalyar, M. A.; Baig, M. A., 2006. The European Physical Journal D, 40, 331- 33
Barklem, P. S., Belyaev, A. K., Dickinson, A. S., & Gadea, F. X. 2010, Astronomy and Astrophysics, 519, A20+
Belyaev, A. K., Barklem, P. S., Dickinson, A. S., & Gadea, F. X. 2010, Physical Review A, 81, 032706
Belyaev, A. K. & Barklem, P. S. 2003, Physical Review A: General Physics, 68, 062703
Croft, H., Dickinson, A. S., & Gadea, F. X. 1999, Monthly Notices of the Royal Astronomical Society, 304, 327
Cyburt, R. H., Fields, B. D., & Olive, K. A. 2008, Journal of Cosmology and Astro-Particle Physics, 11, 12
Drawin, H.-W. 1968, Zeitschrift fur Physik, 211, 404
Feautrier, N., Han, X.-Y., & Lind, K. in preparation, Astronomy and Astrophysics
Gao, X., Han, X., Voky, L., Feautrier, N., & Li, J. 2010, Physical Review A: General Physics, 81, 022703
Gaupp et al. 1982. Physical Review A 26, 3351
Igenbergs, K., Schweinzer, J., Bray, I., Bridi, D., & Aumayr, F. 2008, Atomic Data and Nuclear Data Tables, 94, 981
Lind, K., Asplund, M., & Barklem, P. S. 2009a, Astronomy and Astrophysics, 503, 541
Lind, K., Primas, F., Charbonnel, C., Grundahl, F., & Asplund, M. 2009b, Astronomy and Astrophysics, 503, 545
Lind, K., Charbonnel, C., Decressin, T., et al. submitted, Astronomy and Astrophysics
Lind, K., Asplund, M., Barklem, P. S., & Belyaev, A. K. Submitted to Astronomy and Astrophysics
Nissen, P. E. & Schuster, W. J. 2010, Astronomy and Astrophysics, 511, L10+
Park, C. 1971, Journal of Quantitative Spectroscopy and Radiative Transfer, 11, 7
Peach, G., Saraph, H. E., & Seaton, M. J. 1988, Journal of Physics B Atomic Molecular Physics, 21, 3669
Sansonetti, J. E. 2008, Journal of Physical and Chemical Reference Data, 37, 1659
Schweinzer, J., Brandenburg, R., Bray, I. et al. 1999. Atomic Data and Nuclear Data Tables, 72, 239
Seaton, M. J. 1962, Proceedings of the Physical Society, 79, 1105
Qi, Y. Y.; Wu, Y.; Wang, J. G. 2009. Physics of Plasmas, 16, 033507
van Regemorter, H. 1962, Astrophysical Journal, 136, 906
Wippel, V., Binder, C., Huber, W. et al. 2001. The European Physical Journal D,17, 285
Yan, Z.-C., Tambasco, M., & Drake, G. W. F. 1998, Physical Review A: General Physics, 57, 1652
Yan, Z.-C.& Drake, G. W. F. 1995, Physical Review A: General Physics, 52, 4316