The Broadening of Spectral Lines by Collisions with Neutral Hydrogen Atoms in Cool Stars

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Scientific Motivation

Need accurate stellar chemical abundances from spectroscopy for many problems in modern astrophysics:

- Understanding the chemical and dynamical evolution of the Galaxy, e.g.:
  - Origin and evolution of bulge, thin and thick disks
  - Merger history
  - Astrophysical sites of nucleosynthesis processes
- Solar composition and its place in the solar neighbourhood
- Strong lines are often the best to use - in some cases, e.g. very cool stars, galaxies, there is no choice

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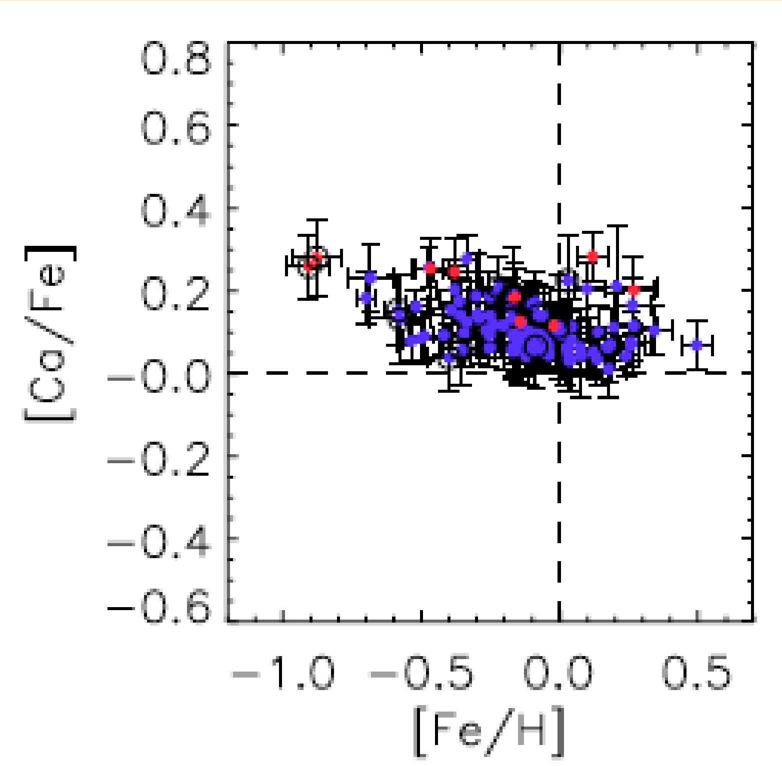
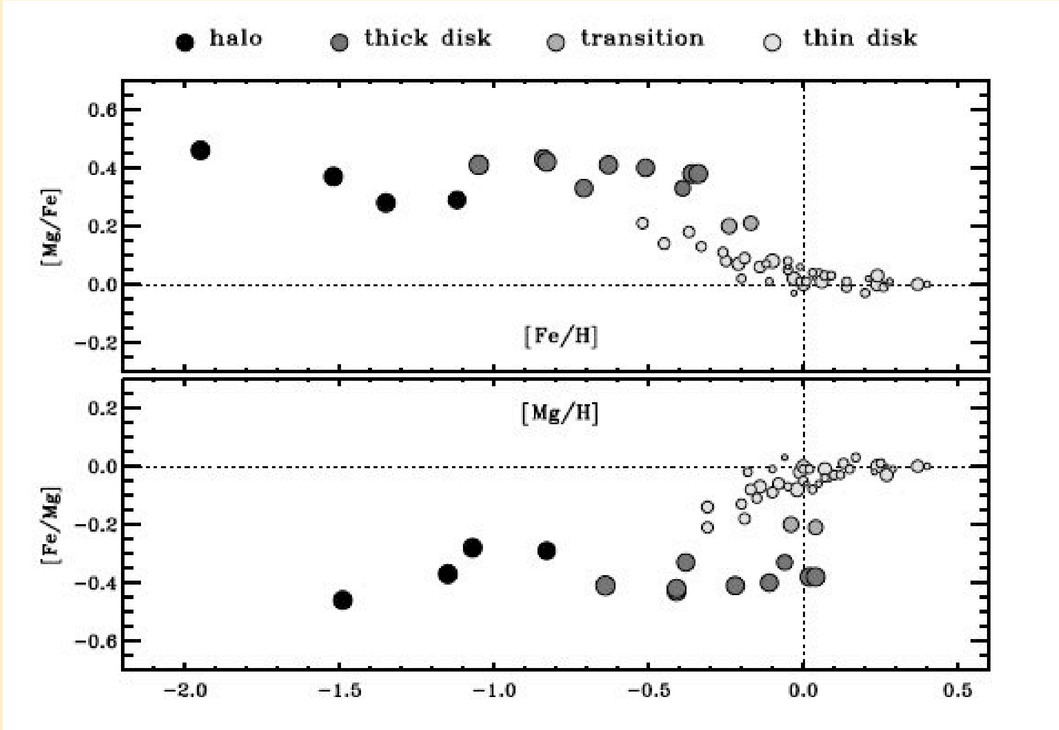
Scientific Motivation

Solar neighbourhood



Galactic Thick and Thin Disks



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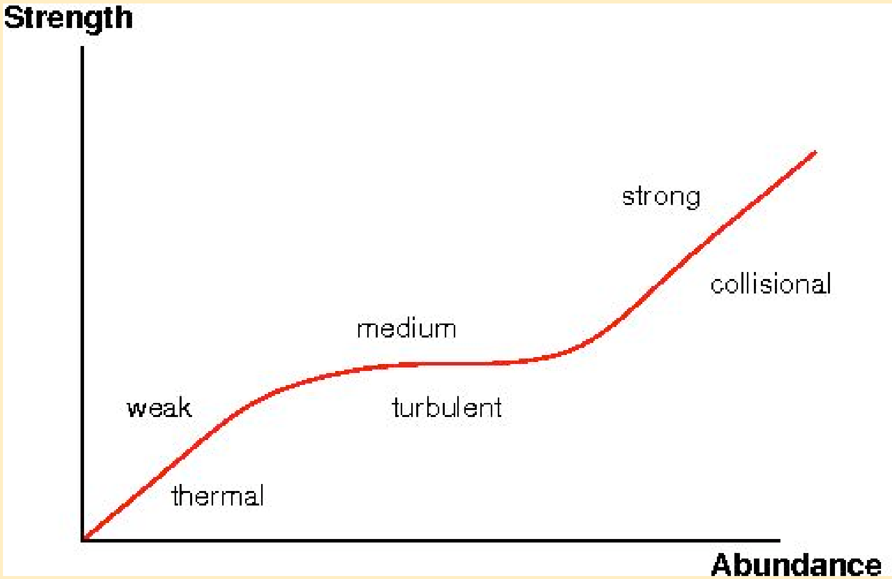
Scientific Motivation



Weak lines are susceptible to blends

Medium strength lines are saturated and insensitive to abundance

Strong lines typically have the best oscillator strengths, and often no choice: E.g. very cool stars, galaxies, distant stars

Cool star atmospheres dominated by neutral hydrogen, in its ground state

90% H, 9% He, 1% metals $$\frac{N_H}{N_e} \approx 10^4$$

Weight of number means generally dominant over electrons

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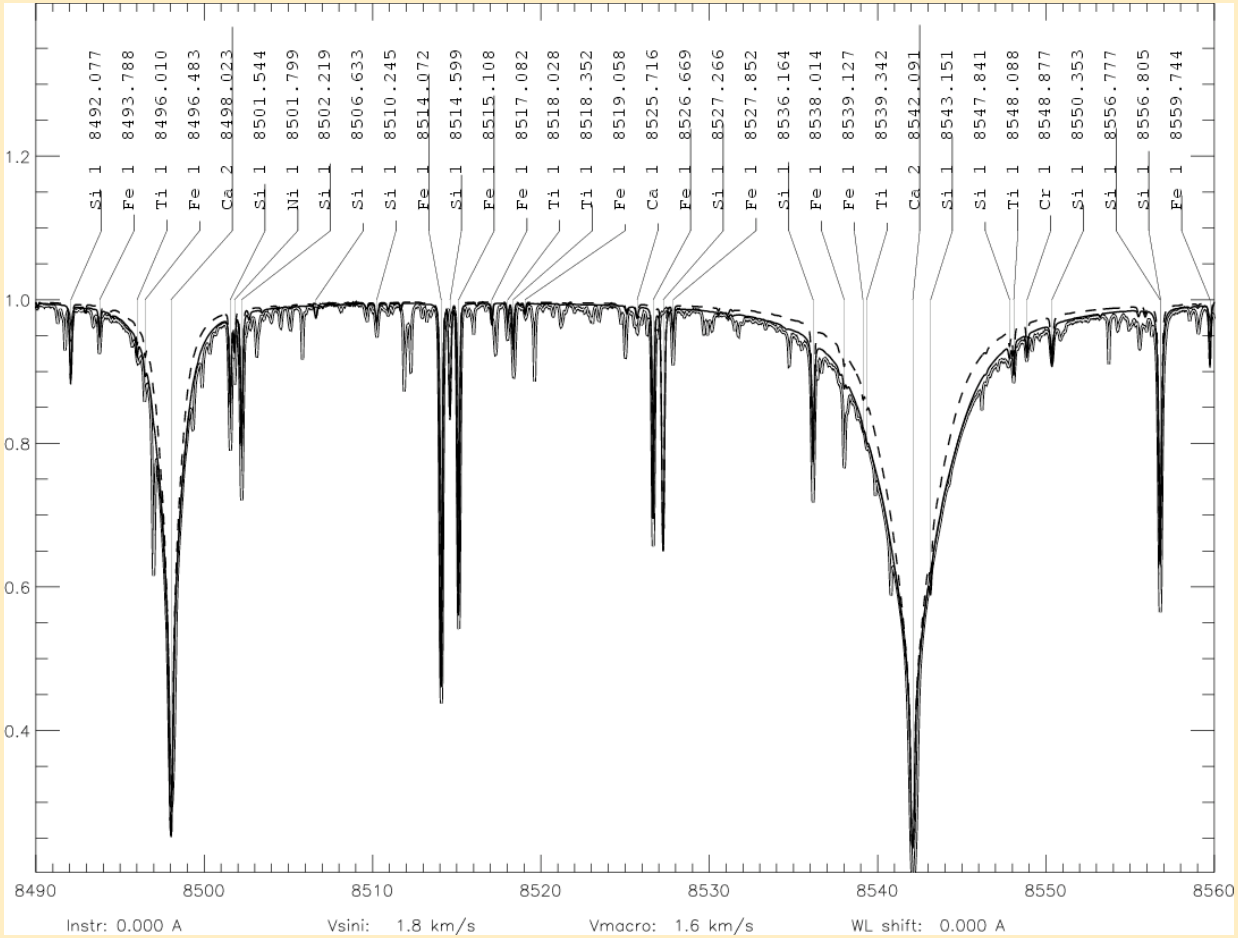
Scientific Motivation

- E.g. Ca II IR triplet in the Sun



History

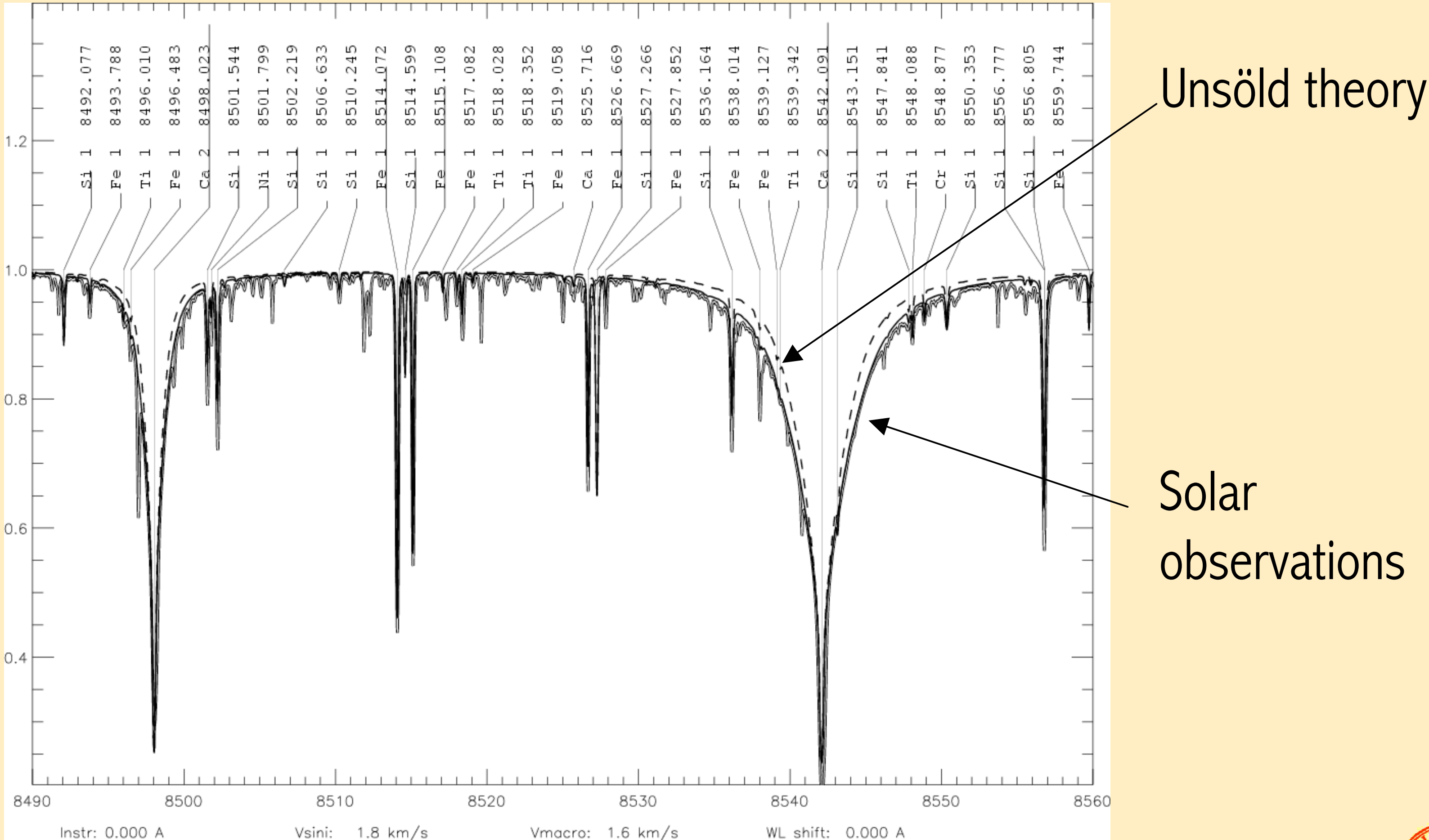
- Lorentz (1906) — Impulse theory (prior to QM)
- Weisskopf/London (1930's) — VdW potential, strong collisions
- Lindholm/Foley (1940's) — weak collisions, averaged interaction
- Unsöld (1950's) — apply VdW + approx, general formula

VdW = van der Waals $\Delta E \approx C_6 / R^6$

$$\Gamma = 17 \upsilon^{3/5} C_6^{2/5} N_H$$

- (1960's -) Accurate calculations for a few specific cases

Scientific Motivation



Need a fudge factor about 1 to 4 to fit solar lines

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Scientific Motivation

- Astrophysical evidence that Unsöld theory is inadequate
- Astrophysics needs a theory to compute data for a large number of lines of various elements (e.g. Fe, Ni, Mg, Ca, etc)
- Theory should ideally to be simple to use!

History

Lorentz (1906)	Impulse theory (prior to QM)
Weisskopf/London (1930's)	VdW potential, strong collisions
Lindholm/Foley (1940's)	weak collisions, averaged interaction
Unsöld (1950's)	apply VdW + approx, general formula
Brueckner (1970's)	numerical RSU perturbation theory
O'Mara (1970's)	analytic RSU perturbation theory
Anstee & O'Mara (1992)	removal of averaged interaction+more
Barklem & O'Mara (1998-)	extension to d and f states, and ions

ABO theory

- isolated lines
- impact approximation (Lorentzian profile)
- classical straight path approximation
- no fine structure (orbital angular momentum basis, *nlm*)
- no quenching

- Important part is the potentials:

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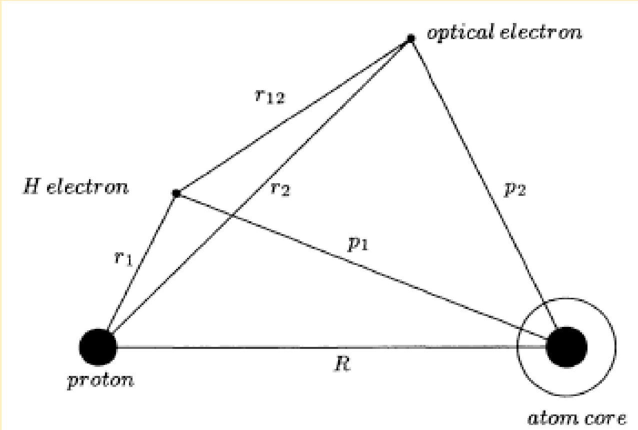
ABO theory: RSU potentials



$$V = \frac{1}{R} + \frac{1}{r_{12}} - \frac{1}{r_2} - \frac{1}{p_1}$$

Covalent partitioning
(Ionic partitioning neglected)

$$\Delta E = \langle i|V|i\rangle + \sum_{j\neq i} \frac{\langle i|V|j\rangle\langle j|V|i\rangle}{E_i - E_j}$$

Rayleigh-Schrödinger Perturbation Theory to 2nd order (no exchange)

$$\approx \langle i|V|i\rangle + \frac{1}{E_p(R)}\langle i|V^2|i\rangle$$

Unsöld approximations

$$E_p(R) \approx E_p(\infty)$$

$$\approx \langle i|V|i\rangle + \frac{1}{E_p}\int_0^\infty R_{nl}^2(p_2) I_{lm}(p_2,R)\, p_2^2\, dp_2$$

Analytic functions where all integrals except the final integral over the radial wavefunction have been performed

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ABO theory: RSU potentials

$$\Delta E = \langle i|V|i\rangle + \sum_{j\neq i} \frac{\langle i|V|j\rangle\langle j|V|i\rangle}{E_i - E_j}$$

$$\approx \langle i|V|i\rangle + \frac{1}{E_p(R)}\langle i|V^2|i\rangle$$

$$\approx \langle i|V|i\rangle + \frac{1}{E_p}\int_0^\infty R_{nl}^2(p_2) I_{lm}(p_2,R) p_2^2 dp_2$$

- Coulomb wavefunctions (n^*, l) $\quad n^* = \left[2E_{binding}\right]^{-1/2}$
- Unsöld approx $E_p = -2/\alpha_H = -4/9$

- Cross sections depend only on n^*, l ⟶ Independent of species!

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ABO theory: Results

Cross section

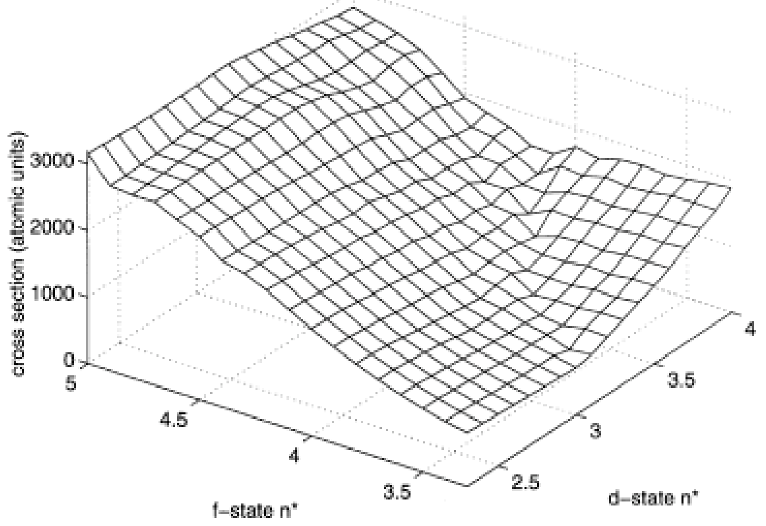

Figure 1. Plot of the cross-section for a perturber velocity of 10^4 m s^{-1} against the effective principal quantum number of the two states.

Velocity dependence

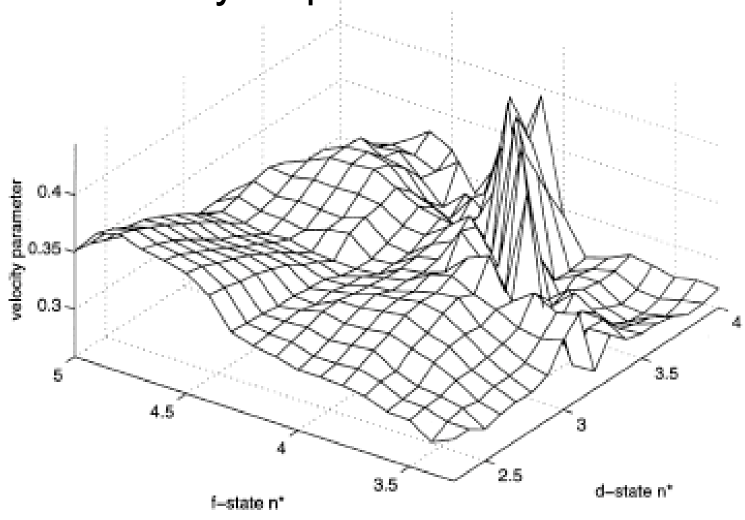

Figure 2. Plot of the velocity parameter α against the effective principal quantum number of the two states.

Tabulated results dependent only on effective principal quantum number

Simple velocity behaviour:

$$\sigma(v) = \sigma(v_0)\left(\frac{v}{v_0}\right)^{-\alpha}$$

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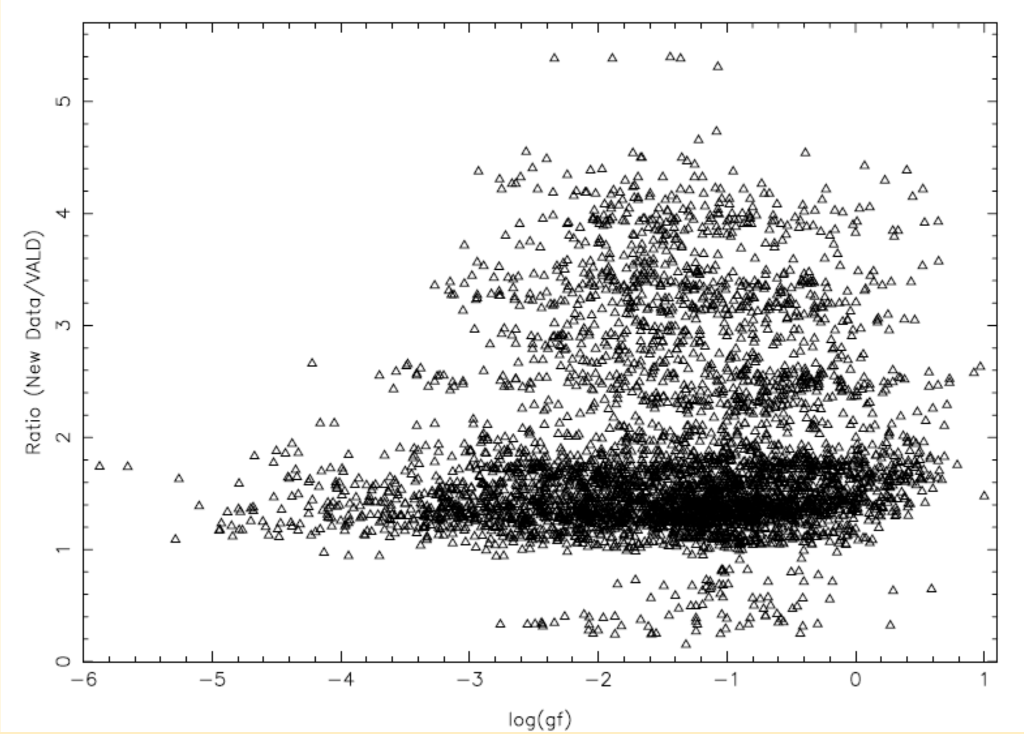
ABO theory: Results

Comparison with Unsöld’s theory for 4891 lines, Li to Ni:



Mean difference of 1.88, in rough agreement with astrophysical fudge factor commonly used of 2

Applications

• Application to lines of Na, Ca and Fe in the solar spectrum indicate uncertainties as low as 5%

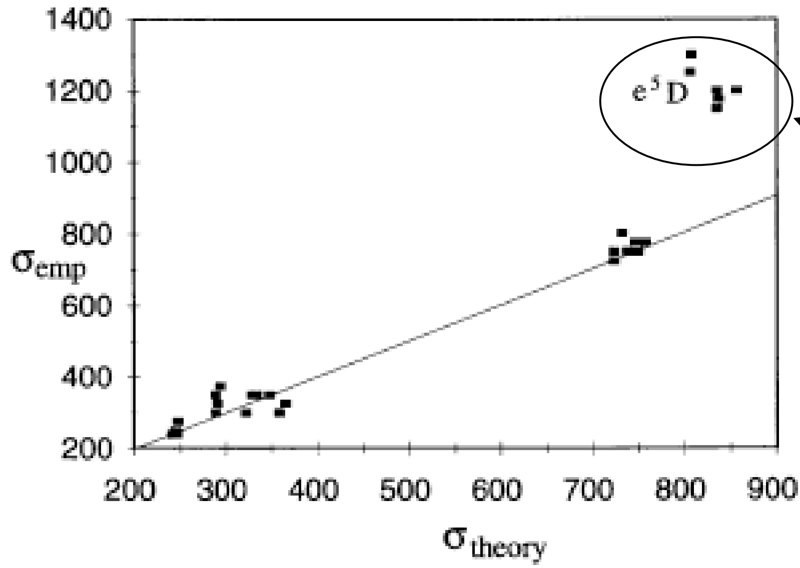


Figure 8. Empirical cross-sections obtained under the assumption that the solar abundance of iron is the same as in meteorites are plotted against theoretical cross-sections. The agreement is good except for lines with upper e^5D upper states.

Strongly Stark broadened

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Testing

• Comparison with more detailed calculations indicates uncertainties of order 5-20%.

Table 1. Comparison of line widths per unit perturber density (w/n_H in units 10^{-8} cm^3 rad s^{-1}) at 5000 K for resonance lines of Mg, Ca and Sr using different potentials and dynamics.

Dynamics →	Quantal	Semi-classical	Semi-classical	Semi-classical
Potentials →	MOLPRO	MOLPRO	ABO	Hybrid
Mg	1.13	1.10	1.01	1.25
Ca	1.23	1.24	1.10	1.28
Sr	1.49	1.48	1.18	1.48

No difference due to dynamics

10-20% due to potentials
-neglect of ionic crossing

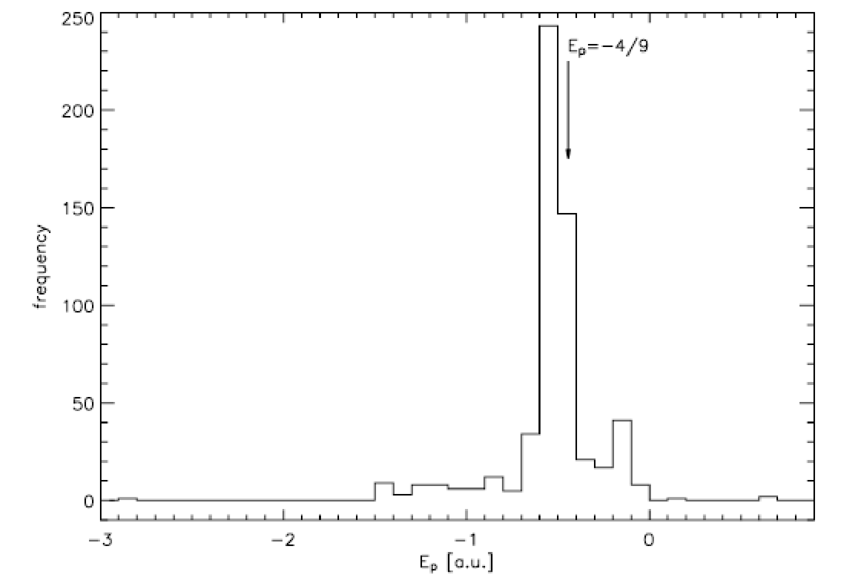
Extension to Ions

- Unsöld approx $E_p = -4/9$ is no longer valid
- Compute via

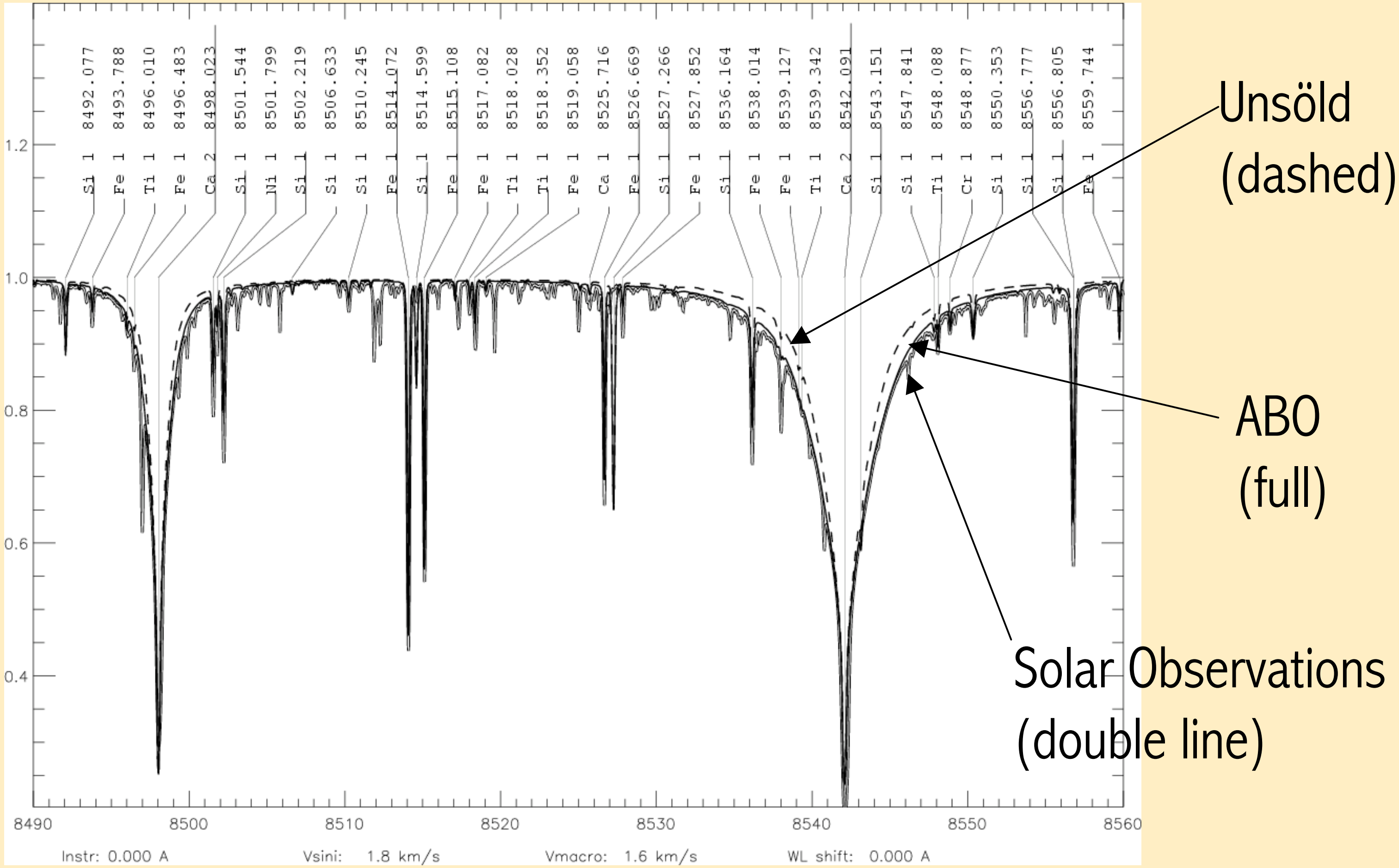
$$C_6 = \frac{3}{2} \sum_{k' \neq k} \sum_{l' \neq l} \frac{f^A_{kk'} f^H_{ll'}}{(\Delta E^A_{k'k} + \Delta E^H_{l'l}) \Delta E^A_{k'k} \Delta E^H_{l'l}},$$

$$E_{\rm p} = -\frac{2 \langle p_2^2 \rangle}{C_6}.$$

Large Scale calculations for Fe II using large scale semi-empirical atomic data calculations by Kurucz



Applications



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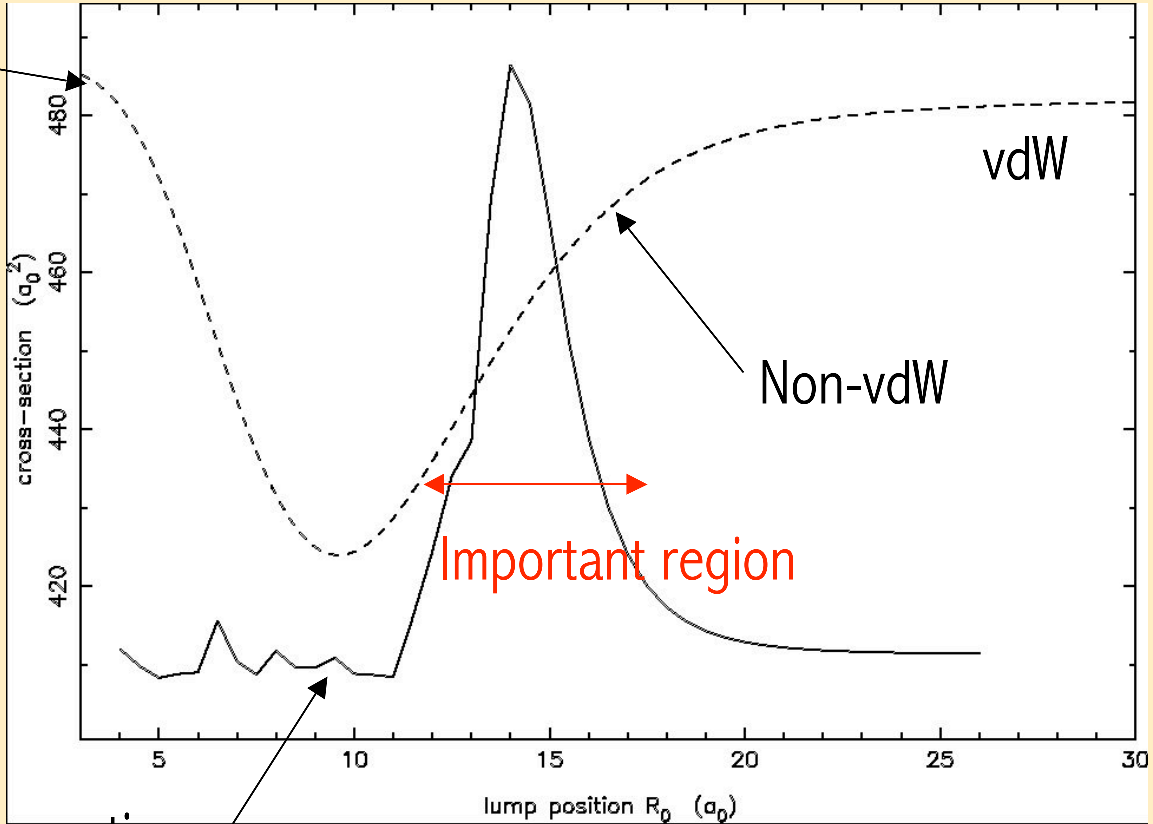
ABO theory: Why it works

"Intermediate" separations most important:

Potential
$\times R^6$



Response of cross section
To local perturbation in potential

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ABO theory: Why it works

Often, avoided ionic crossings either diabatic, or in the strong collision regime:

Crossing or Weisskopf Radius

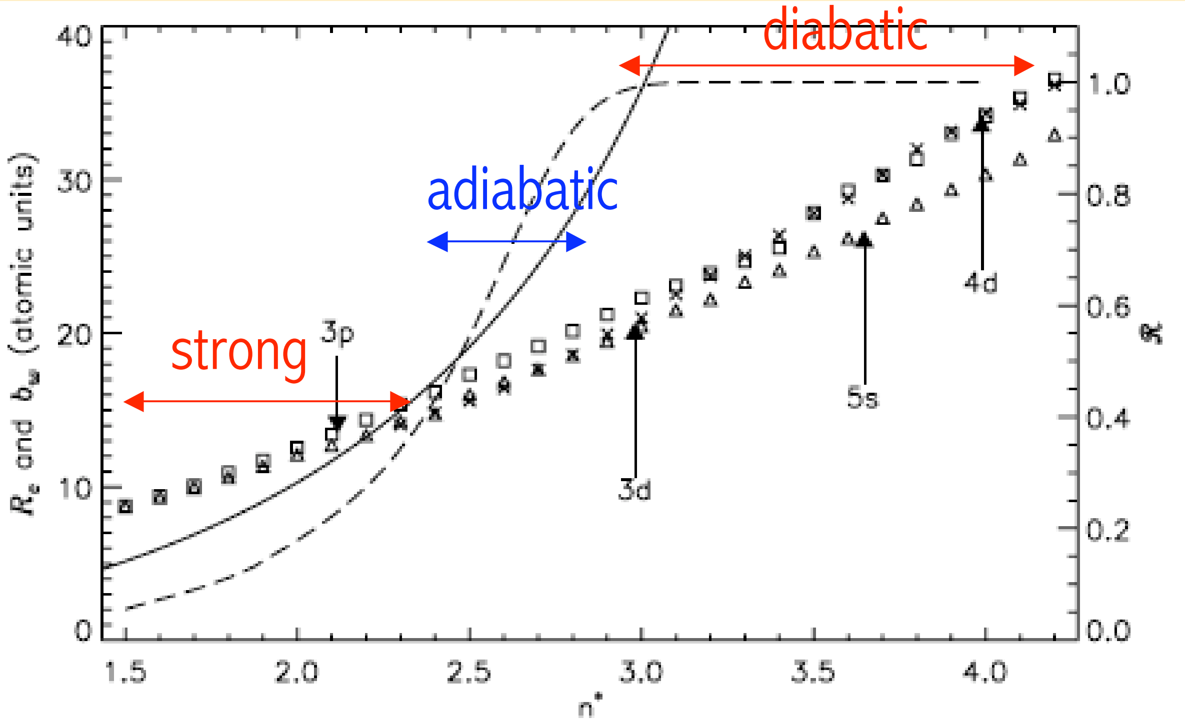

Figure 4. Plots demonstrating various collision regimes. b_w plotted against n^* for s states (triangles), p states (squares) and d states (crosses) for $v = 10^4$ ms^{-1}. The full curve is R_c. The reflection coefficient $\mathcal{R}$, is plotted as the dashed curve.

Impedance to tunnelling to ionic configuration

Summary of Results

• Tables of general data for transitions in neutrals involving s, p, d and f states
• Code for interpolating in tables available
• Table of 4891 strong lines, Li to Ni, mostly neutral + important ionised lines
• Table of 24188 Fe II lines
• Table of 13167 Cr II lines (unpublished)

• Also extended to H Balmer lines

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Conclusions

- ABO theory provides a general and widely applicable theory, with accuracy of better than 20%
- Strong lines can now be used with confidence in analysis of cool star spectra (no fudge factors)
- Theory is gaining wide use

- Future: inclusion of ionic state should lead to some improvement

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