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

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Acknowledgements

- Jim O'Mara
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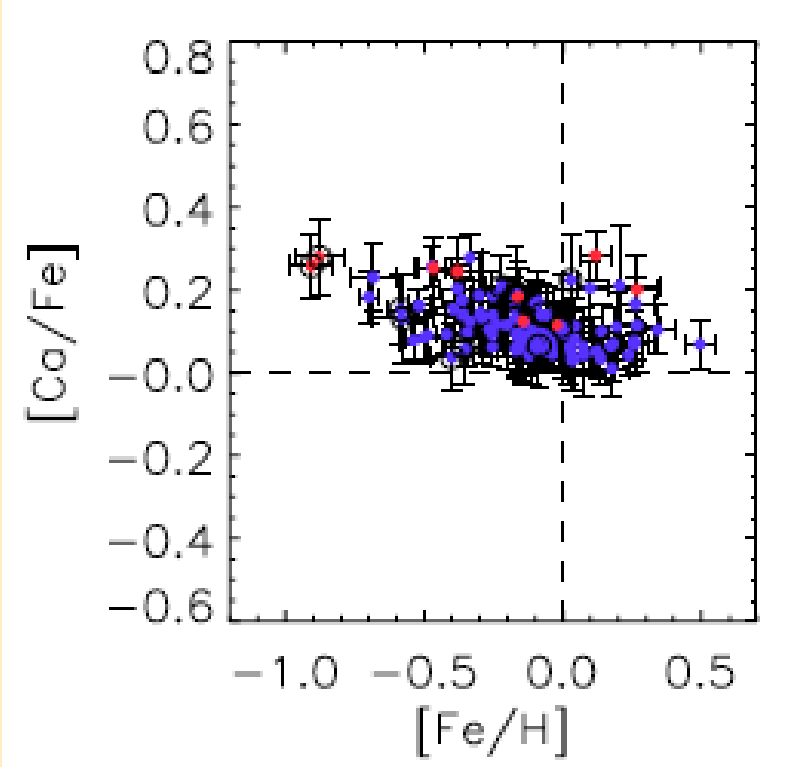
Scientific Motivation

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

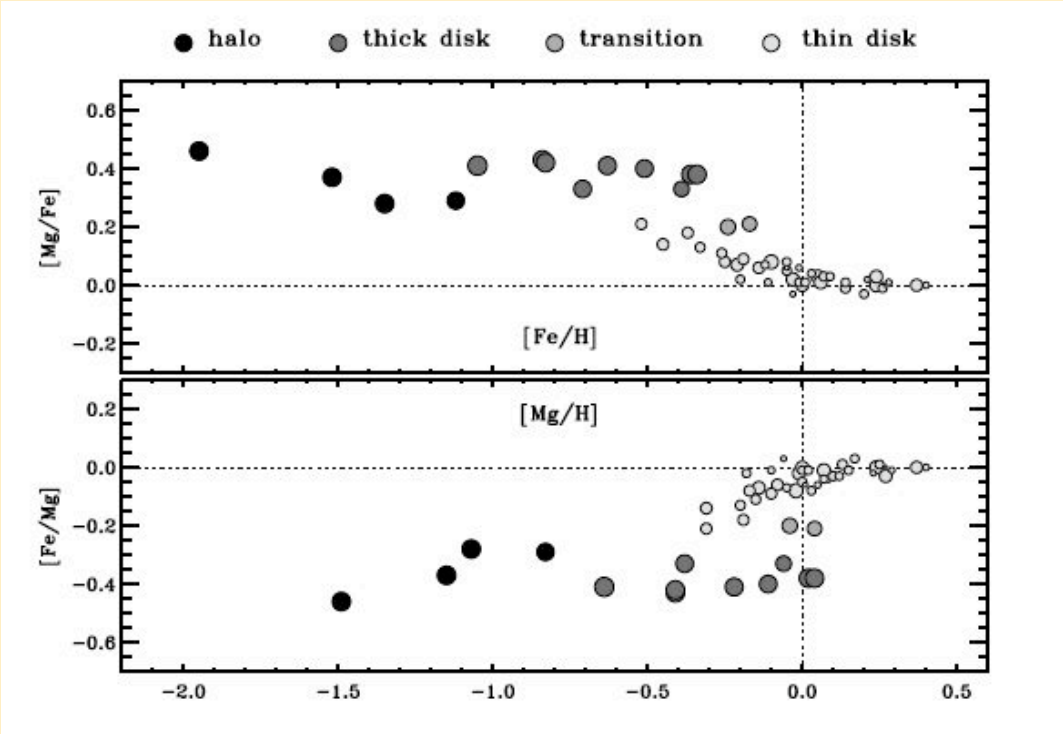
- Understanding the chemical and dynamical evolution of the Galaxy, e.g.:
  - Origin and evolution of bulge, thin and thick disks
  - Merger history
  - Astrophysical sites of nucleosynthesis processes
- Solar composition and its place in the solar neighbourhood
- Strong lines are often the best to use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

Scientific Motivation

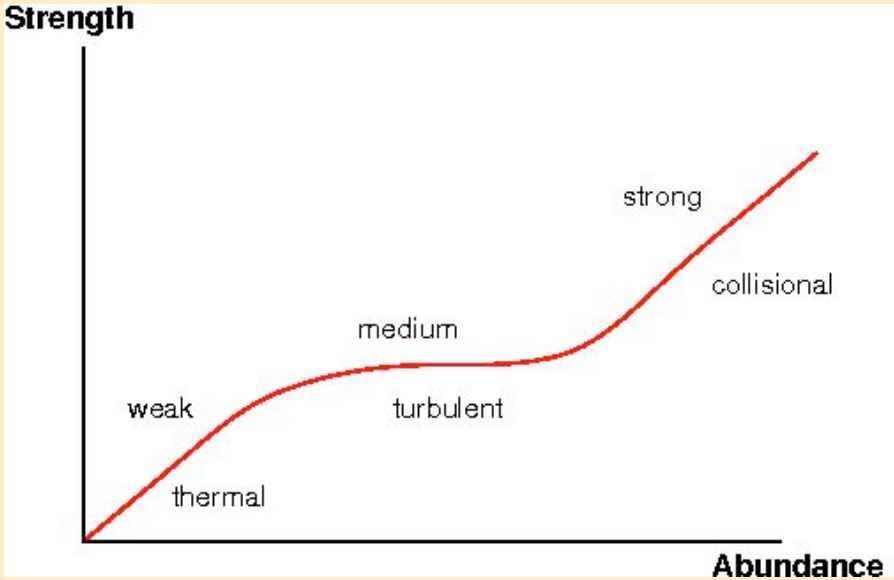
Solar neighbourhood



Galactic Thick and Thin Disks



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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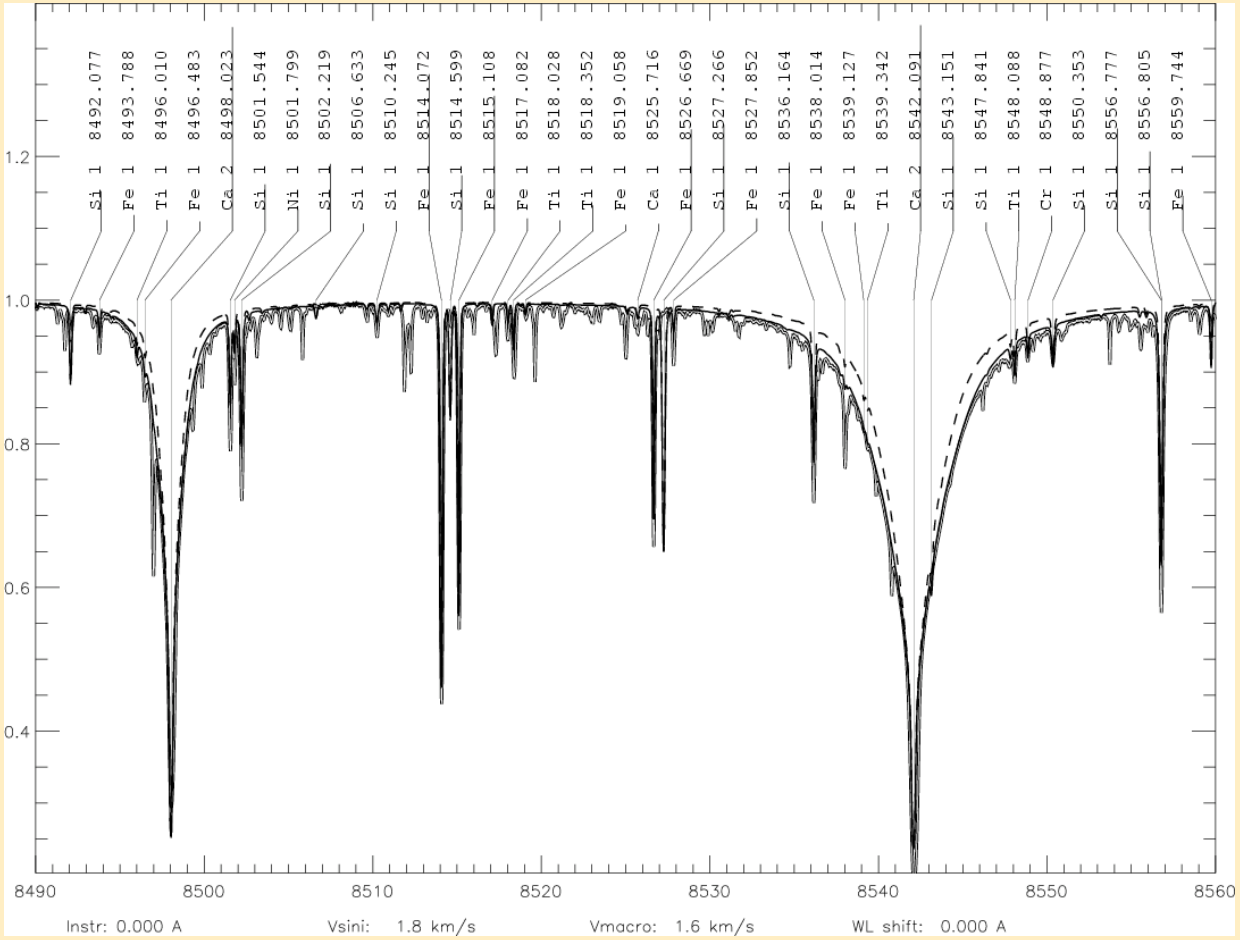
Scientific Motivation

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



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History

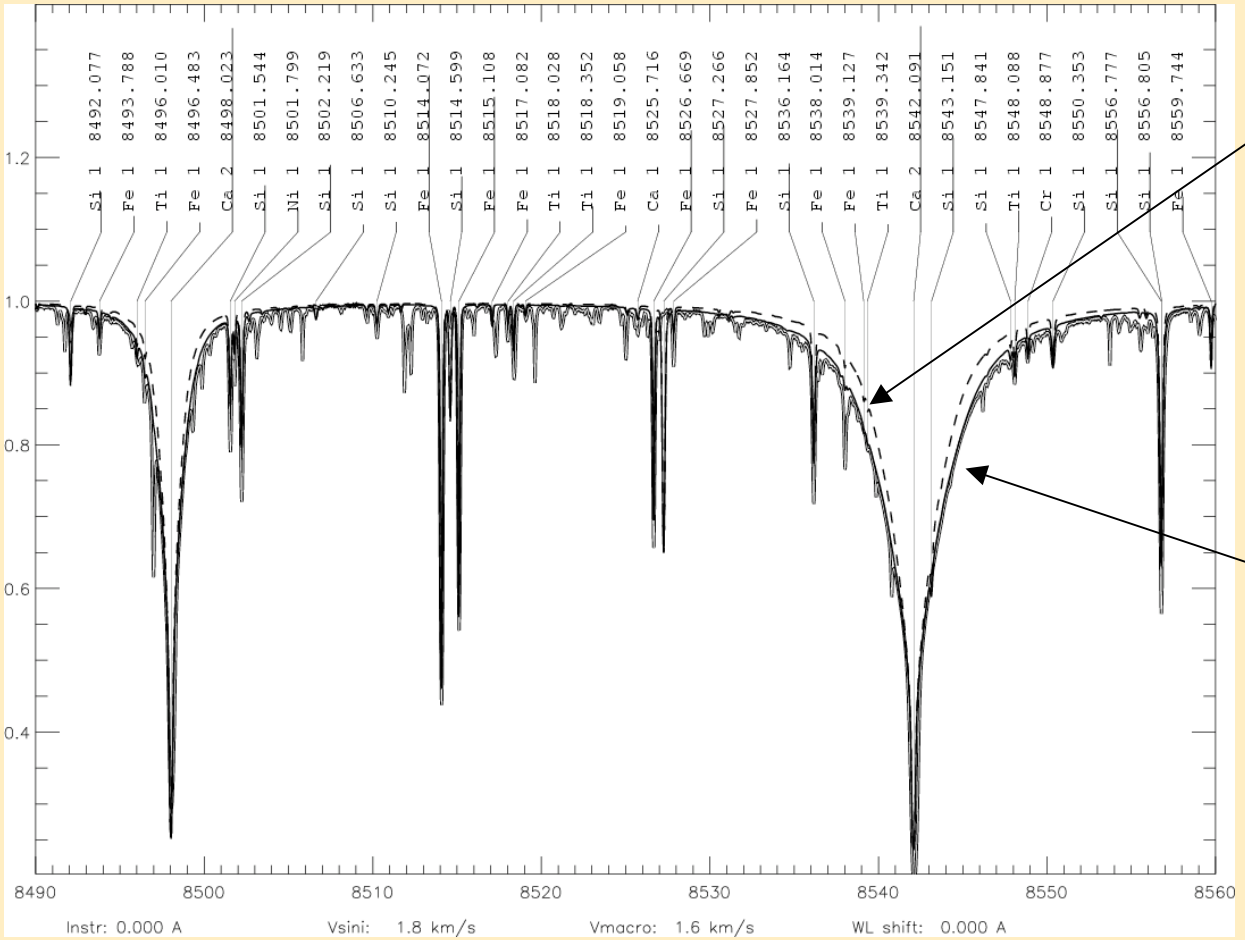
- Lorentz (1906) — Impulse theory (prior to QM)
- Weisskopf/London (1930's) — VdW potential, strong collisions
- Lindholm/Foley (1940's) — weak collisions, averaged interaction
- Unsöld (1950's) — apply VdW + approx, general formula

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



Unsöld theory

Solar observations

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

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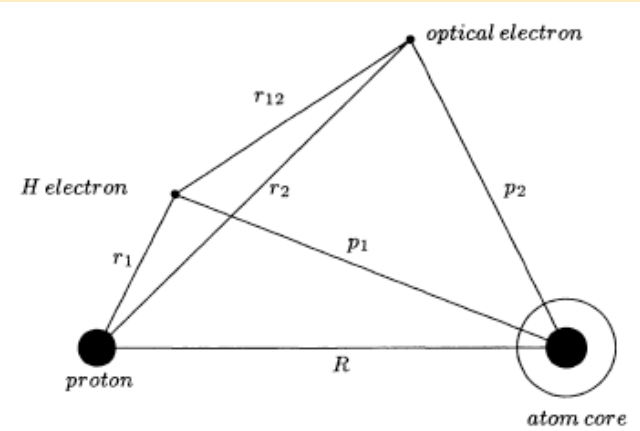
- Brueckner (1970's) — numerical RSU perturbation theory
- O'Mara (1970's) — analytic RSU perturbation theory
- Anstee & O'Mara (1992) — removal of averaged interaction+more
- Barklem & O'Mara (1998-) — extension to d and f states, and ions

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:

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

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

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

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)

$$n^* = \left[2E_{binding}\right]^{-1/2}$$

- Unsöld approx $E_p = -2/\alpha_H = -4/9$

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

ABO theory: Results

Cross section

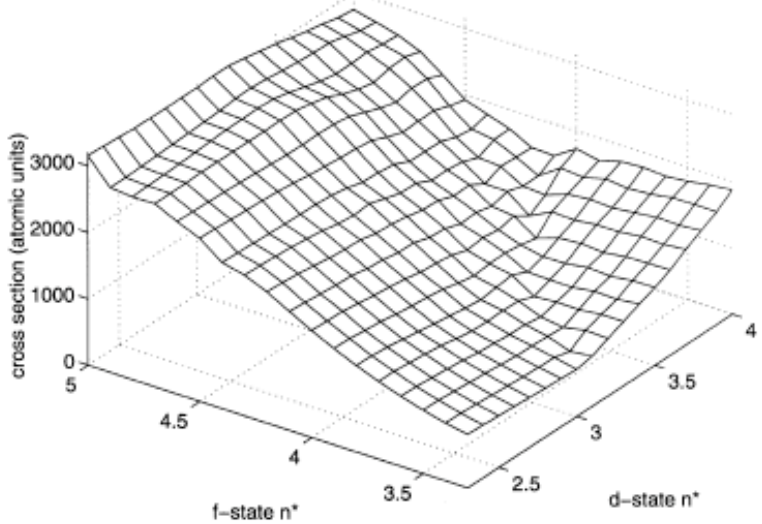


Figure 1. Plot of the cross-section for a perturber velocity of 10^4 m s^{-1} against the effective principal quantum number of the two states.

Velocity dependence

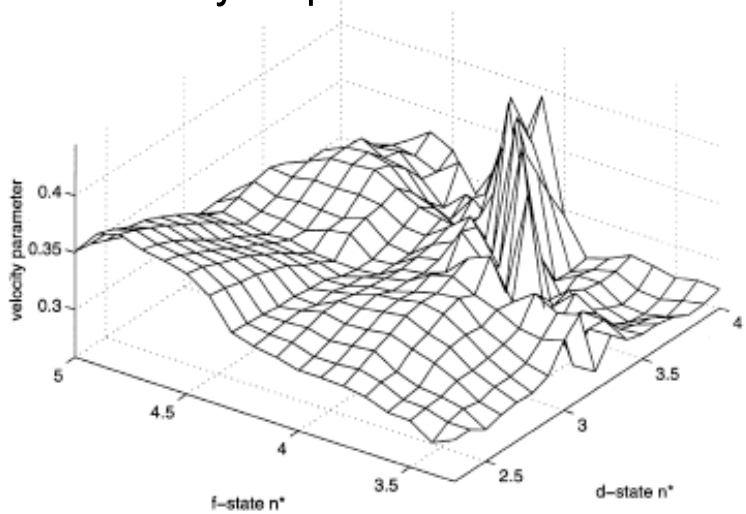


Figure 2. Plot of the velocity parameter α against the effective principal quantum number of the two states.

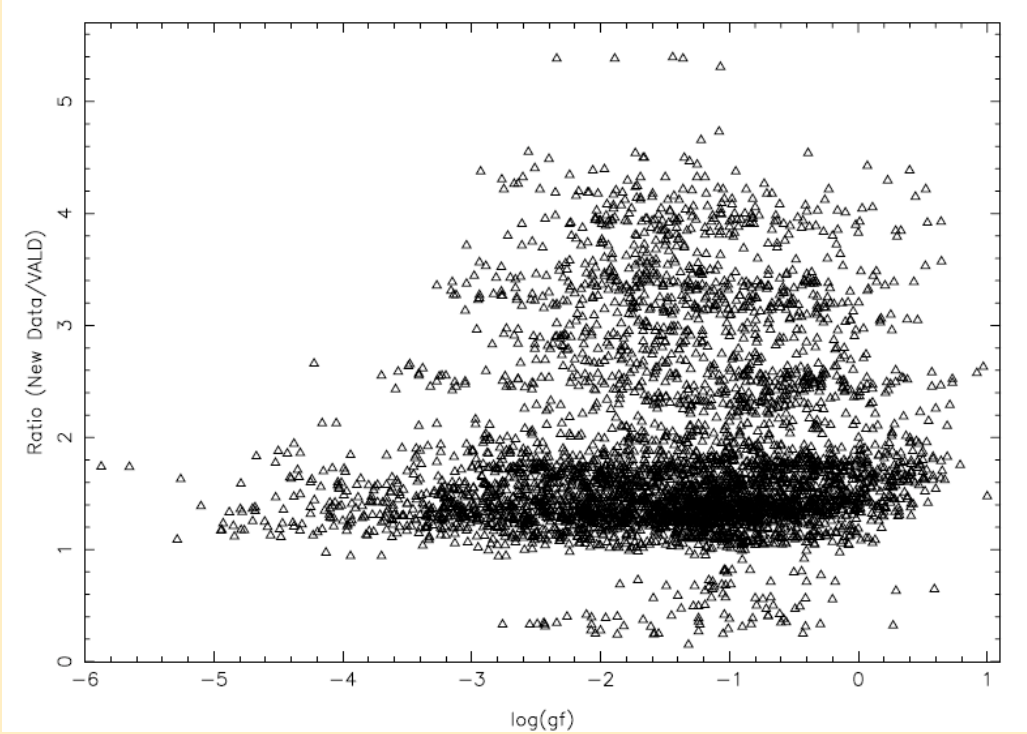
Tabulated results dependent only on effective principal quantum number

Simple velocity behaviour:

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

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

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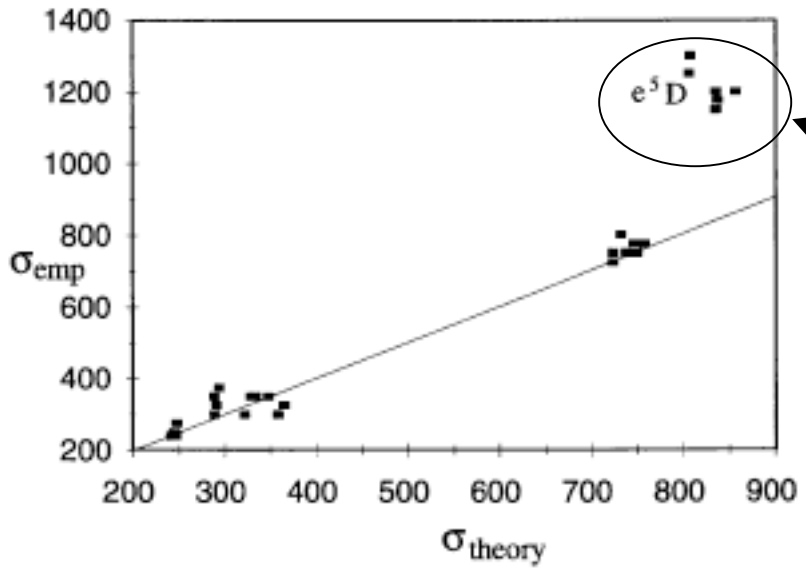
Applications

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



Strongly Stark broadened

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.

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

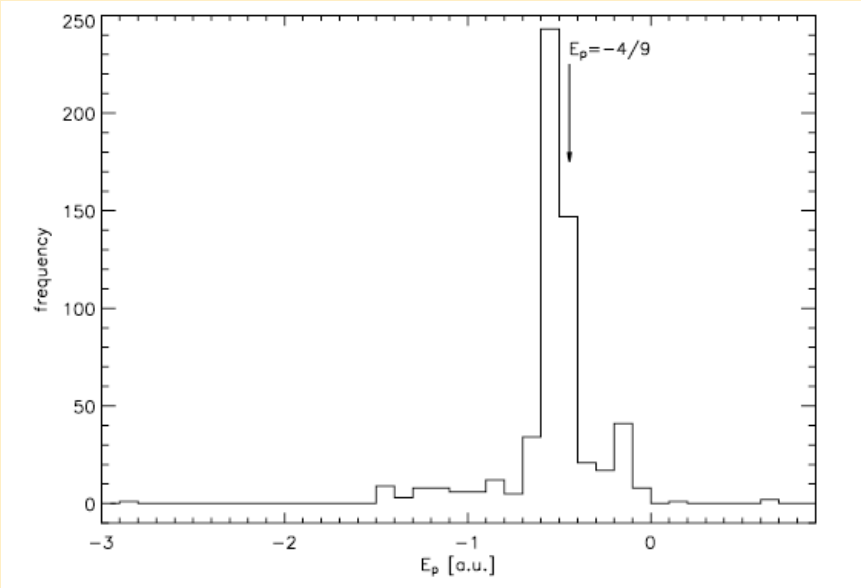
Extension to Ions

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

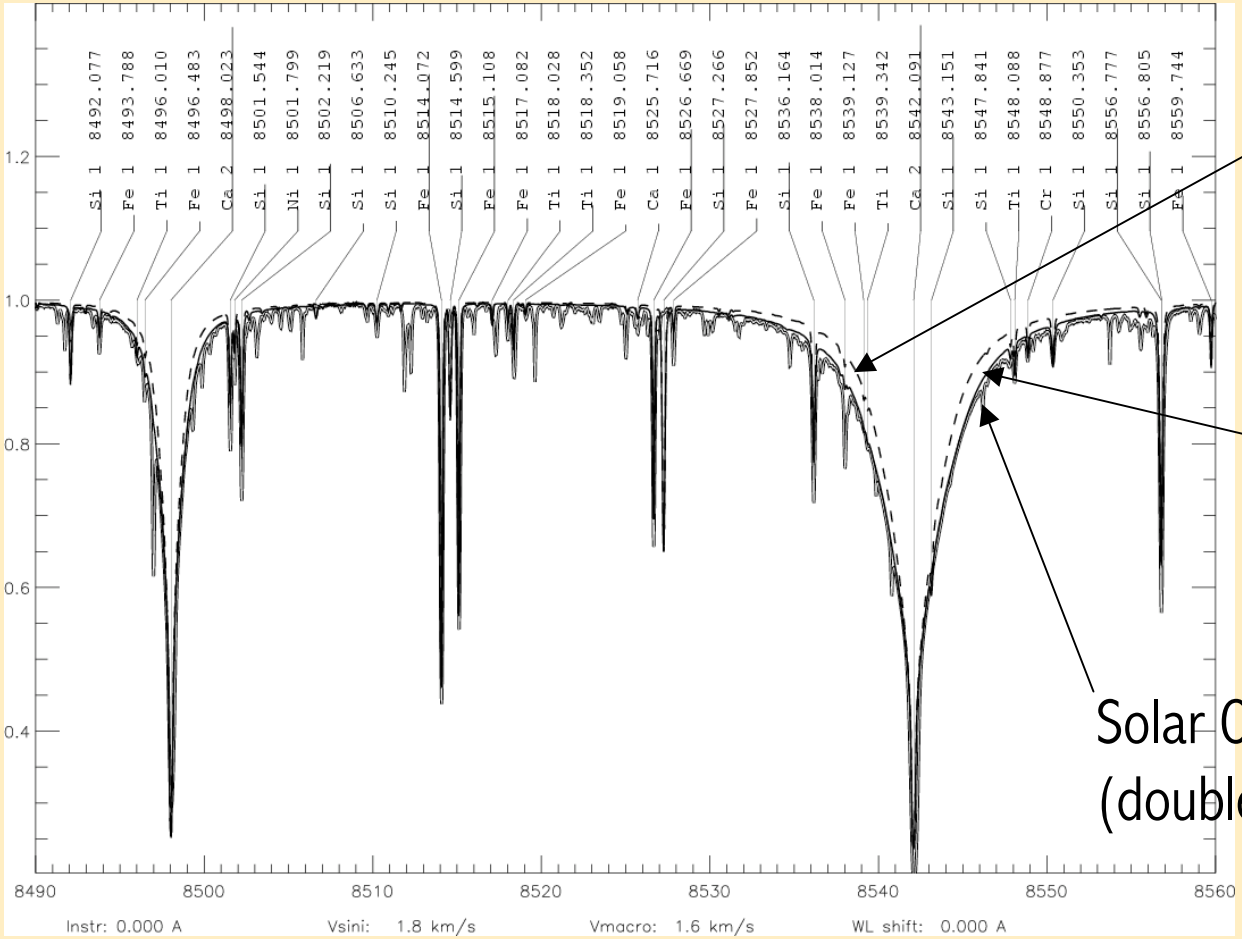
$$C_6 = \frac{3}{2} \sum_{k' \neq k} \sum_{l' \neq l} \frac{f^A_{kk'} f^H_{ll'}}{(\Delta E^A_{k'k} + \Delta E^H_{l'l}) \Delta E^A_{k'k} \Delta E^H_{l'l}},$$

$$E_p = -\frac{2\langle p_2^2 \rangle}{C_6}.$$

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



Applications



Unsöld
(dashed)

ABO
(full)

Solar Observations
(double line)

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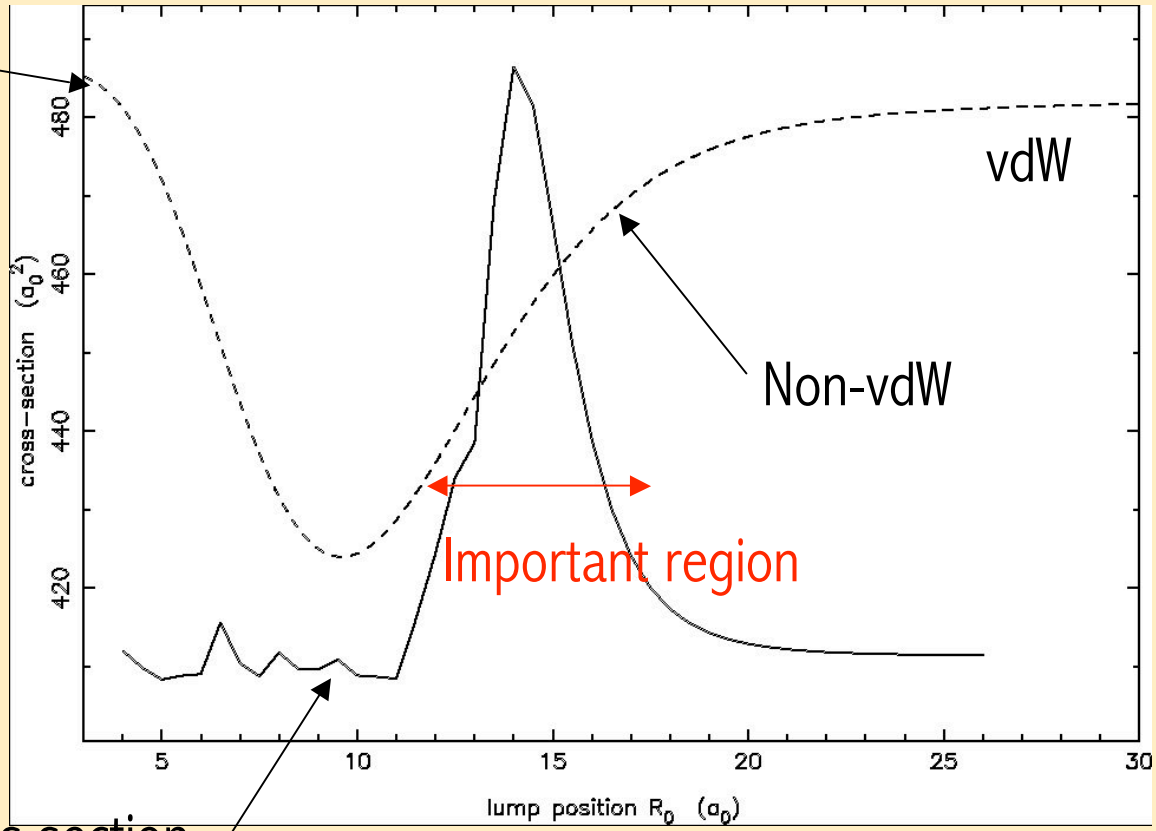
ABO theory: Why it works

"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

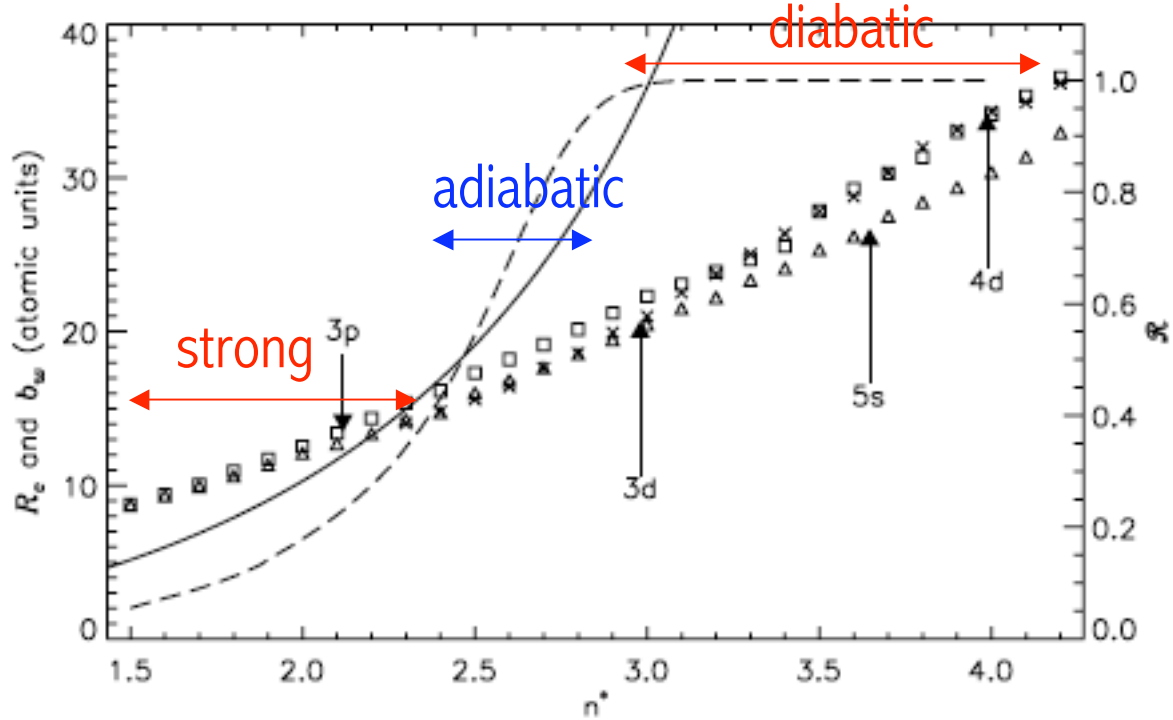

Figure 4. Plots demonstrating various collision regimes. b_w plotted against n^* for s states (triangles), p states (squares) and d states (crosses) for $v = 10^4$ ms^{-1}. The full curve is R_c. The reflection coefficient $\mathcal{R}$, is plotted as the dashed curve.

Impedance to tunnelling to ionic configuration

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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