DEPOLARIZING COLLISIONS WITH HYDROGEN: Neutral and singly ionized alkaline earths

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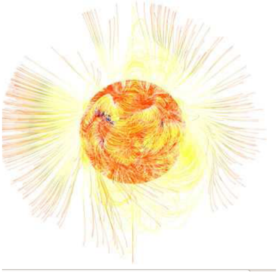
Outline:

Why depolarizing collisions?

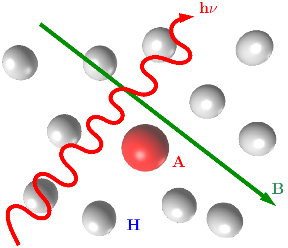
- Magnetic fiel, **B**,
  drives energy flux to the corona and its dynamics
- **B** is high in solar atmosphere
  B is low in solar corona
- High **B** measured using Zeeman splittings
  Low **B** from polarization of spectral lines
- Line polarization arises from anisotropic light in the upper solar atmosphere
- **B** reduces polarization through Hanle effect
- Other depolarization processes needed
  Eg. collisions with Hydrogen atoms

Raouafi, Solank & Wiegelmann ('09)



Atomic spectral lines: reduced density matrix

- Upper atmosphere at T$>$ 5000 K
- High density of H atoms, n_H
- Weak magnetic fields, **B**
- Anisotropic radiation, hν



– Mixture state described density matrix: $\rho = \rho_A \otimes \rho_B \otimes \rho_{h\nu} \otimes \rho_H$

– Only A detected, and the rest remain in their ground state

– Only the reduced matrix $\rho_{\alpha\mathbf{J}}(\mathbf{M},\mathbf{M}')$ described by master equation

Statistical equilibrium equation for Atom $\mathbf{A}(^{2S+1}L_J)$

The reduced density matrix $\rho_{\alpha\mathbf{J}}(\mathbf{M},\mathbf{M}')$ of atom $\mathbf{A}(^{2S+1}\mathbf{L_J})$ governed by

Bommier & Sahal-Brechot ('78), Landi Degl'Innoccenti & Landolfi ('04) , etc

$$
\begin{aligned}
\frac{d}{dt}\rho_{\alpha J}(M,M') &= -2\pi i\nu(JM,JM')\rho_{\alpha J}(M,M') \qquad \text{Hanle}\\
&+ \left[\frac{d}{dt}\rho_{\alpha J}(M,M')\right]_{radiative}\\
&+ \left[\frac{d}{dt}\rho_{\alpha J}(M,M')\right]_{collision}
\end{aligned}
$$

Impact approximation: radiative and collisional are obtained separately

Lamb & ter Haar ('71)

$$
\begin{aligned}
\frac{d}{dt}\rho_{\alpha J}(M_1,M_2) = &\sum_{\alpha' J' M_1' M_2'} C(\alpha J M_1 M_2 \leftarrow \alpha' J' M_1' M_2') \quad \rho_{\alpha' J'}(M_1',M_2')\\
&- \sum_{\alpha' J' M_1' M_2'} C(\alpha' J' M_1' M_2' \leftarrow \alpha J M_1 M_2) \quad \rho_{\alpha J}(M_1,M_2)
\end{aligned}
$$

Collisional rate constants

Thermal Rate Constants, C

For a collisional event at relative speed $\mathbf{v}$

$$A(\alpha, J, M) + H(^2S) \rightarrow A(\alpha', J', M')$$

the rate equation is

$$\frac{d\rho_{\alpha' J'}(M', M')}{dt} = C(\alpha' J' M' M' \leftarrow \alpha J M M; \mathbf{v}) \quad \rho_{\alpha J}(M, M) \quad n_H$$

- $[C] \equiv 1/(\text{concentration} \times \text{time}) \equiv \text{volume}/(\text{no.atoms} \times \text{time})$

"Effective volume per atom and time":

$$C(\mathbf{v}) = n_H \quad \sigma(\mathbf{v}) \times L/t \qquad \begin{cases} \sigma : \text{cross section}, [L]^2 \\ L = \mathbf{v}t, (\text{t} : \text{unit of time}) \end{cases}$$

Assuming a Boltzman distribution of velocities, the thermal rate constant is

$$C(T) = \left(\frac{\mu}{2\pi k_B T}\right)^{3/2} n_H \int_0^\infty \mathbf{v}\, \sigma(\mathbf{v})\, e^{-E_{kin}/k_B T} \quad 4\pi \mathbf{v}^2 d\mathbf{v}$$

Expansion in Spherical Tensors

- $\rho^K_Q(\alpha J)$: an irreducible representation under rotation Fano ('57), Omont ('77)

$$\rho^K_Q(\alpha J) = \sum_{M_1 M_2} (-1)^{J-M} \sqrt{2K+1} \begin{pmatrix} J & J & K \\ M_1 & -M_2 & -Q \end{pmatrix} \rho_{\alpha J}(M_1, M_2)$$

Expansion in Spherical Tensors

- $\rho^K_Q(\alpha J)$: an irreducible representation under rotation — Fano ('57), Omont ('77)
- Similar expansion of the rates, $C^K(\alpha' J' \leftarrow \alpha J)$
  Due to isotropic distribution of H atoms — Landi Degl'Innoccenti & Landolfi ('04)

$$C(\alpha' J' M_1' M_2' \leftarrow \alpha J M_1 M_2) = \sqrt{\frac{2J+1}{2J'+1}} \sum_K (-1)^{J-M_1+J'-M_1'} (2K+1) \begin{pmatrix} J & J & K \\ M_1 & -M_2 & -Q \end{pmatrix} \begin{pmatrix} J' & J' & K \\ M_1' & -M_2' & -Q \end{pmatrix} C^{(K)}(\alpha' J' \leftarrow \alpha J)$$

Expansion in Spherical Tensors

- $\rho^K_Q(\alpha J)$: an irreducible representation under rotation Fano ('57), Omont ('77)
- Similar expansion of the rates, $C^K(\alpha' J' \leftarrow \alpha J)$
- Rate equation for multipolar moments Landi Degl'Innoccenti & Landolfi ('04)

$$\begin{aligned}\frac{d}{dt}\rho^K_Q(\alpha J) &= \sum_{J'\neq J}\sqrt{\frac{2J'+1}{2J+1}}C^{(K)}(\alpha J \leftarrow \alpha' J')\rho^K_Q(\alpha' J') \\ &- \left[\sum_{\alpha' J'\neq \alpha J} C^{(0)}(\alpha' J' \leftarrow \alpha J) + D^{(K)}(\alpha J)\right]\rho^K_Q(\alpha J)\end{aligned}$$

Expansion in Spherical Tensors

- $\rho^K_Q(\alpha J)$: an irreducible representation under rotation — Fano ('57), Omont ('77)
- Similar expansion of the rates, $C^K(\alpha' J' \leftarrow \alpha J)$
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$$\frac{d}{dt}\rho^K_Q(\alpha J) = \sum_{J' \neq J} \sqrt{\frac{2J'+1}{2J+1}} C^{(K)}(\alpha J \leftarrow \alpha' J') \rho^K_Q(\alpha' J') - \left[\sum_{\alpha' J' \neq \alpha J} C^{(0)}(\alpha' J' \leftarrow \alpha J) + D^{(K)}(\alpha J) \right] \rho^K_Q(\alpha J)$$

- Calculation with Quantum Dynamical methods of
  $C^{(K)}(\alpha' J' \leftarrow \alpha J)$
  $D^{(K)}(\alpha J) = C^{(0)}(\alpha J \leftarrow \alpha J) - C^{(K)}(\alpha J \leftarrow \alpha J)$
  $g^{(K)}(\alpha J) = D^{(K)}(\alpha J) + \sum_{\alpha' J' \neq \alpha J} C^{(0)}(\alpha' J' \leftarrow \alpha J)$ — Omont, Kerkeni

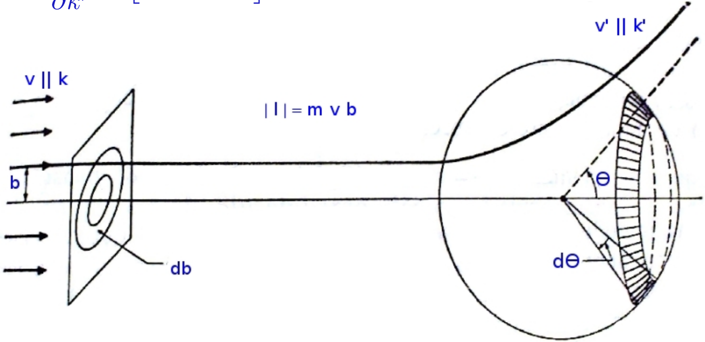
Outline:

Collision Cross Section, $\boldsymbol{\sigma}$

A single collisional event has cylindrical symmetry around $\hat{\boldsymbol{k}}$

Differential cross section: flux collected at $\hat{\boldsymbol{k}}'$

$$\frac{\partial\sigma}{\partial\hat{k}'} = \left[f^{\beta_1}_{\beta_{1'}}(\hat{k},\hat{k}')\right]^* \quad f^{\beta_2}_{\beta_{2'}}(\hat{k},\hat{k}')$$

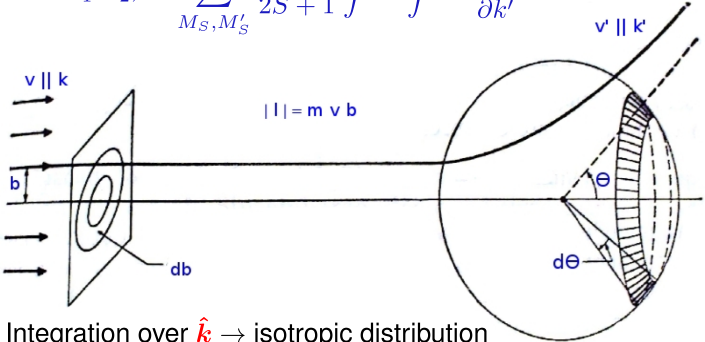


$f^{\beta_1}_{\beta_{1'}}(\hat{k},\hat{k}')$: Scattering amplitude $\quad\quad \beta \equiv \alpha J M_1 S M_S$ in A +H collisions

Collision Cross Section, σ

Integral cross section:

$$\sigma^0(\alpha J M_1 M_2; \alpha' J' M_1' M_2') = \sum_{M_S, M_S'} \frac{1}{2S+1} \int d\hat{k} \int d\hat{k}' \frac{\partial \sigma}{\partial \hat{k}'}$$



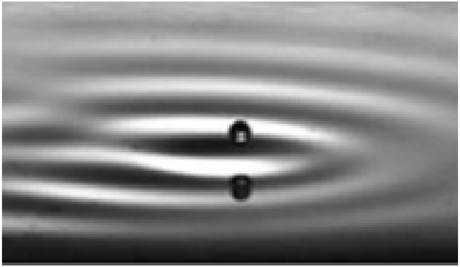
Integration over $\hat{k}$ $\rightarrow$ isotropic distribution

Thermal rate constant:

$$C(\alpha' J' M_1' M_2' \leftarrow \alpha J M_1 M_2) = N_{H^\circ} \int v^2 dv\, f(T, v)\, \sigma^0(\alpha J M_1 M_2; \alpha' J' M_1' M_2')$$

Scattering Amplitude $\mathbf{f}_{\beta'}^{\beta}(\hat{\mathbf{k}}, \hat{\mathbf{k}}')$

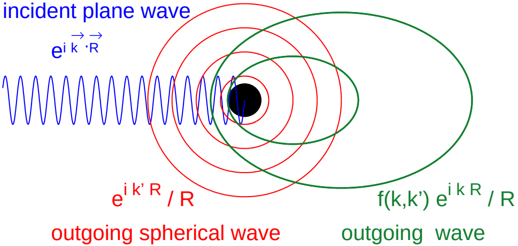
Asymtptotic Conditions of the total Wave function



Scattering Amplitude $\mathrm{f}_{\beta'}^{\beta}(\hat{\mathrm{k}}, \hat{\mathrm{k}}')$

Asymtptotic Conditions of the total Wave function

$$\lim_{R\to\infty} \Phi_\beta(\boldsymbol{k}, \hat{k}') = e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |\alpha JM\rangle |SM_S\rangle + i \sum_{\beta'} f_{\beta'}^{\beta *}(\hat{k}, \hat{k}') \frac{e^{ik'R}}{R\sqrt{k' k_\alpha}} |\alpha' J' M'\rangle |S' M'_S\rangle$$



$f_{\beta'}^{\beta}(\hat{k}, \hat{k}')$

outgoing amplitude on

$$\beta' \equiv A(\alpha' J' M') + H(S' M'_S)$$

Simplified considering

$$\mathbf{J}_t = \mathbf{J} + \mathbf{S} + \ell = \text{cte.}$$

Amplitude f, S-Matrix: under central forces

Total angular momentum conserved $\rightarrow$ Partial wave expansion

ℓ =cte

$$\Phi(\vec{R}) = \frac{1}{R}\sum_{\ell=0}^{\infty} A_\ell\, \Phi_\ell(R)\, Y_{\ell m}(\hat{R})$$

$3-D$ | $1-D$

$\Phi(\vec{R})$ are eigenfunctions of

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(R) - E\right]\Phi(\vec{R}) = 0$$

with boundary conditions

$$\Phi(\vec{R}) \underset{R\rightarrow\infty}{\propto} e^{-i\vec{k}\cdot\vec{R}} + f(\vec{k},\vec{k}')\frac{e^{ik'R}}{R}$$

$\Phi_\ell(R)$ are eigenfunctions of

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu R^2} + V(R) - E\right]\Phi_\ell(R) = 0$$

$$\Phi_\ell(\mathbf{R}) \underset{R\rightarrow\infty}{\propto} e^{-ikR} + S(E)e^{ikR}$$

Amplitude f, S-Matrix: A(α, J, M) + $H(S, M_S)$ case

- Scattering amplitude partial wave expansion

$$f^{\beta}_{\beta'}(\hat{k},\hat{k}') = \sum_{J_t M_t} \sum_{\ell m_\ell} \sum_{\ell' m'_\ell} B\, Y^{*}_{\ell m_\ell}(\hat{k})\, Y_{\ell' m'_\ell}(\hat{k}') \left(\delta_{n,n'} - S^{J_t}_{n,n'}(E)\right)$$

where B is a geometric factor

$$\begin{aligned} B &= \frac{2\pi}{k}(-1)^{\ell} \sum_{jj'} \sum_{mm'} (-1)^{j+j'+J+J'-\ell-\ell'-2S+2M_t+m+m'} (2J_t+1)\sqrt{(2j+1)(2j'+1)} \\ &\times \begin{pmatrix} j & \ell & J_t \\ m & m_\ell & -M_t \end{pmatrix} \begin{pmatrix} j' & \ell' & J_t \\ m' & m'_\ell & -M_t \end{pmatrix} \begin{pmatrix} J & S & j \\ M & M_S & -m \end{pmatrix} \begin{pmatrix} J' & S & j' \\ M' & M'_S & -m' \end{pmatrix} \end{aligned} \quad (1)$$

Amplitude f, S-Matrix: A(α, J, M) + $H(S, M_S)$ case

- Scattering amplitude state multipoles (Alexander & Davis ('83))

$$f^{K''}_{Q''}(\alpha J S M_S, \hat{k} \to \alpha' J' S' M'_S, \hat{k}') = \sum_{\ell m_\ell} \sum_{\ell' m'_\ell} \sum_{K} \sum_{K'} b^{\ell K}_{\ell' K'}(K'') G \, Y_{\ell m_\ell}(\hat{k}) \, Y_{\ell' m'_\ell}(\hat{k}')$$

with

$$\begin{aligned} b^{\ell K}_{\ell' K'}(K'') &= \frac{2\pi}{k} \sum_{J_t j j'} \Big(\delta_{n,n'} - S^{J_t}_{n,n'}(E)\Big)(-1)^{J_t+J+S} \sqrt{(2j+1)(2j'+1)} \\ &\times \quad (2J_t+1) \begin{Bmatrix} \ell & J_t & j \\ J & S & K \end{Bmatrix} \begin{Bmatrix} \ell' & J_t & j' \\ J' & S' & K' \end{Bmatrix} \begin{Bmatrix} J' & K' & J_t \\ K & J & K'' \end{Bmatrix} \end{aligned}$$

$$\begin{aligned} G &= (-1)^{\ell+2K''+2M_S+2M'_S-Q+2Q''} (2K+1)(2K'+1)\sqrt{2K''+1} \\ &\times \begin{pmatrix} K' & K & K'' \\ Q' & -Q & -Q'' \end{pmatrix} \begin{pmatrix} S & \ell & K \\ M_S & m_\ell & Q \end{pmatrix} \begin{pmatrix} S' & \ell' & K' \\ M'_S & m'_\ell & Q' \end{pmatrix}, \end{aligned}$$

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- Scattering amplitude state multipoles (Alexander & Davis ('83))

$$f^{K''}_{Q''}(\alpha J S M_S, \hat{k} \rightarrow \alpha' J' S' M'_S, \hat{k}') = \sum_{\ell m_\ell} \sum_{\ell' m'_\ell} \sum_K \sum_{K'} b^{\ell K}_{\ell' K'}(K'') G\, Y_{\ell m_\ell}(\hat{k})\, Y_{\ell' m'_\ell}(\hat{k}')$$

with

$$b^{\ell K}_{\ell' K'}(K'') = \frac{2\pi}{k} \sum_{J_t j j'} \left(\delta_{n,n'} - S^{J_t}_{n,n'}(E)\right)(-1)^{J_t+J+S}\sqrt{(2j+1)(2j'+1)} \times (2J_t+1) \begin{Bmatrix} \ell & J_t & j \\ J & S & K \end{Bmatrix} \begin{Bmatrix} \ell' & J_t & j' \\ J' & S' & K' \end{Bmatrix} \begin{Bmatrix} J' & K' & J_t \\ K & J & K'' \end{Bmatrix}$$

- Cross section state multipoles (Kerkeni *et al.* ('00))

$$\sigma^K_{\alpha J \rightarrow \alpha' J'}(E) = \sum_{K'} (-1)^{J+J'+K+K'} \frac{(2K'+1)}{4\pi(2S+1)} \begin{Bmatrix} J' & J & K' \\ J & J' & K \end{Bmatrix} \sum_{NN'} (2N+1)(2N'+1) \left| b^{\ell N}_{\ell' N'}(K') \right|^2$$

- Rate constants (Landi Degl'Innoccenti & Landolfi ('04))

$$C^{(K)}(\alpha' J' \leftarrow \alpha J) = \sqrt{\frac{2J'+1}{2J+1}} N_{H^\circ} \int v^2 dv\, f(T, v)\, \sigma^K_{\alpha J \rightarrow \alpha' J'}(E)$$

Representation of A$(\alpha, J, M) + H(S, M_S)$ collisions

- Basis set for A(α, J, M): $\mathbf{J} = \mathbf{L} + \mathbf{S}_A$

$$|JM; \alpha \equiv L, S_A\rangle$$

- Basis set for A$(\alpha, J, M) + H(S, M_S)$ fragments: $\mathbf{j} = \mathbf{J} + \mathbf{S}$

$$|jm; \alpha J, S\rangle$$

- Angular basis set: $\mathbf{J}_t = \mathbf{j} + \boldsymbol{\ell}$

$$|\mathcal{Y}_n^{J_t M_t}\rangle \qquad \text{with} \qquad n \equiv j\ell\alpha JS$$

- Total wave function: in a space-fixed basis set representation

$$\left|\Psi_E^{J_t M_t n}\right\rangle = \sum_{n'} \frac{\Phi_{n'}^{J_t M_t n}(R; E)}{R} |\mathcal{Y}_{n'}^{J_t M_t}\rangle.$$

where $\Phi_{n'}^{J_t M_t n}(R; E)$ are obtained numerically

Close coupling equations and S-matrix

- Total Hamiltonian

$$H = -\frac{\hbar^2}{2\mu}\left(\frac{2}{R}\frac{\partial}{\partial R} + \frac{\partial^2}{\partial R^2}\right) + \frac{\boldsymbol{\ell}^2}{2\mu R^2} + H_{el} + H_{SO}^{A}$$

- Close Coupling equations: $n \equiv j\ell\alpha JS$

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu R^2} + E^{A}_{LS,J} - E\right\}\Phi_n^{J_t M_t n}(R;E) = -\sum_{n'}\left\langle \mathcal{Y}_n^{J_t M_t}\,|\mathcal{H}_{el}|\,\mathcal{Y}_{n'}^{J_t M_t}\right\rangle \Phi_{n'}^{JM\ell n}(R;E)$$

- Asymptotic boundary conditions

$$\Phi_{n'}^{J_t M_t n}(R\to\infty;E) \propto \sqrt{\frac{\mu}{2\pi\hbar^2}}\left\{\delta_{nn'}\frac{e^{-i(kR-\ell\pi/2)}}{\sqrt{k}} - S^{J_t}_{nn'}(E)\frac{e^{i(k'R-\ell'\pi/2)}}{\sqrt{k'}}\right\}$$

The problem is the evaluation of electronic matrix elements

$$\langle \mathcal{Y}_n^{J_t M_t}|\mathcal{H}_{el} + H_{SO}|\mathcal{Y}_{n'}^{J_t M_t}\rangle$$

Electronic Matrix elements

- $|\mathcal{Y}_{n'}^{J_t M_t}\rangle$ are defined in a space fixed such as

$$H^A \quad |\mathcal{Y}_{n'}^{J_t M_t}\rangle = E_{\alpha J} \quad |\mathcal{Y}_{n'}^{J_t M_t}\rangle \qquad \text{with} \qquad n \equiv j\ell\alpha JS$$

- Total electronic Hamiltonian

$$H^A + \mathcal{H}_{el} \qquad \text{with} \qquad H^A = H^A_{el} + H_{SO}$$

- $\mathcal{H}_{el}$: $A(\alpha JM) + H(S, M_S)$ interaction in a body-fixed frame $\hat{z}' \parallel \mathbf{R}$

$$H_{el}|\varphi^{S_t}_{L\Lambda}\rangle = V^{S_t}_{L\Lambda}(R)|\varphi^{S_t}_{L\Lambda}\rangle \qquad \text{with} \qquad \Lambda = L_{z'}$$

- Body-fixed $\rightarrow$ Space-fixed transformation

$$\langle\mathcal{Y}_{n}^{J_t M_t}|\mathcal{H}_{el}|\mathcal{Y}_{n'}^{J_t M_t}\rangle = \sum_{\Omega}\sum_{\Lambda}\sum_{S_t} G \quad V^{S_t}_{L\Lambda}(R)$$

Born-Oppenheimer approximation: calculation of $V^{S_t}_{L\Lambda}(R)$ at each R value

Outline:

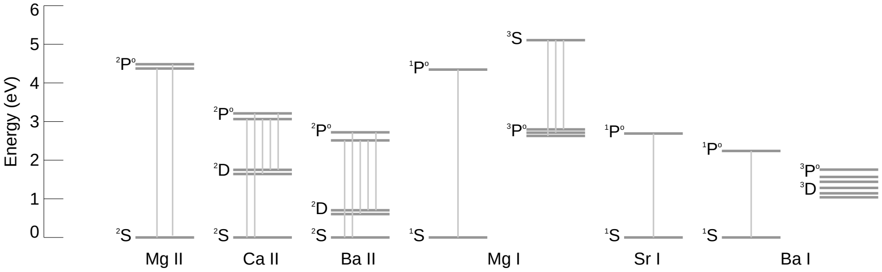
Summary of the Quantum method

For a particular $A(J;\alpha = LS)$: (neglecting transitions between different α)

Conference by C. Sanz

- Calculation of $\mathcal{V}^{S_t}_{L\Lambda}(R)$
  - for a collection of distances R_i
  - for $|\Lambda| \leq L$
  - for $S_t = S - 1/2, S + 1/2$
- Use the experimental H_{SO} energies
- Resolution of the coupled equations to obtain $S^{J_t}_{n,n'}(E)$
  - for 1000-10000 energies in the interval 1 meV - 50 eV
  - for J_t=0 or 1/2 up to 1000 or 2000
- Calculation of $\sigma^{K}_{\alpha J \rightarrow \alpha' J'}(E)$
- Numerical integration to get: $C^{(K)}(\alpha' J' \leftarrow \alpha J)$
  and fit them to analytical functions

Results: Neutral and singly ionized Alkaline Earths



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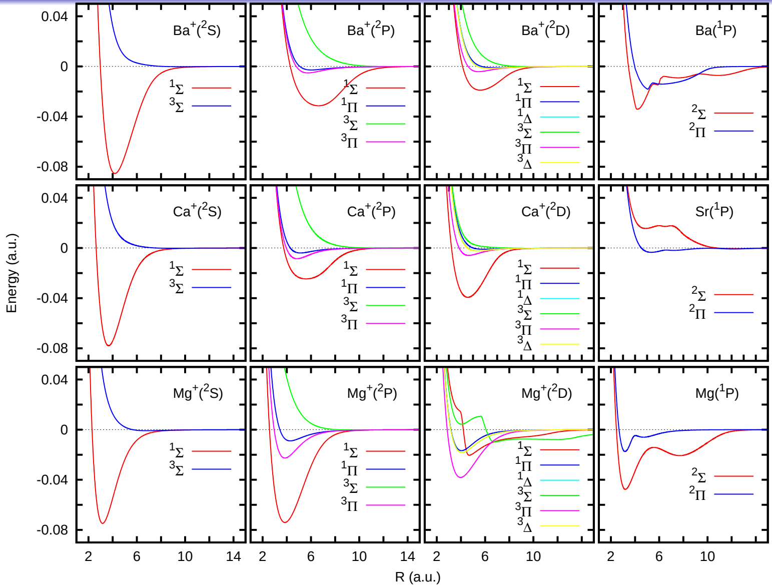
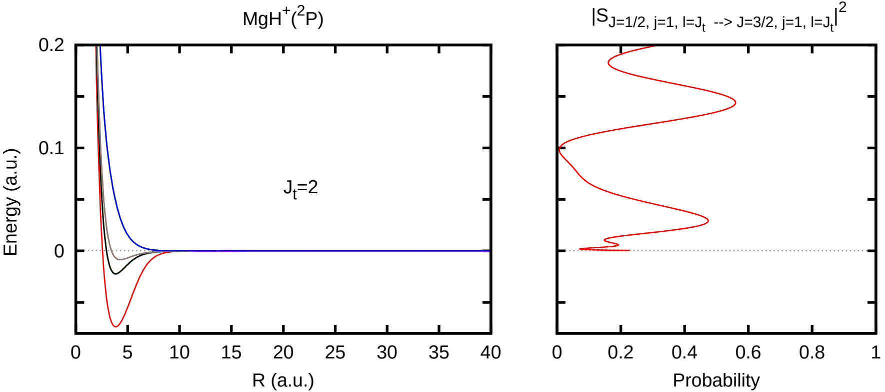


$Mg^+(^2P)$ example; S-matrices for several J_t

$J = 1/2, 3/2$ $\quad$ $j = J \pm S =$ 0,1,2 $\quad$ $\ell = |J_t - j|, ..., J_t + j$

12 channels

Effective potential: $H_{el} + H_{SO} + \dfrac{\ell(\ell+1)}{2\mu R^2}$



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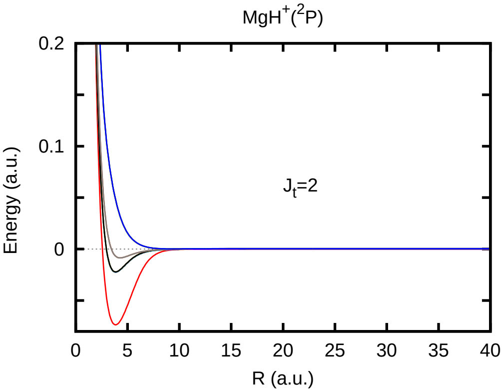
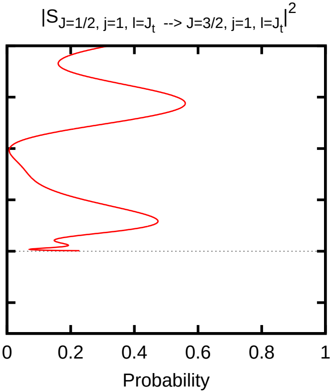
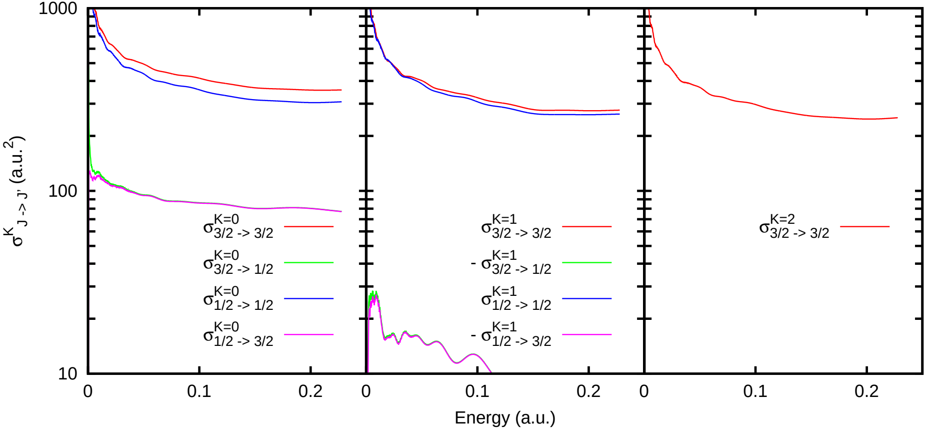




$Mg^{+}(^{2}P)$ example: cross-section σ^{K}

Inelastic cross section:

$$\sigma_{\alpha J\to\alpha' J'}(E) = \frac{1}{2J+1}\sum_{MM'}\sigma_{\alpha JM\to\alpha' J'M'}(E) = \sqrt{\frac{2J'+1}{2J+1}}\,\sigma^{K=0}_{\alpha J\to\alpha' J'}(E)$$

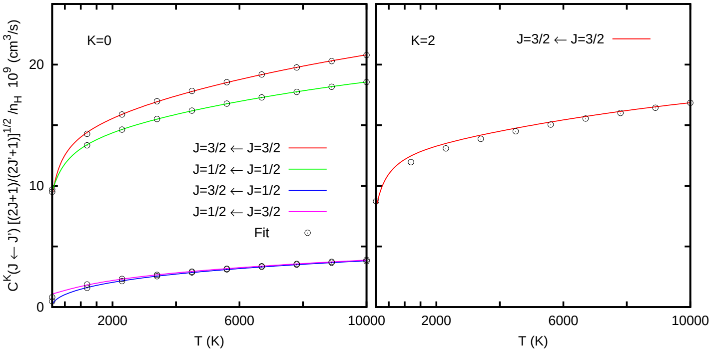


$Mg^+(^2P)$ example: rates C^K

Rate constants

(Landi Degl'Innoccenti & Landolfi ('04))

$$C^{(K)}(\alpha' J' \leftarrow \alpha J) = \sqrt{\frac{2J'+1}{2J+1}} N_{H^\circ} \int v^2 dv\, f(T,v)\, \sigma^K_{\alpha J \rightarrow \alpha' J'}(E)$$



Analytical fit:

$$C^{(K)}(\alpha' J' \leftarrow \alpha J) = \sqrt{\frac{2J'+1}{2J+1}} \; a \left(\frac{T}{5000}\right)^b c^{T/5000} \quad 10^{-9} N_{H^\circ} s^{-1}$$

Comparison with other studies

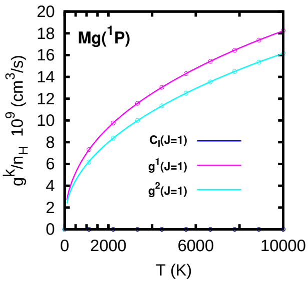
Quantum and Semi-classical total depolarization rate

$$g^{(K)}(\alpha J) = \left[C^{(0)}(\alpha J \to \alpha J) - C^{(K)}(\alpha J \to \alpha J)\right] + \sum_{J' \neq J} C^{(0)}(\alpha J \to \alpha' J')$$

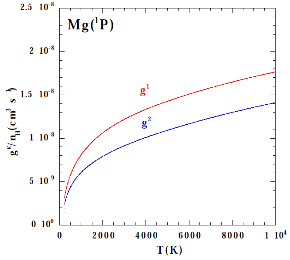
- Faurobert-Scholl *et al.* ('95): Sr I, Ca I
- Kerkeni ('02) : Mg I, Ca I, Sr I, Na I
- Kerkeni *et al.* ('03) : Ca I
- Derouich *et al.* ('03): Mg I, Ca I, Na I
- ⋮
- This work ('14): Mg (I, II), Ca(II), Sr(I), Ba(I,II)
  ApJ in press, ArXiv 1404.6339

Mg(^2P): Quantum versus Semiclassical ($\approx 10\,\%$)

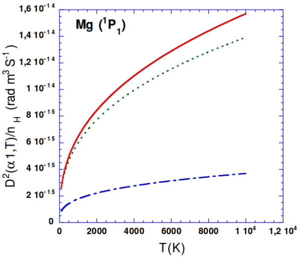
Quantum this work



Quantum Kerkeni ('02)



Semiclassical Derouich et el. ('03)

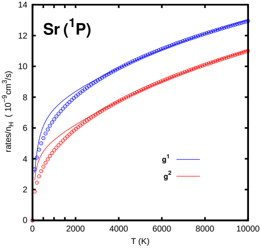


$g^K \times N_H 10^{-9}$ cm ^{3}/s at T=5000K

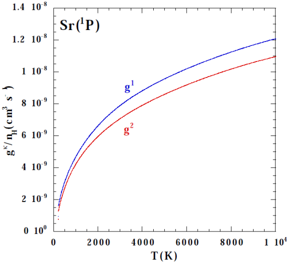
K	This work	Kerkeni ('02)	Derouich *et al.* ('03) (n*=2.03)
1	13.696	13.836	–
2	11.944	10.79	11.767

Sr(^2P): Quantum versus Semiclassical

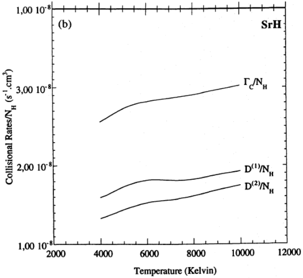
Quantum this work



Quantum Kerkeni ('02)



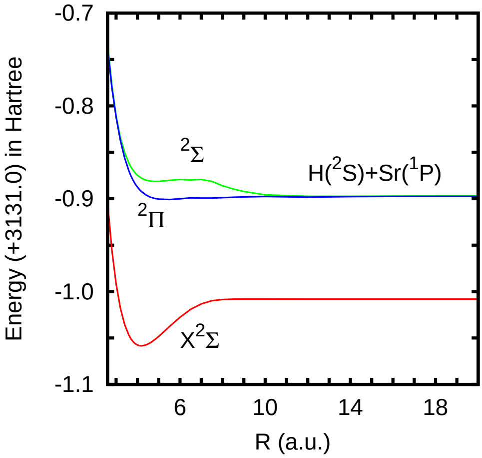
Faurobert-Scholl et el. ('95)



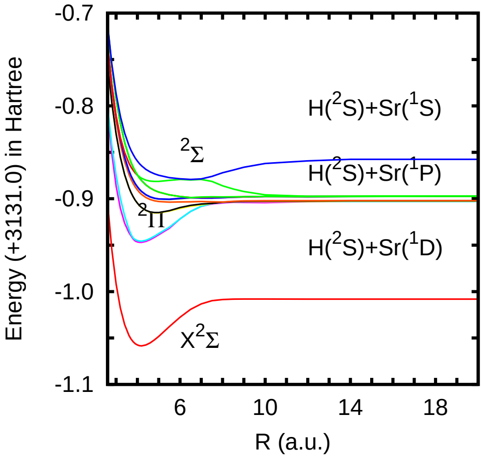
g^K at T=5000K	This work	Kerkeni ('02)	Faurobert-Scholl *et al.* ('95)
1	10.543	8.9875	$\approx$ 17.5
2	8.42791	8.0015	$\approx$ 14

Larger differences → curve crossing effects?

Curve crossings and failure of B.O. approx.



Curve crossings and failure of B.O. approx.

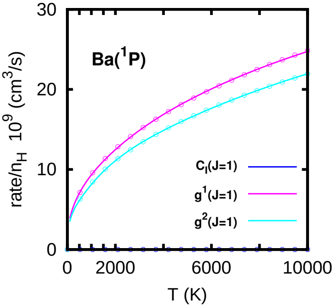


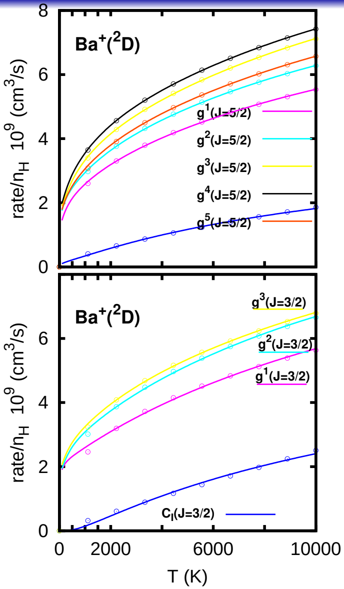
- Close lying electronic states
  $M^+ + H^-$ cross $M(L, S) + H$
- Adiabatic approximation fails at crossings
- Couplings between different L, S
  Diabatization: C. Sanz
- Anstee, Barklem and O'Mara
  use a single electron model
  no ionic states

Results for Ba I and Ba II: l=0

Valid for:

^{134}Ba	$2{,}4\,\%$
^{136}Ba	$7{,}8\,\%$
^{138}Ba	$71{,}7\,\%$





Results for Ba I and Ba II: I$>$0

For:

$$\begin{array}{lll} {}^{135}Ba & I = 3/2 & 6{,}6\,\% \\ {}^{137}Ba & I = 3/2 & 11{,}2\,\% \end{array}$$

Hyperfine structure

$$\vec{F} = \vec{J} + \vec{I}$$

Hyperfine splitting $<<$ Temperature

J-transitions independent of I

Recoupling approach Faure & Lique ('12)

$$\sigma_{JF\to J'F'}(E) = (2F'+1)\sum_k \left\{ \begin{array}{ccc} J & J' & K \\ F' & F & I \end{array} \right\}^2 \sigma^K_{J\to J'}(E)$$

Outline:

Conclusions

- Full Quantum treatment for A($^{2S+1}L_J$)+H depolarizing collisions has been developed and applied to Mg(I, II), Sr(I), Ca(II), Ba(I,II)
- Based on adiabatic electronic approximation within the same (L,S) level: quasi-elastic collisions

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- Based on adiabatic electronic approximation within the same (L,S) level: quasi-elastic collisions
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- Inclusion of hyperfine structure in progress recoupling techniques

Conclusions

- Full Quantum treatment for A($^{2S+1}L_J$)+H depolarizing collisions has been developed and applied to Mg(I, II), Sr(I), Ca(II), Ba(I,II)
- Based on adiabatic electronic approximation within the same (L,S) level: quasi-elastic collisions
- Inclusion of $(L, S) \rightarrow (L', S')$ transitions in progress diabatization techniques (C. Sanz)
- Inclusion of hyperfine structure in progress recoupling techniques
- Possible application to H + MgH collision: inclusion of exchange reaction: H + MgH $\rightarrow$ HMg + H
- He($^3S,^3P,^3D$) + H also under consideration: problem of autoionization He(^1S) $+ H^+$ + e

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