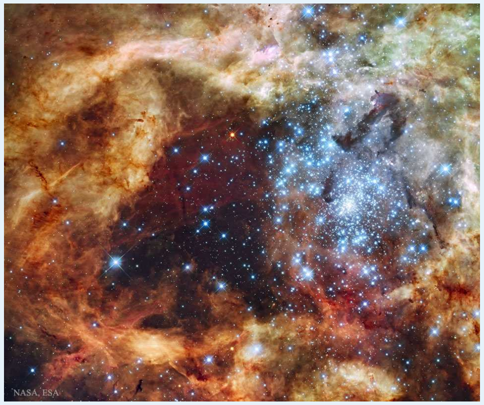
Radiative Transfer, Spectroscopy & Collisions - II

Jacques Le Bourlot
Observatoire de Paris & Université Paris-Cité



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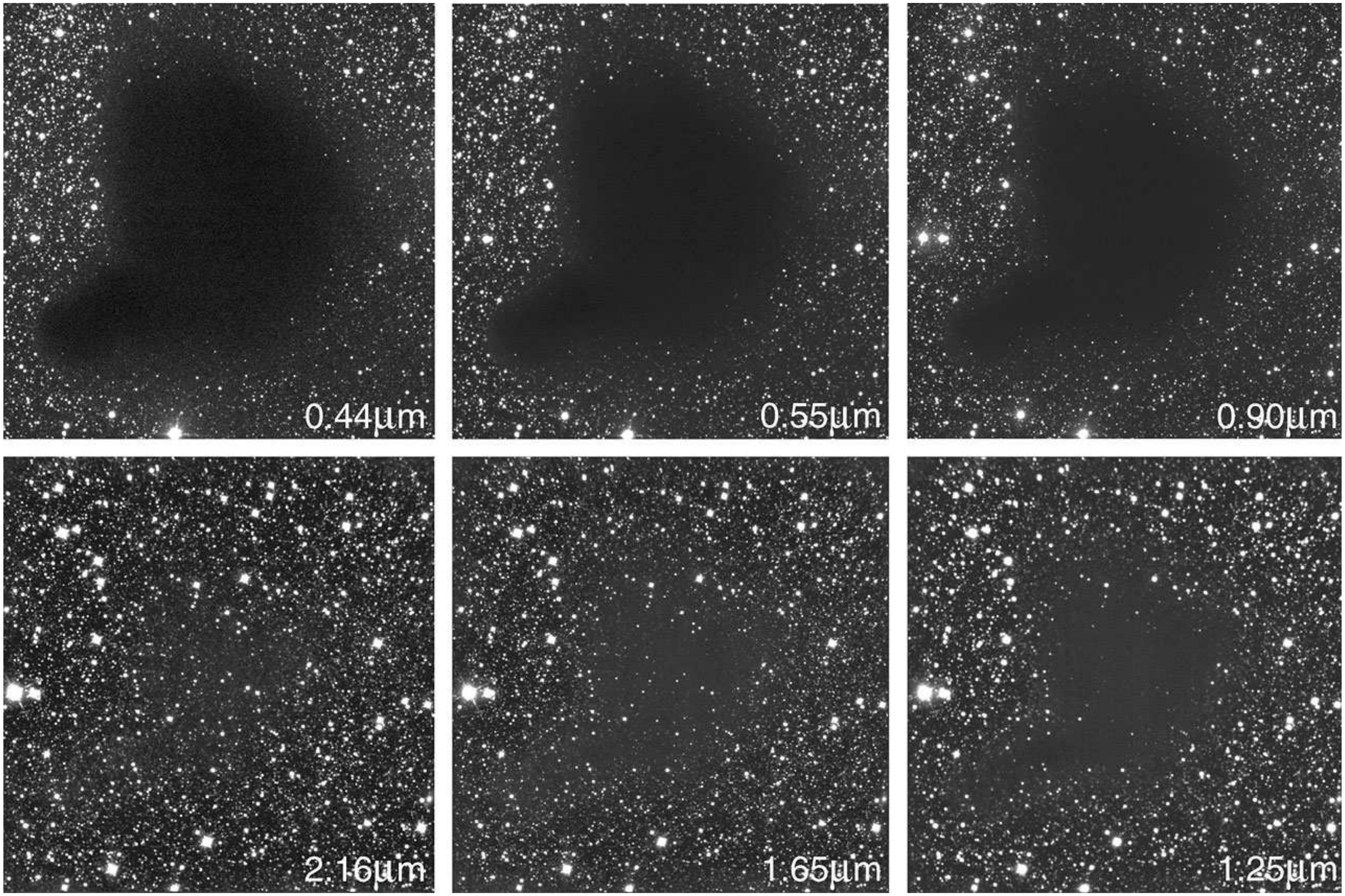
Intermezzo: Interstellar extinction



Barnard 68 - © ESO

Definitions

- $m_1 - m_2$: magnitude difference between λ_1 (flux f_1) and λ_2 (flux f_2):

$$m_1 - m_2 = -2.5 \log_{10}\left(\frac{f_1}{f_2}\right)$$

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  With D in pc, and no absorption:

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$$m_\lambda - M_\lambda = 5 \log_{10} D - 5$$

- A_λ: Extinction at λ. With absorption.

$$m_\lambda - M_\lambda = 5 \log_{10} D - 5 + A_\lambda$$

$$A_\lambda = 2.5 \log_{10}(e)\, \tau_\lambda \simeq 1.086\, \tau_\lambda$$

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- Photometric bands:

Band	U	B	V	R	I	K
λ (μm)	0.365	0.445	0.551	0.658	0.806	2.2

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- C_D (non standard!): Hydrogen column density to color index:

$$C_D = \frac{N_{\mathrm{H}}}{E_{\mathrm{B-V}}}$$

Extinction curve

- Standard definition:

$$Ext\left(\lambda\right) = \frac{E_{\lambda-\mathrm{V}}}{E_{\mathrm{B}-\mathrm{V}}} = \frac{A_\lambda - A_\mathrm{V}}{A_\mathrm{B} - A_\mathrm{V}} = \frac{\tau_\lambda - \tau_\mathrm{V}}{\tau_\mathrm{B} - \tau_\mathrm{V}}$$

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- WARNING !! By construction:

$$Ext\,(V) = 0\,; \quad Ext\,(B) = 1$$

Adapted to visible and near UV, but **NOT** to infrared and radio!

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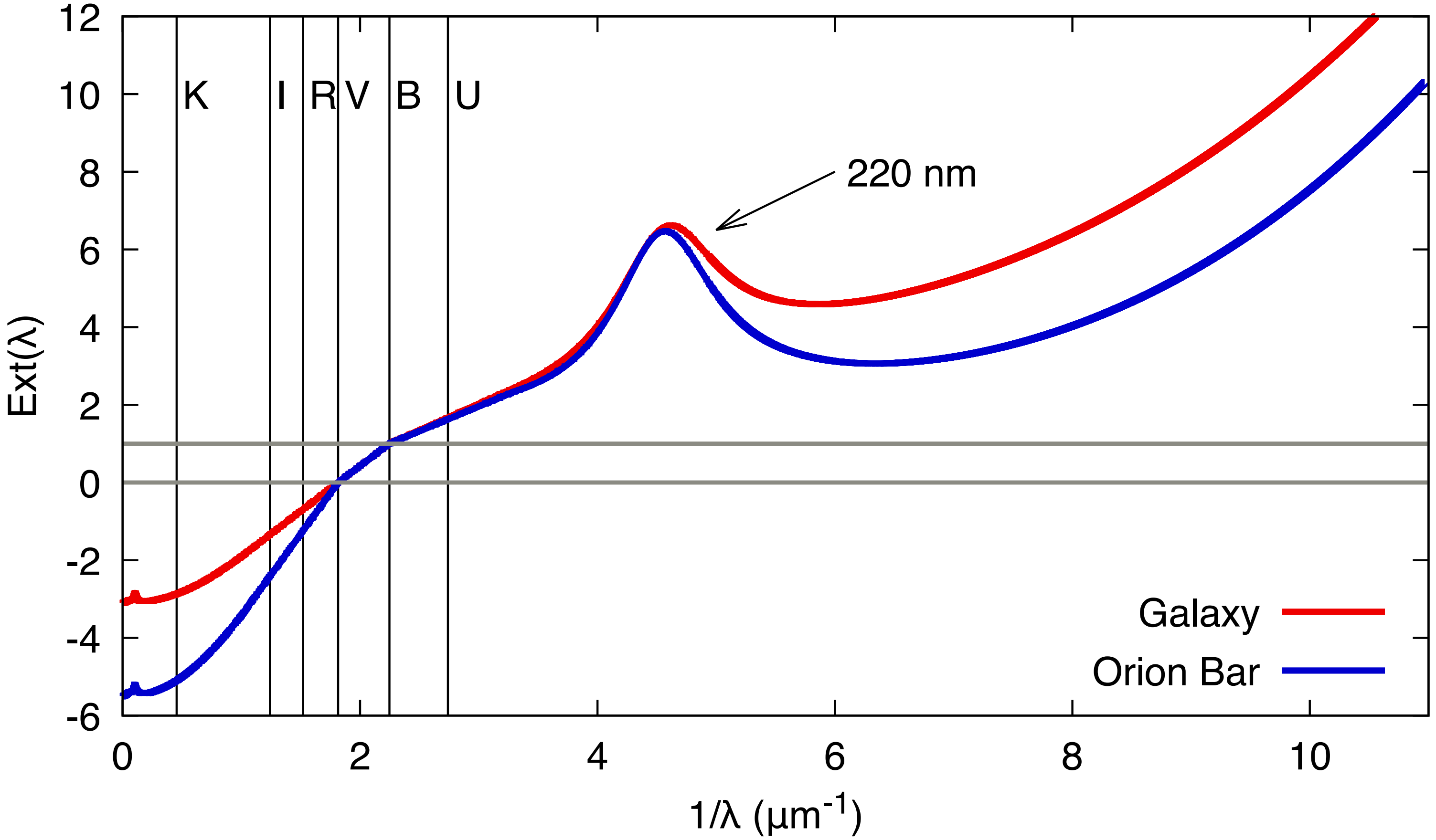
- Inversion:

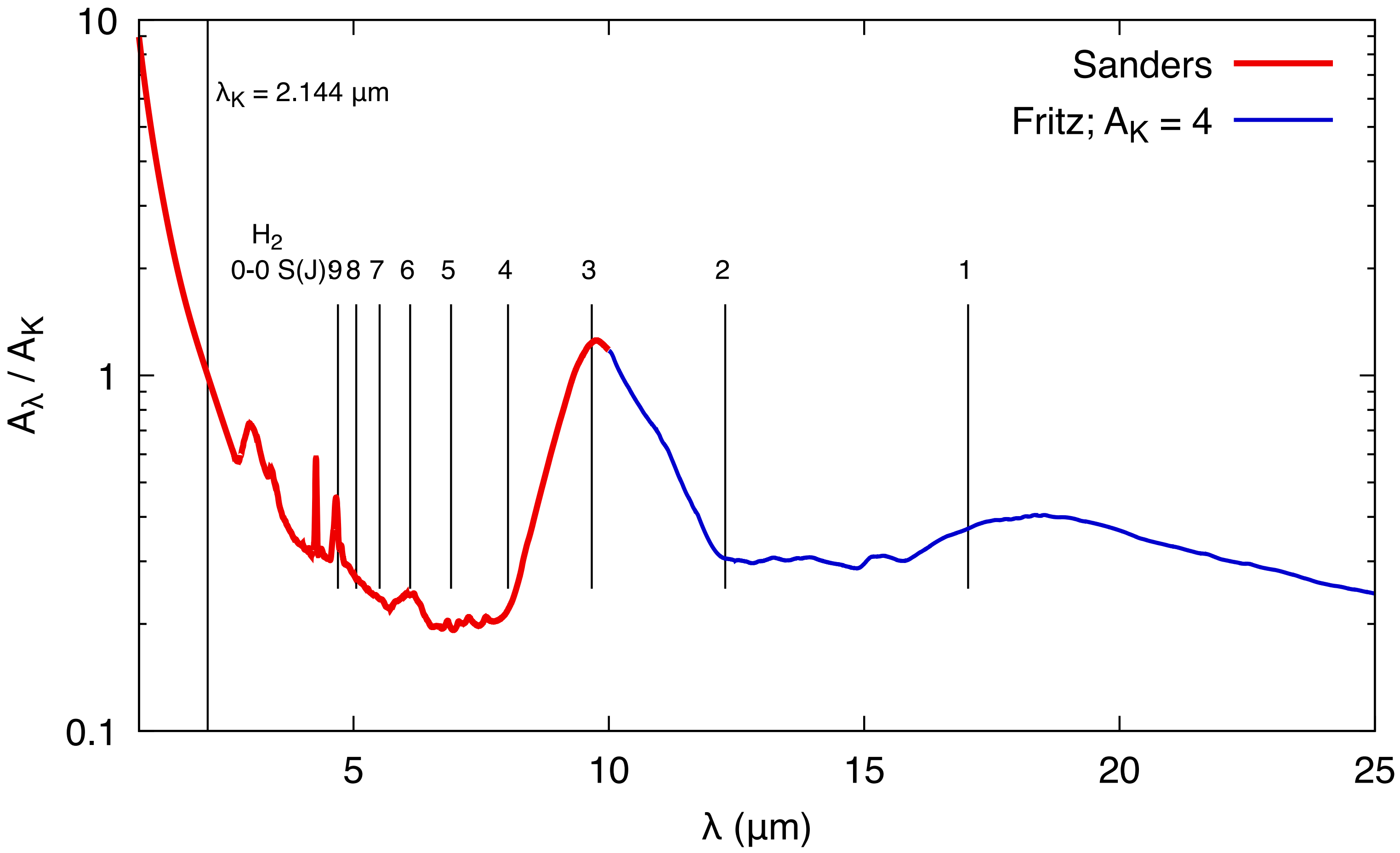
$$A_\lambda = A_\mathrm{V}\left(1 + \frac{Ext\,(\lambda)}{R_\mathrm{V}}\right)$$

Extinction curve



Galaxy: $R_\mathrm{V} \simeq 3.1$, $C_D \simeq 5.8\,10^{21}\,\mathrm{cm}^{-2}$.
Orion Bar: $R_\mathrm{V} \simeq 5.5$, $C_D \simeq 1.57\,10^{22}\,\mathrm{cm}^{-2}$.

Extinction curve



Galactic Center LoS - Fritz (2011) + Sanders (2022)

Size to extinction conversion

- Column density:

$$N_{\mathrm{H}} = \int_{LoS} n_{\mathrm{H}} \, ds = \frac{C_D}{R_{\mathrm{V}}} \, 2.5 \, \log_{10}(e) \int_{LoS} d\tau_{\mathrm{V}}$$

- So:

$$ds = 2.5 \, \log_{10}(e) \, \frac{C_D}{R_{\mathrm{V}}} \, \frac{1}{n_{\mathrm{H}}} \, d\tau_{\mathrm{V}}$$

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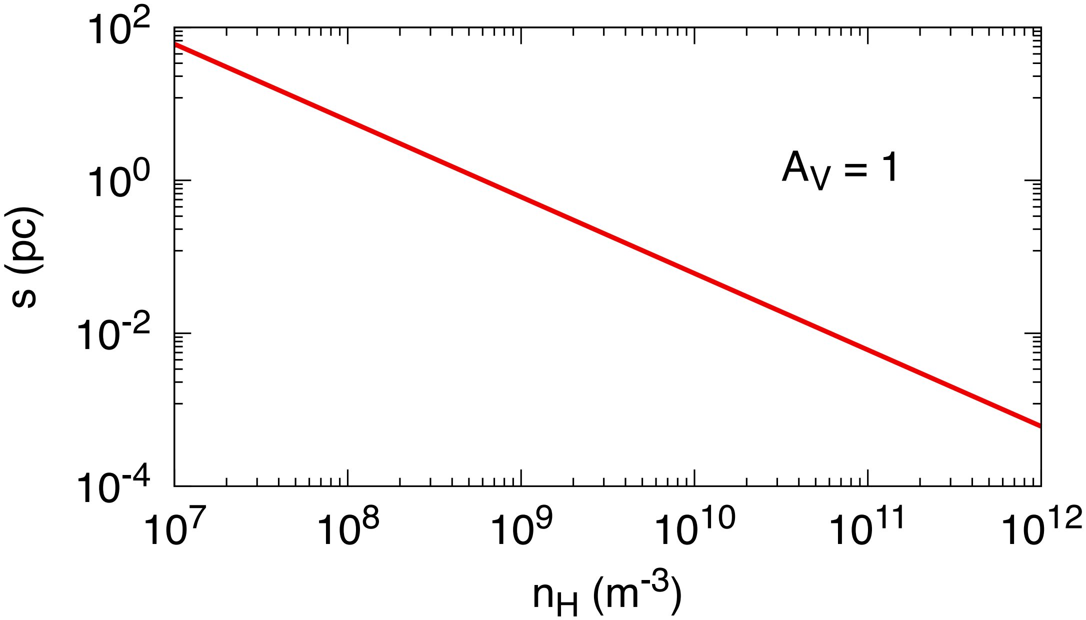
Galaxy:

$$s = \frac{1}{n_\mathrm{H}}\, \frac{C_D}{R_\mathrm{V}}\, A_\mathrm{V}$$



Non LTE situation

- Transfer equation (no scattering):

$$\frac{\partial I}{\partial s} = -\left(\kappa_D + \kappa_{lu}\right) I + \eta_{ul} + \eta_D$$

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- Line absorption and emission coefficients:

$$\kappa_{lu} = \frac{h\,c}{4\pi\,\lambda}\left(B_{lu}\,n_l - B_{ul}\,n_u\right)\phi_\lambda$$

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- Detailed balance:

$$n_l \left(B_{lu}\, \bar{J}_{lu} + k_{lu}^X\, n_X + D_l \right) = n_u \left(A_{ul} + B_{ul}\, \bar{J}_{ul} + k_{ul}^X\, n_X \right) + F_l$$

$$n_u \left(A_{ul} + B_{ul}\, \bar{J}_{ul} + k_{ul}^X\, n_X + D_u \right) = n_l \left(B_{lu}\, \bar{J}_{lu} + k_{lu}^X\, n_X \right) + F_u$$

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- $n_u\left(s_0\right)$ and $n_l\left(s_0\right)$ depend on mean radiation field $\bar{J}_{ul}$ at s_0.

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$\Rightarrow$ The problem is fully coupled!

- **If** $\bar{J}_{ul}$ is known, **then** all positions uncouple.

So, how can we estimate it?

Transfer equation revisited

- Along a sight line, without scattering (D: Dust):

$$\frac{\partial I}{\partial s} = -\left(\kappa_D + \kappa_{lu}\right) I + \eta_{ul} + \eta_D$$

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- Introducing populations:

$$\frac{\partial I}{\partial s} = \left[-E_{ul}\,\left(x_l - x_u\right)\,\phi_\nu\, I - \sigma_D\, I + D_{ul}\, x_u\, \phi_\nu + \epsilon_D\right]\, n_H$$

$$E_{ul} = \frac{c^2}{8\pi\,\nu_{ul}^2}\, g_u\, A_{ul}\,; \quad D_{ul} = \frac{h\nu_{ul}}{4\pi}\, g_u\, A_{ul}$$

$$\kappa_D = \sigma_D\, n_{\mathrm{H}}\,; \quad \eta_D = \epsilon_D\, n_{\mathrm{H}}$$

Optical depth

- Dust contribution:

$$\tau^D(s) = \int_0^s \sigma_D(t)\, n_H(t)\, dt$$

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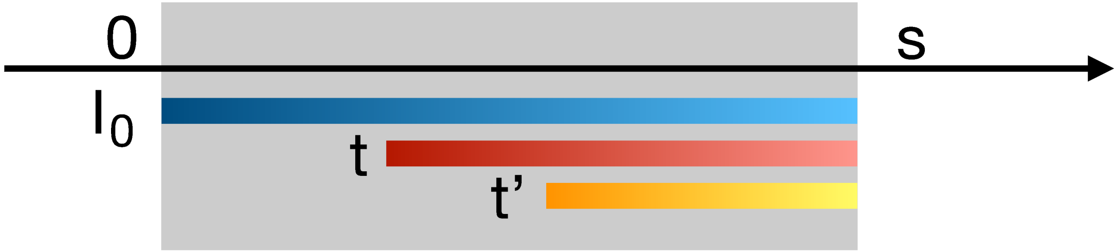
- Total:

$$\tau_T^\nu(s) = \tau^D(s) + \tau_\nu^L(s)$$

  - CO rot: Line dominates
  - H_2 vib: Dust dominates

Formal solution for I_ν



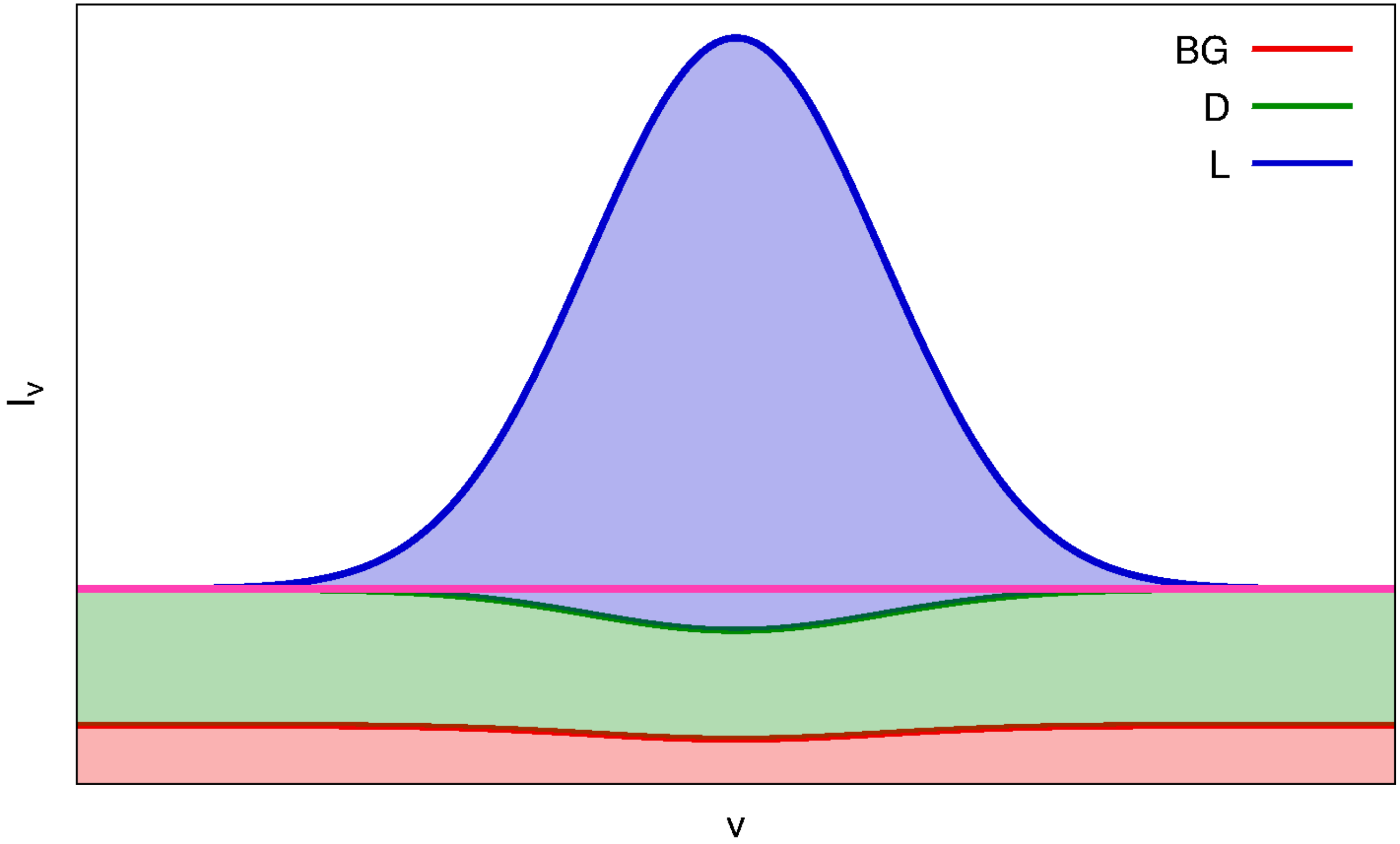
- Taking $\tau = 0$ at the "far end":

$$I_\nu(s) = I_\nu^0 \exp\left(-\tau_T^\nu(s)\right) + \int_0^s D_{ul}\, x_u \phi_\nu\, n_H \exp\left(\tau_T^\nu(t) - \tau_T^\nu(s)\right)\, dt + \int_0^s \epsilon_D\, n_H \exp\left(\tau_T^\nu(t) - \tau_T^\nu(s)\right)\, dt$$

- 3 contributions:

$$I_\nu(s,\mu) = I_\nu^{ext}(s,\mu) + I_{D,\nu}^{int}(s,\mu) + I_{ul,\nu}^{int}(s,\mu)$$

Contributions



Thick lines absorb the background!

Mean intensity (the tricky part)

- We need:

$$\bar{J}_{ul} = \int_{-\infty}^{+\infty} \left(\frac{1}{2} \int_{-1}^{+1} I_\nu \left(s, \mu\right) \, d\mu \right) \phi_\nu \, d\nu$$

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- Play with integration order if needed.
- Compute separately each contribution
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  - $\Rightarrow$ Helps understanding the origin of various approximations.
- External contribution ("Left" side):

$$\bar{J}_{ul}^{ext} = \int_{-\infty}^{+\infty} \left(\frac{1}{2} \int_{0}^{+1} I_\nu^0 \, \exp\left(-\tau_T^\nu \left(s, \mu \right) \right) \, d\mu \right) \phi_\nu \, d\nu$$

External contribution (Left)

- Angle integration:

$$J_\nu^{ext}\left(s\right) = \frac{I_\nu^0}{2}\int_0^1 \exp\left(-\frac{\tau_T^\nu\left(s\right)}{\mu}\right)d\mu$$

External contribution (Left)

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$$J_\nu^{ext}\left(s\right) = \frac{I_\nu^0}{2} \int_0^1 \exp\left(-\frac{\tau_T^\nu\left(s\right)}{\mu}\right) d\mu$$

- Frequency integration:

$$\begin{aligned} J_\nu^{ext}\left(s\right) &= \frac{I_\nu^0}{2} \int_{-\infty}^{+\infty} \left(\int_0^1 \exp\left(-\frac{\tau_T^\nu\left(s\right)}{\mu}\right) d\mu\right) \phi_\nu \, d\nu \\ &= I_\nu^0 \, \beta_L\left(s\right) \end{aligned}$$

$\Rightarrow$ Escape probability!

Escape probability (single side)

- Change of variable: $\alpha = 1/\mu$, $d\alpha/\alpha = -d\mu/\mu$:

$$\int_0^1 \exp\left(-\frac{\tau_T^\nu(s)}{\mu}\right) d\mu = \int_1^\infty \exp\left(-\alpha\,\tau_T^\nu(s)\right) \frac{d\alpha}{\alpha^2} = E_2\left(\tau_T^\nu(s)\right)$$

E_2: Exponential integral of the second kind.

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- Gaussian profile: use $z = \frac{\nu-\nu_{ul}}{\nu_{ul}}\ \frac{c}{v_T(s)}$ so $d\nu = dz\, \frac{v_T(s)}{c}\, \nu_{ul}$

$$\phi_z(s) = \frac{1}{\sqrt{\pi}\, \nu_{ul}}\, \frac{c}{v_T(s)}\, e^{-z^2}$$

$$\beta_L(s) = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-z^2}\, E_2\left(\tau_T^z(s)\right)\, dz$$

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$$\times \int_0^s \frac{n_H\left(t\right)}{v_T\left(t\right)}\, \left(x_l\left(t\right) - x_u\left(t\right)\right) \exp\left[-\left(\frac{\nu-\nu_0}{\nu_{ul}}\, \frac{c}{v_T\left(t\right)}\right)^2\right] dt$$

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- If $r = \frac{v_T(s)}{v_T(t)} \sim 1$:

$$\tau_T^z\left(s\right) = \tau_D\left(s\right) + e^{-z^2}\, \tau_L^0\left(s\right)$$

- $\tau_L^0\left(s\right)$: Line optical depth at line center $(z = 0)$.

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$\Rightarrow$ Gauss-Hermite integration is possible.

Line width

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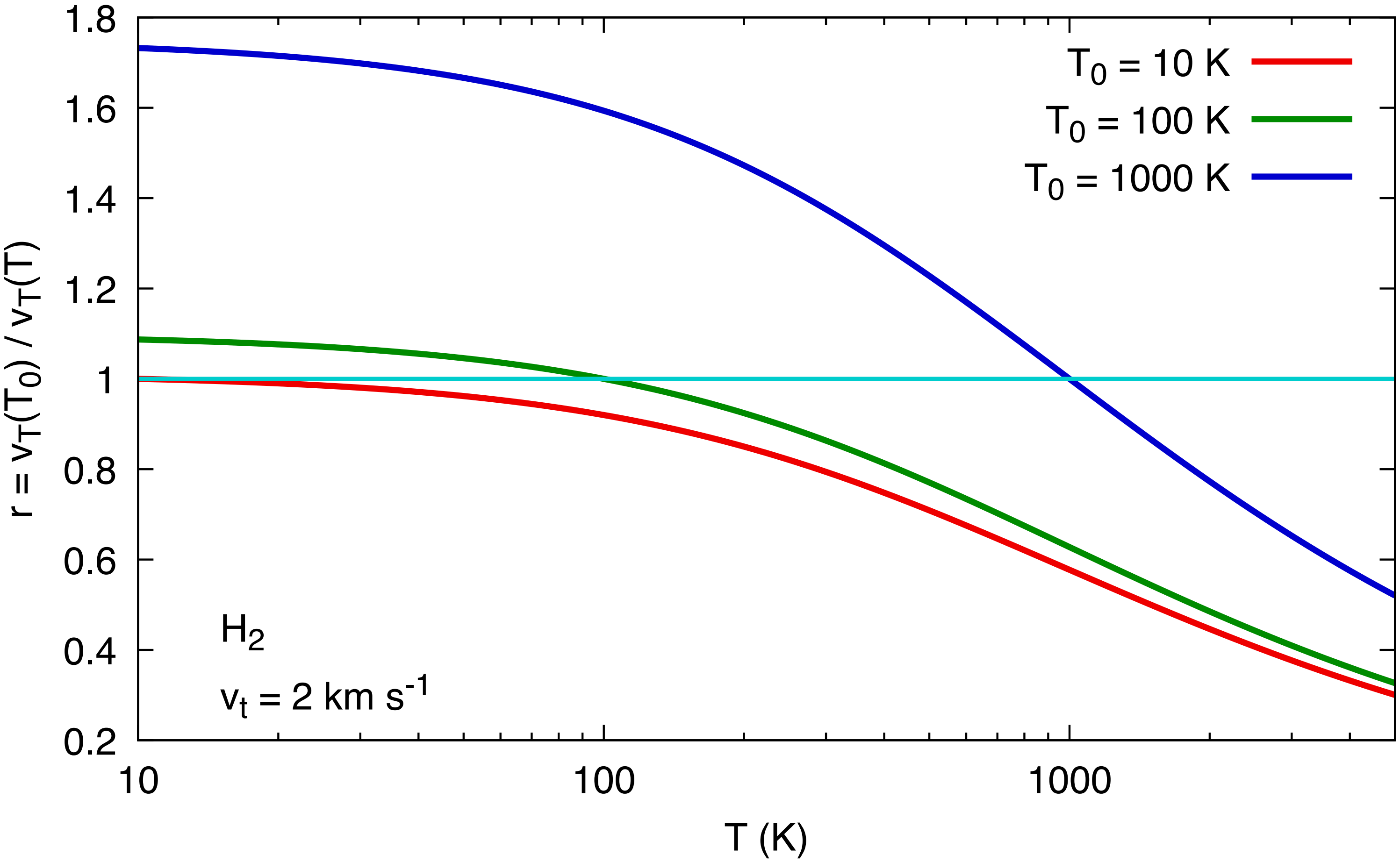
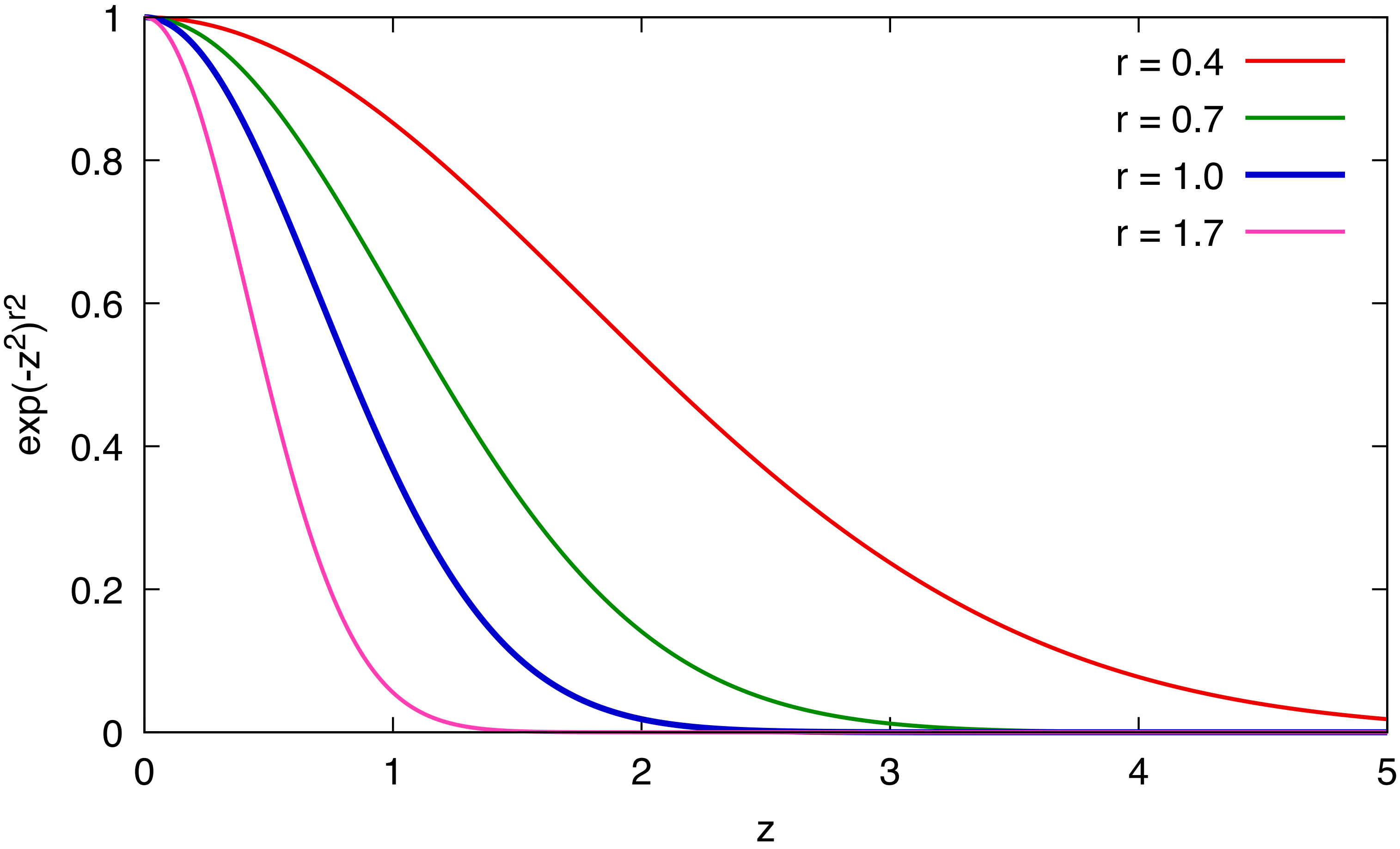


Depends on position in cloud and ratio of Turbulence / Thermal.

Line width



Approximation may be badly off ($r = \frac{v_T(s)}{v_T(t)}$)!

Various approximations for β

- Constant width approximation:

$$\beta_L\left(\tau_0\right) = \frac{1}{2\,\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-z^2}\, E_2\left(e^{-z^2}\,\tau^0\right)\, dz$$

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- RADEX LVG and Slab approximations:

$$\beta_{LVG}\left(\tau_0\right) = \frac{1}{2}\,\frac{1-e^{-\tau_0}}{\tau_0}\,;\;\; \beta_{PP}\left(\tau_0\right) = \frac{1}{2}\,\frac{1-e^{-3\tau_0}}{3\,\tau_0}$$

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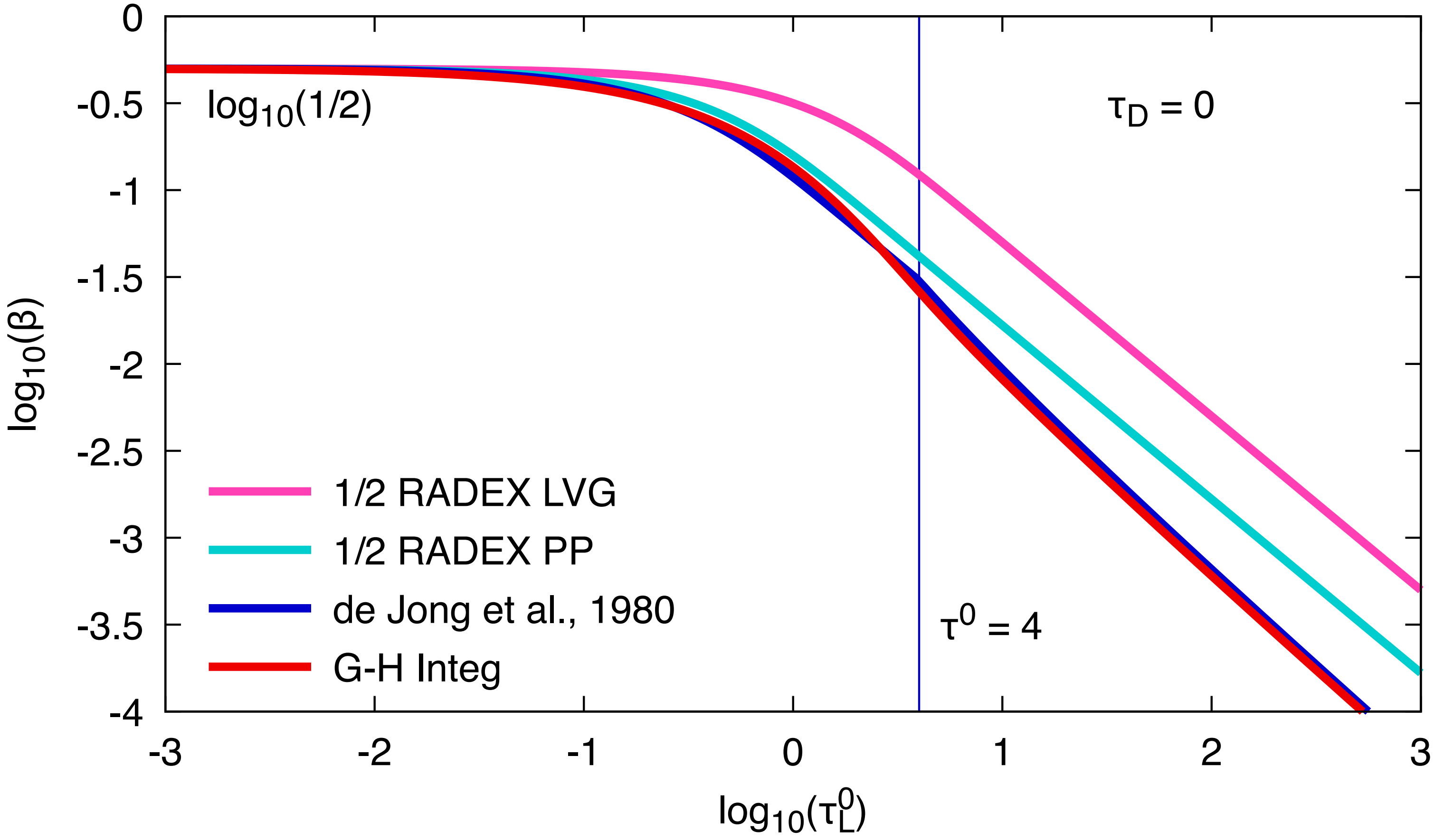
- de Jong, Boland, Dalgarno (1980)
(warning: $\tau = \tau_0\,\sqrt{\pi}$ in Appendix B):

$$\beta_{dJ}\left(\tau_0 < 4\right) = \frac{1}{2}\,\frac{1 - e^{-4.15\,\tau_0}}{4.15\,\tau_0}\,; \quad \beta_{dJ}\left(\tau \geqslant 4\right) = \frac{1}{4\sqrt{\pi}\,\tau_0\,\sqrt{\ln\left(\tau\right)}}$$

Escape probability (single side)



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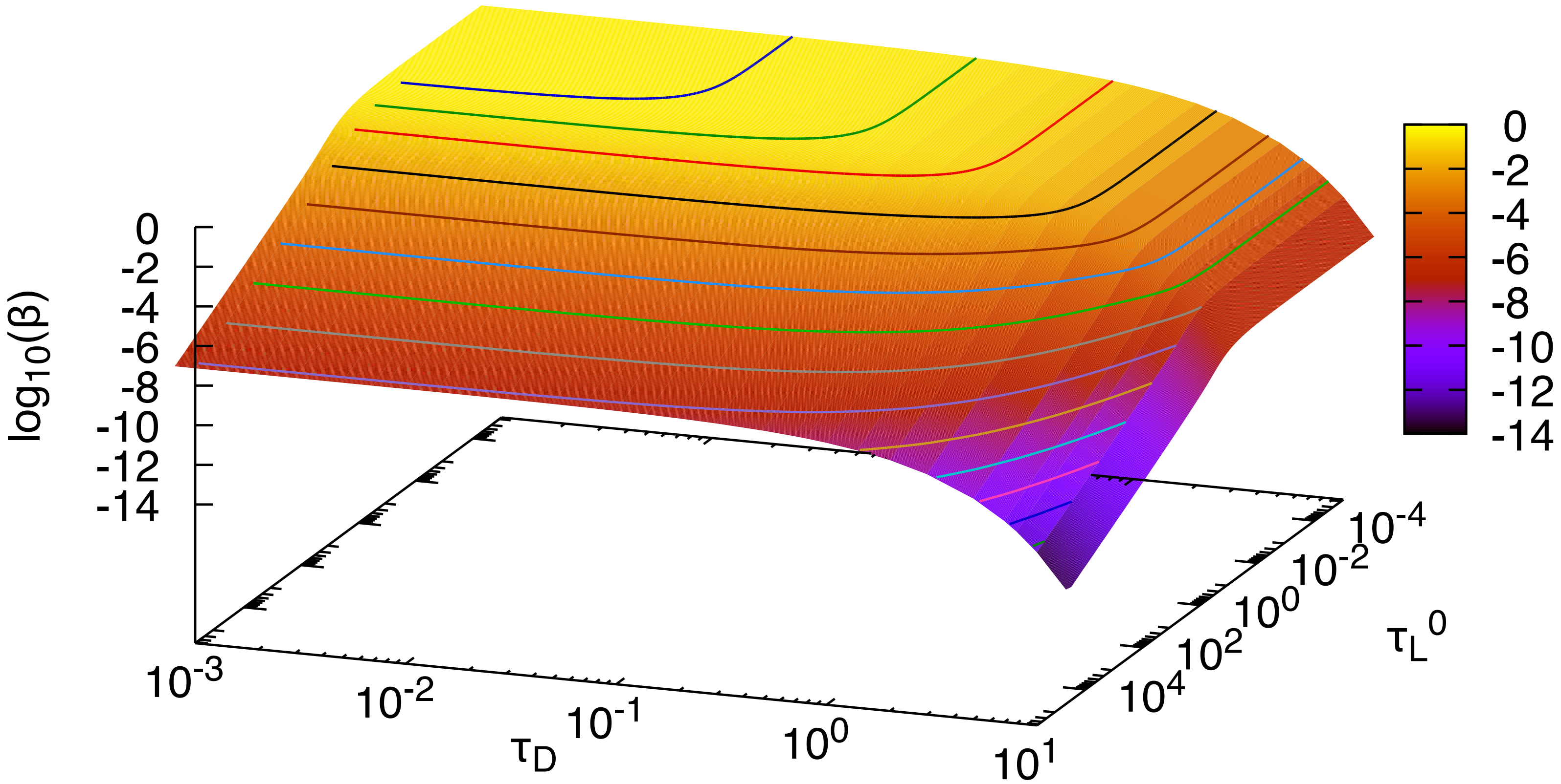

Gauss-Hermite integration

$$\beta \simeq \beta_{dJ}\left(\tau_0^L\right)\, E_2\left(\tau^D\right)$$

Internal contributions

- with $\Delta_s t = -\left|\tau_T^\nu(t) - \tau_T^\nu(s)\right|$:

$$\bar{J}_D^{int}(s) = \int_0^{s_{max}} \epsilon_D(t)\; n_H(t)\; L_{1,s}(\Delta_s t)\; dt$$

$$\bar{J}_{ul}^{int}(s) = \frac{h\nu_{ul}}{4\pi}\,\frac{A_{ul}}{\nu_{ul}}\,\int_0^{s_{max}} n_u(t)\; K_{1,s}(\Delta_s t)\; dt$$

- Interpretation is simple:
  - $\begin{cases} \epsilon_D(t)\; n_H(t) \\ \frac{h\nu_{ul}}{4\pi}\,\frac{A_{ul}}{\nu_{ul}}\, n_u(t) \end{cases}$: Photons emitted at t.
  - $\begin{cases} L_{1,s}(\Delta_s t) \\ K_{1,s}(\Delta_s t) \end{cases}$: Fraction of photons that reach s from t.

Kernel functions

Interstellar extinction
Non LTE situation
Coupled problem
Transfer equation
Optical depth
Formal solution
Contributions
Mean intensity
External contribution
Escape probability
Line width
Various approximations
Internal contributions
Kernel functions
Conclusion
Some codes
Collisions
H_3^+ excitation
Conclusions

- Kernel function $L_{1,s}$ (dust) and $K_{1,s}$ (line):

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- If $v_T \sim Cte$:

$$L_{1,s}(\Delta_s t) = \frac{1}{2\sqrt{\pi}}\int_{-\infty}^{+\infty} e^{-z^2}$$

$$E_1\left(\left(\tau_D(t) - \tau_D(s)\right) + e^{-z^2}\,\left(\tau_L^0(t) - \tau_L^0(s)\right)\right)\, dz$$

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Conclusion

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  - Long.
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  - Define what you need.
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- Various codes offer various degrees of approximation.
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  - Then (and only then) chose your best bet.
- If none exists: you're on your own...

Some codes

Simple review paper: van der Tak (2011)
(but see Asensio Ramos, 2018).

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- Fast and simple:
  - LTE ⇒ Too crude.
  - LVG (Sobolev) ⇒ Limited use for ISM.
    - But see RADMC-3D, Section 7.6 of manual.
  - RADEX ⇒ “Simple” Escape probability.

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    - But see RADMC-3D, Section 7.6 of manual.
  - RADEX ⇒ "Simple" Escape probability.
- CPU demanding:
  - MALI ("Multilevel Accelerated Lambda Iteration") ⇒ Accurate and complex. E.g.: RH.
  - LIME (no update since 2018), MCFOST ⇒ Monte-Carlo
  - MOLPOP-CEP ⇒ "Think different"!
  - Meudon PDR ⇒ "More specific"

Local approximations

- Use only local values for computations
- Various levels of approximation:
    - $v_T = Cte$ (neglect variations of line profile)
    - n_{H}, T, ... $= Cte$ (uniform profile)
    - Escape probability prescription (LVG or not)
    - 0D vs. 1D

Sobolev Approximation and RADMC-3D

- Sobolev: “Large Velocity Gradient”.
- Crudest approximation possible.
- Use only for **large** velocity gradients!
- Fallback for computationally intensive codes:
    - See doc at RADMC-3D

Take Away Message: Do not use if you can avoid it.

But only solution for time dependent MHD simulations.

RADEX

- van der Tak et al. (2007).
  - Non-LTE
  - Isothermal, homogeneous medium.
  - 3 options for β, all simple.
- Available at: RADEX

Take away message (by Floris...):
“Proper modeling of optically thick lines requires programs that resolve the source both spectrally and spatially”
(end of Appendix A)

ALI and MALI

- Best reference: Rybicki and Hummer (1991) and (1992)
  - Simple operator splitting:

$$J = \Lambda \left[S \left(J \right) \right]$$

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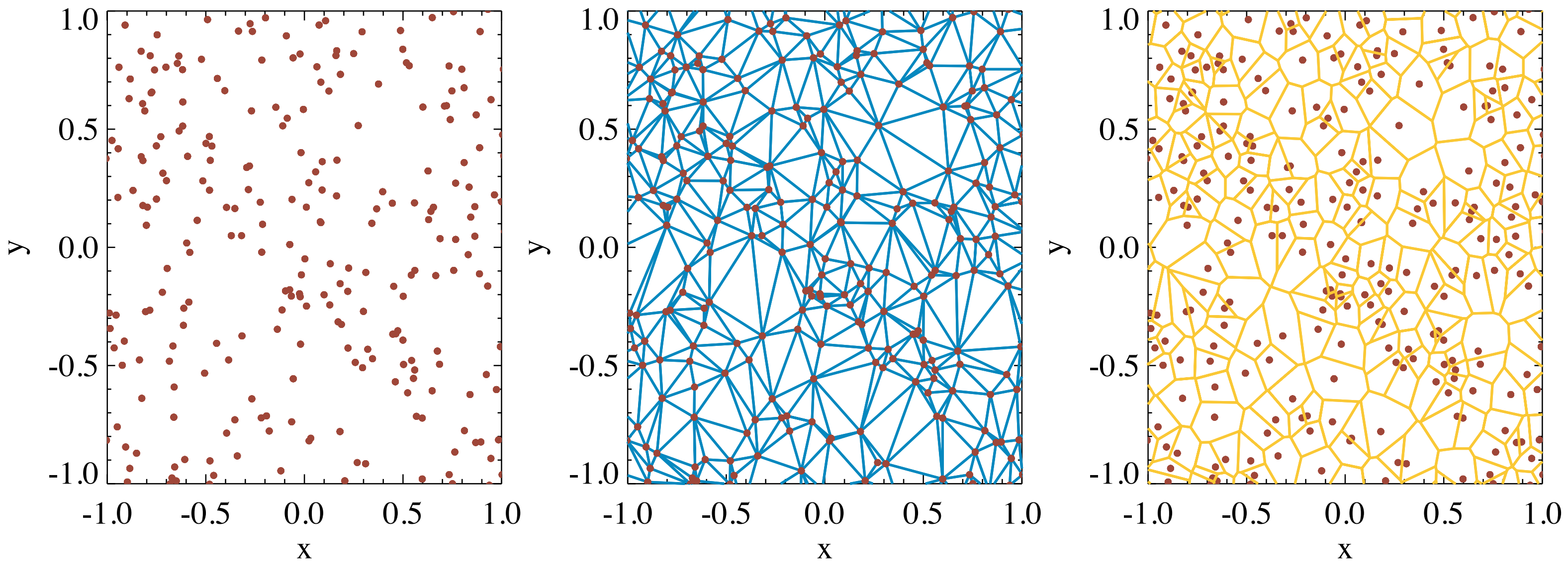
  - Requires simultaneous solution on full spatial grid
    ⇒ coupling with chemistry and thermal balance difficult.
  - Most widely used method. e.g.:
    - MALI or NLTE2D
      (MEDOC and F. Paletou)
    - RH 1.5D: Documentation and Git lab
      (Uitenbroeck and Pereira)
    - Daniel & Cernicharo (2008) and (2013)
      (Availability unknown...)

Monte-Carlo

- Mika Juvela family of codes:
    - Cppsimu, CRT, DIES, LOC, PEP, SOC.
    - Sophisticated transfer (polarization...), simple micro-physics.
- LIME: Based on RATRAN. See Brinch and Hogerheijde (2010).
    - Uses Delaunay triangulation and Voronoi tesselation.



MOLPOP-CEP

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  - n_i depend on $\bar{J}_\nu$.

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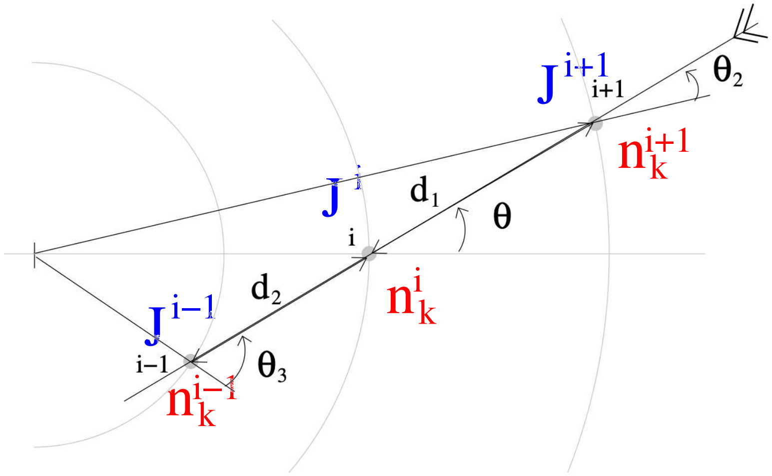
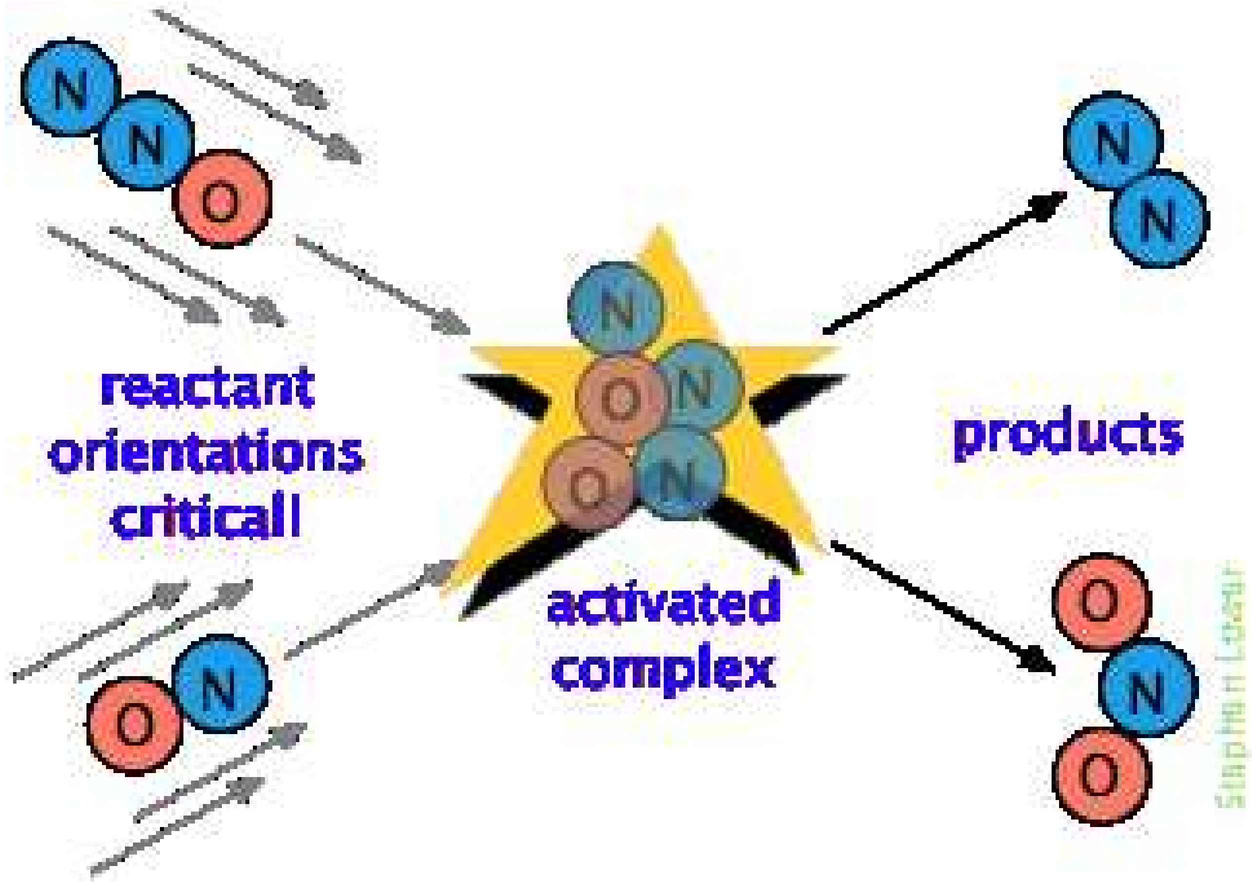
  - n_i depend on $\bar{J}_\nu$.
  - $\bar{J}_\nu$ depend on n_i
  - Replace $\bar{J}_\nu$ by its expression in balance equations for n_i.
  - One (huge) non linear system of equations for n_i at every positions, **without** computing the radiation field!
- Could be used more often.



© Daniel & Cernicharo (2008)

Collisions



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Type of collisions

- Most general binary collision:

$$A\left(St1\right)+B\left(St2\right)\rightarrow C\left(st3\right)+D\left(St4\right)$$

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◆ $(St2) = (St4)$: Simple inelastic collisions. E.g.:

$$\mathrm{C}^+\left({}^2P_{1/2}\right) + \mathrm{H} \rightleftharpoons \mathrm{C}^+\left({}^2P_{3/2}\right) + \mathrm{H}$$

Collisions computation

- Strategy:
  - Compute Potential Energy Surface (PES).
  - Compute deexcitation rates.
    Quasi-Classical or Full Quantum
  - Deduce excitation by detailed balance.

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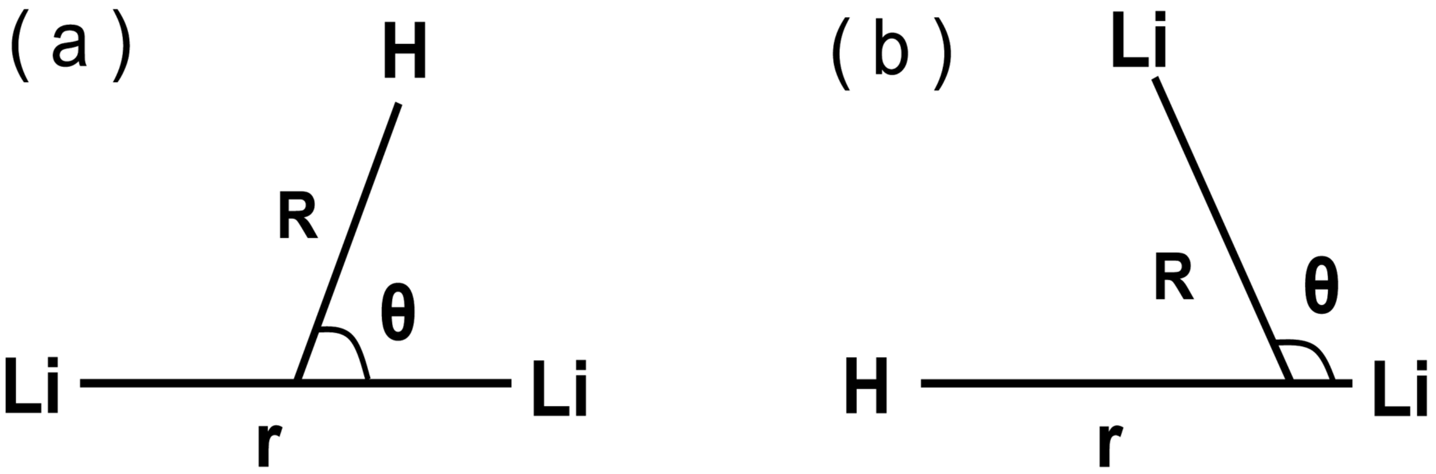
    Quasi-Classical or Full Quantum
  - Deduce excitation by detailed balance.
- Configurations. Jacobi coordinates
  (all geometry required):



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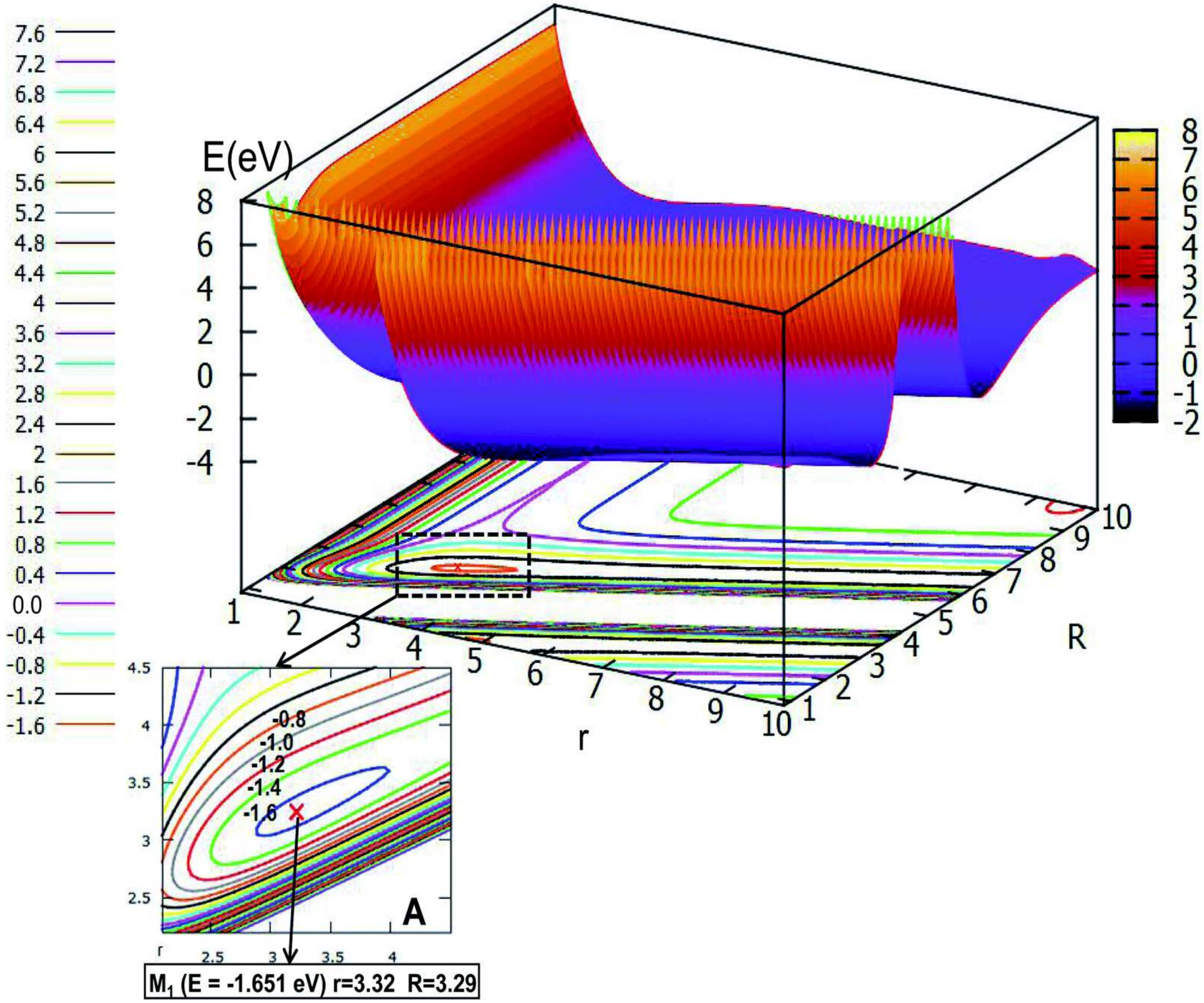
Example: $\mathrm{Li}_2 + \mathrm{H}$



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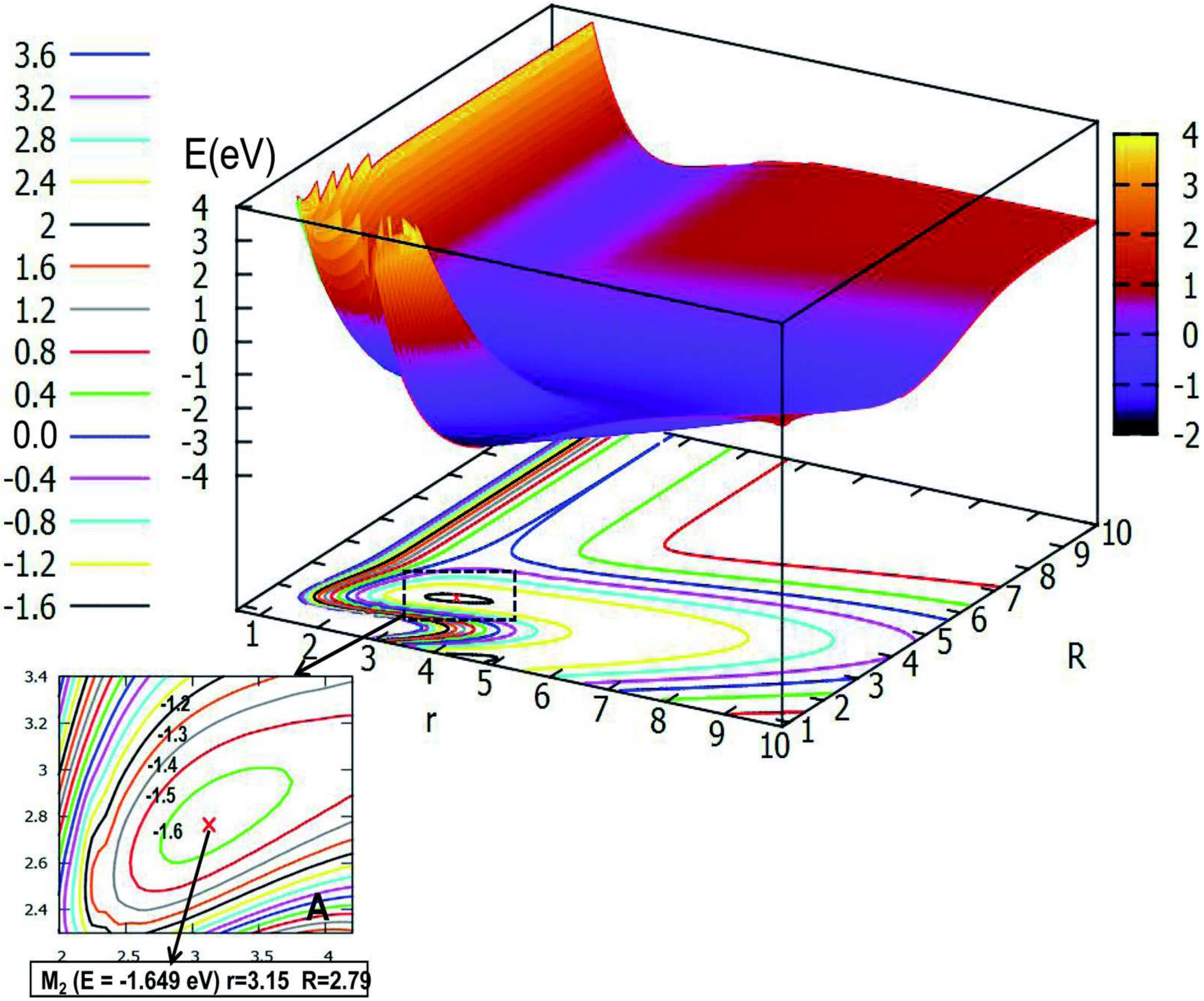

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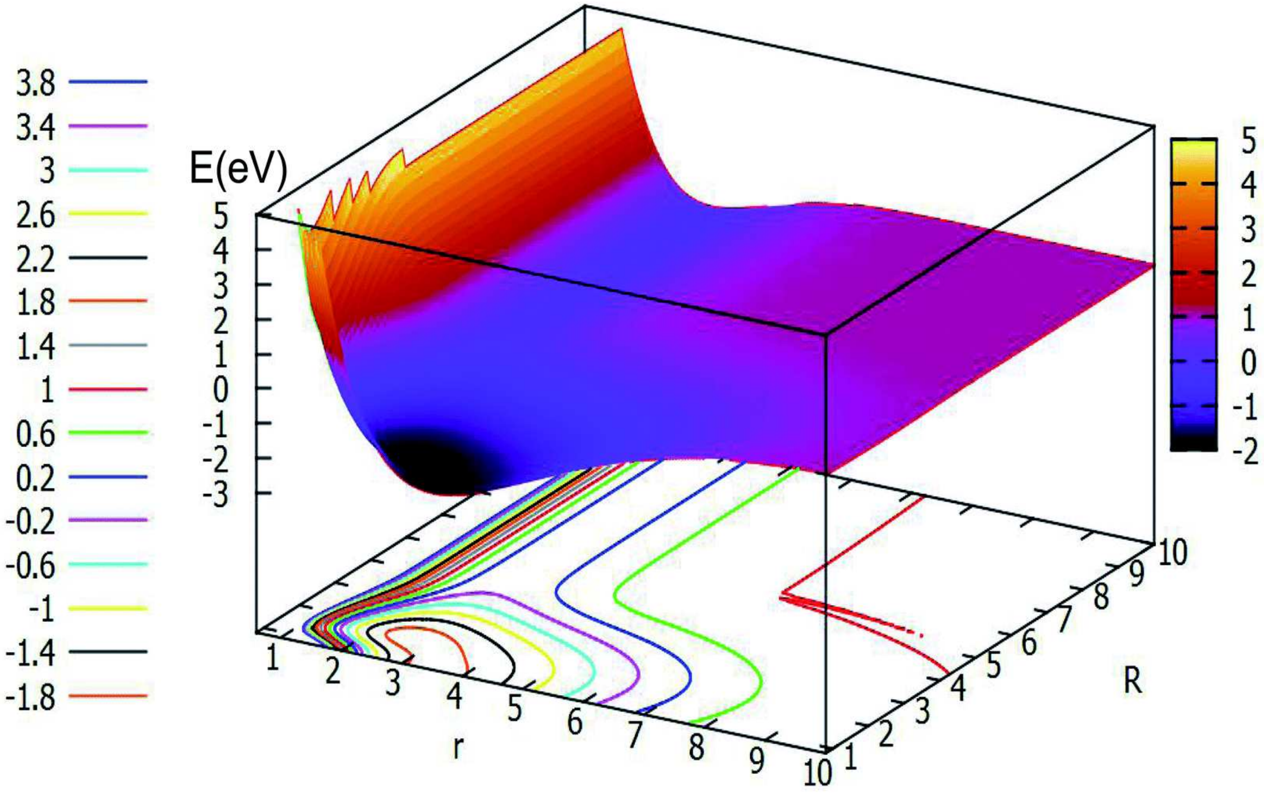

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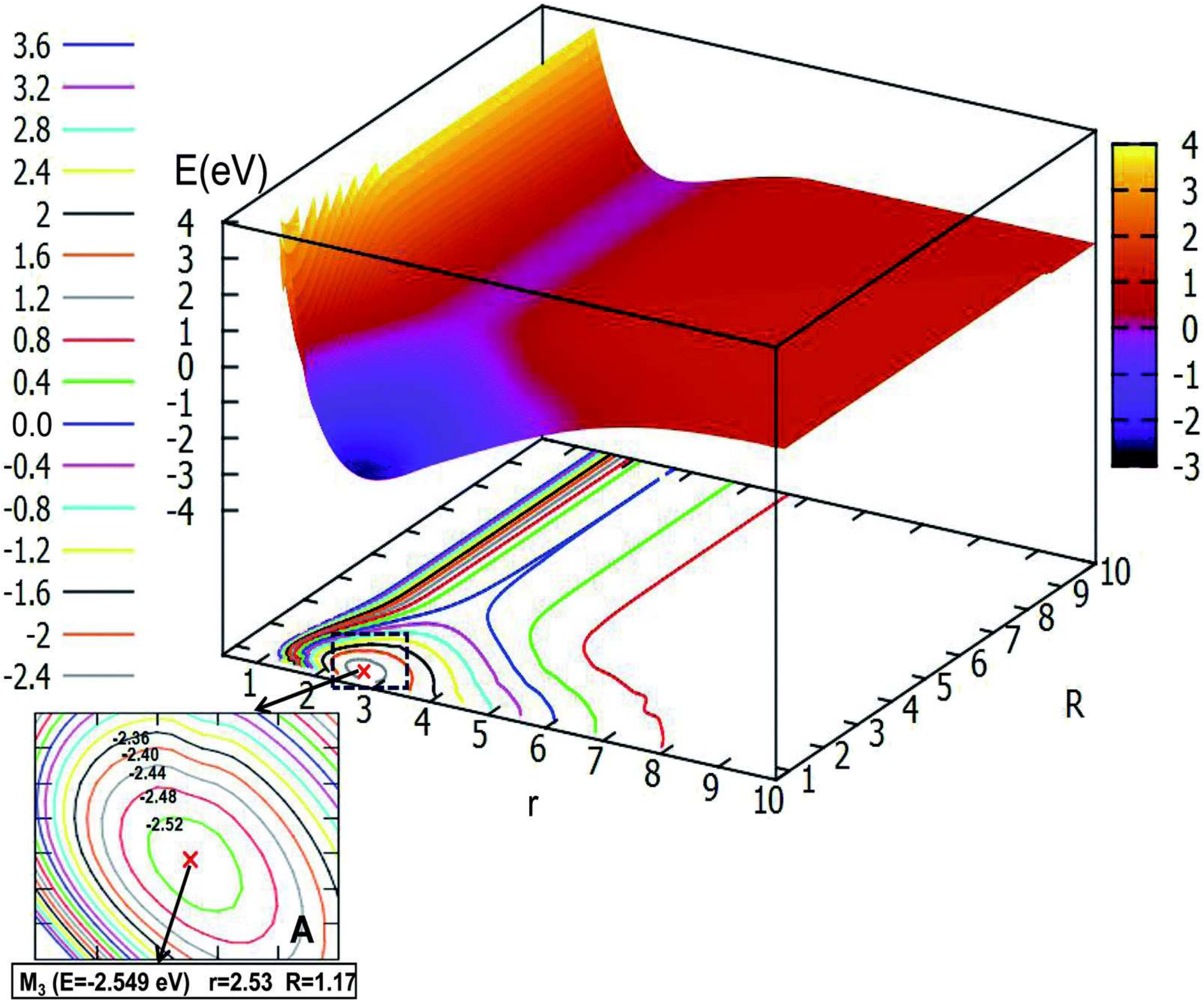

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Conclusion

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    - Always long and expensive.
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  - More reliable if properly done.

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  - Always long and expensive.
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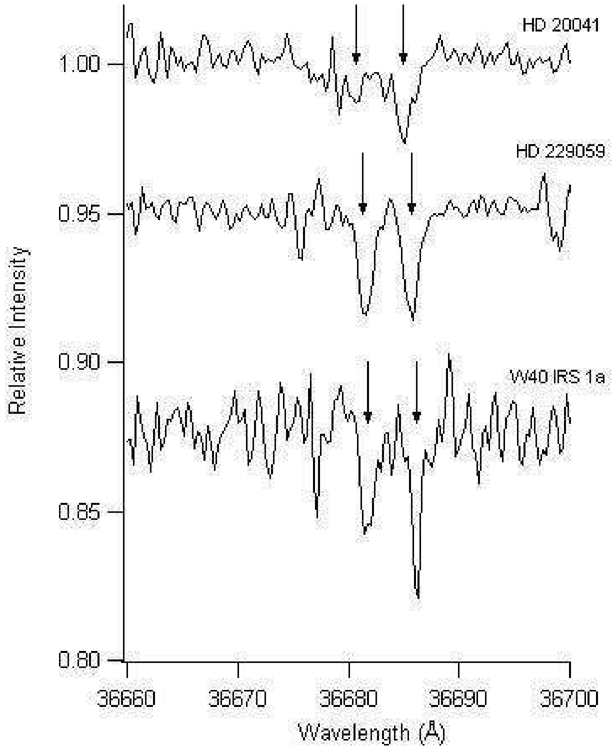
- Experiments:
  - Not always possible.
  - Always long and expensive.
  - More reliable if properly done.
- Databases:
  - EMAA (Grenoble)
  - Basecol.
  - LAMBDA (Leiden).
  - CHIANTI.
  - ...

H_3^+ excitation



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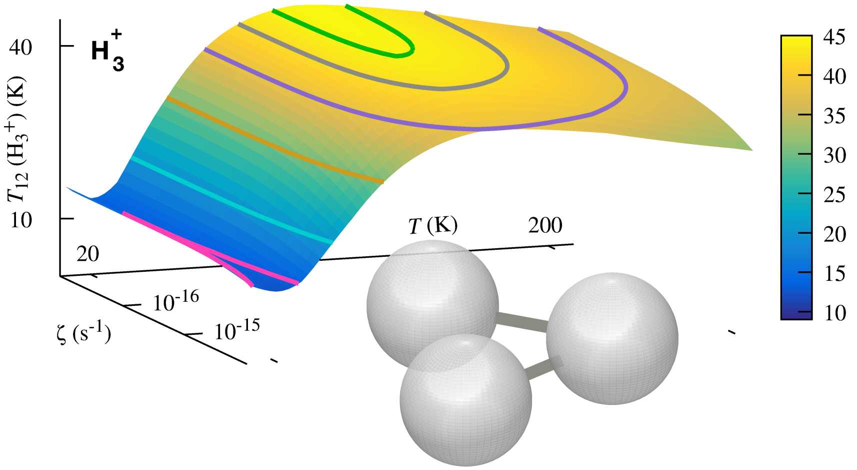

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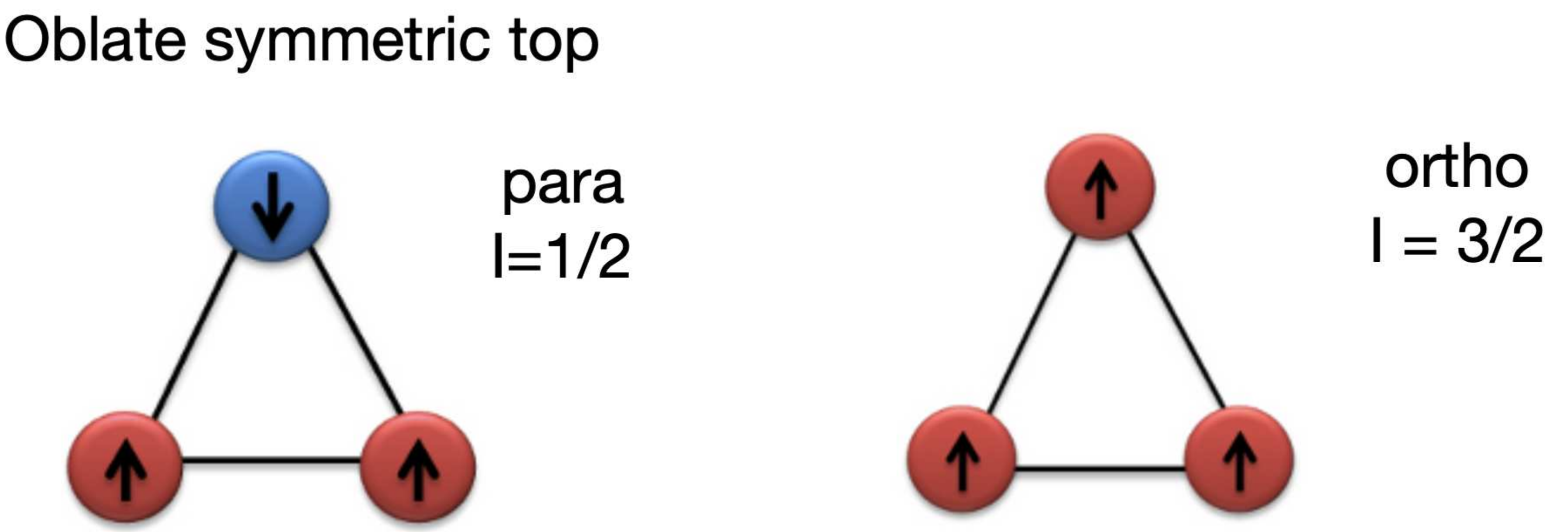
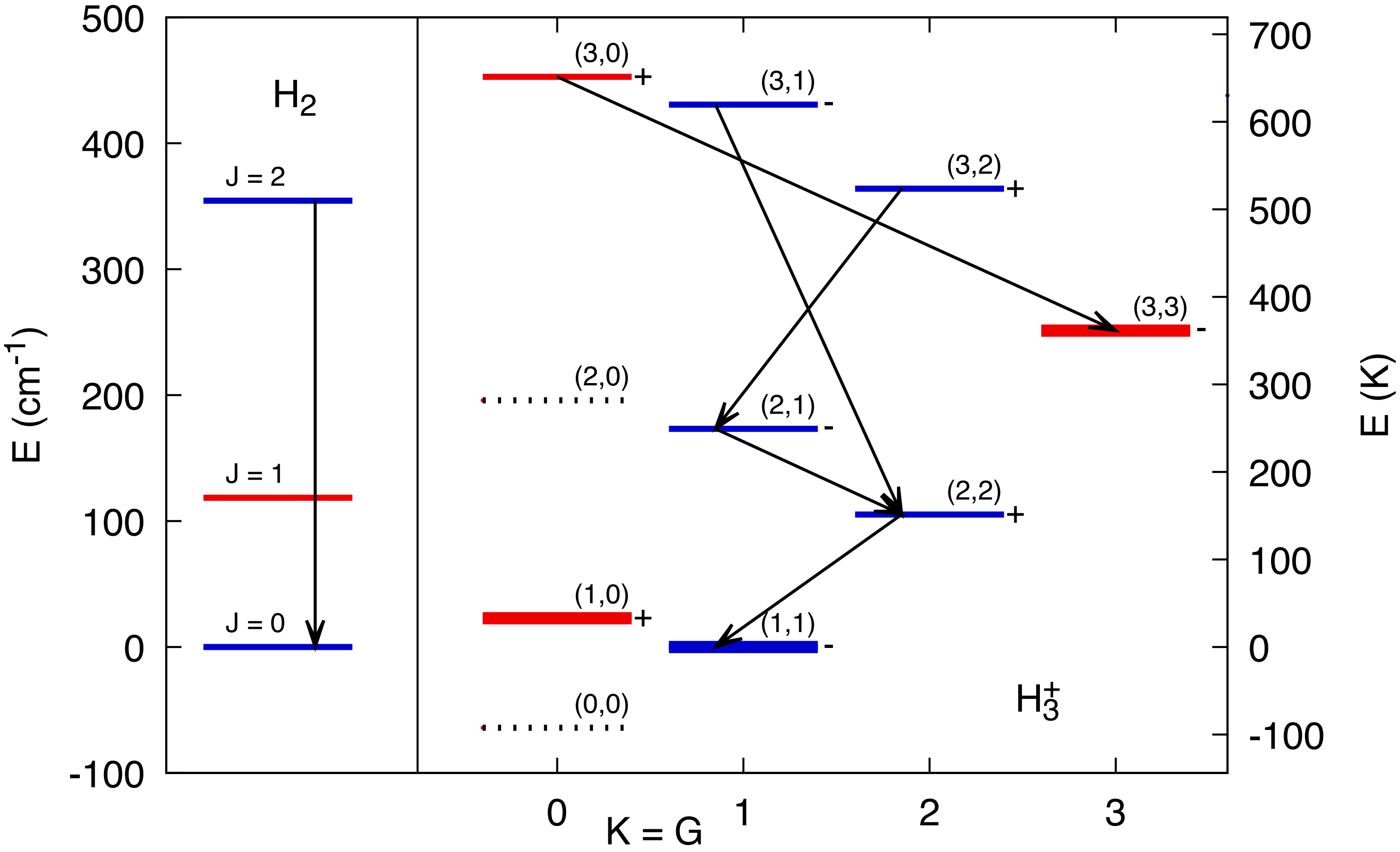
H_3^+ structure



- Quantum numbers (see Lindsay & McCall, 2001):
  - I: Nuclear spin ($1/2$ or $3/2$). $P \nleftrightarrow O$.
  - J: Total angular momentum.
  - G: Projection on symmetry axis.
- For $v = 0$: levels labeled with (G, J).
- Ortho: $G = 3\,n$, Para: $G = 3\,n \pm 1$.

H_3^+ structure (pure rotation)



Blue: para, Red: ortho
Note metastable levels $(1,0)$ and $(3,3)$

H_3^+ chemistry

- Formation:

$$H_2 + \zeta \rightarrow H_2^+ + e^-$$

$$H_2^+ + H_2 \rightarrow H_3^+ + H \ + \ 20000\,\mathrm{K}$$

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$$H_3^+ + e^- \rightarrow H_2 + H$$

$$H_3^+ + X \rightarrow HX^+ + H_2$$

H_3^+ is **very** strongly coupled to H_2.

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- Excitation temperature:

$$T_{ex}\left(H_3^+\right) = T_{21} = \frac{\Delta E/k}{\ln\left(\frac{g_{1,0}}{g_{1,1}}\frac{N_{1,1}}{N_{1,0}}\right)}$$

H_2 and H_3^+ observations

Source	n_{H}	$T_{ex}\,(\mathrm{H_2})$	$T_{ex}\,(\mathrm{H_3^+})$
	(cm^{-3})	(K)	(K)
HD154368	240	51 ± 8	20 ± 4
HD73882	520	51 ± 6	23 ± 3
HD27778 (62 Tau)	280	55 ± 7	29 ± 4
HD24398 (ζ Per)	215	57 ± 6	28 ± 4
HD24534 (χ Per)	325	57 ± 4	46^{+21}_{-13}
HD41117 (χ^2 Ori)	200	60 ± 7	29 ± 13
HD110432	140	68 ± 5	30 ± 2
HD210839 (λ Cep)	115	72 ± 6	34 ± 2
HD43384 (9 Gem)	120	74 ± 15	38 ± 11

Why is $T_{ex}\,(\mathrm{H_3^+}) \neq T_{ex}\,(\mathrm{H_2})$?

Processes affecting H_3^+ excitation

- Radiative transitions:
  - Do not change spin.

Processes affecting H_3^+ excitation

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H_3^+ chemistry
H_3^+ observations
Processes affecting H_3^+ excitation
Reactive collisions
Chemical formation
Chemical destruction
Detailed balance
Impact of N
Why?
Observations
Conclusions

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- Chemical formation.
  - Depends on Ortho or Para state of reactants (H_2^+ and H_2).
- Chemical destruction.
  - Maybe state dependent.

Reactive collisions with H_2

- 3 different channels:

$$H_3^+\,(J',G') + H_2 \rightarrow H_3^+\,(J",G") + H_2$$

$$H_3^+\,(J',G') + H_2 \rightarrow H_2 + (HH_2)^+\,(J",G")$$

$$H_3^+\,(J',G') + H_2 \rightarrow HH + (H_2H)^+\,(J",G")$$

- Or:
  - Inelastic
  - Proton - Hop (reactive)
  - Exchange (reactive)
- Rates deduced from PES of H_5^+ (O. Roncero and collab.) following arguments of Crabtree (2011).

Chemical formation

- Define:

$$p_2 = \frac{n\left(p-\mathrm{H}_2\right)}{n\left(p-\mathrm{H}_2\right)+n\left(o-\mathrm{H}_2\right)}\ ;\ p_3 = \frac{n\left(p-\mathrm{H}_3^+\right)}{n\left(p-\mathrm{H}_3^+\right)+n\left(o-\mathrm{H}_3^+\right)}$$

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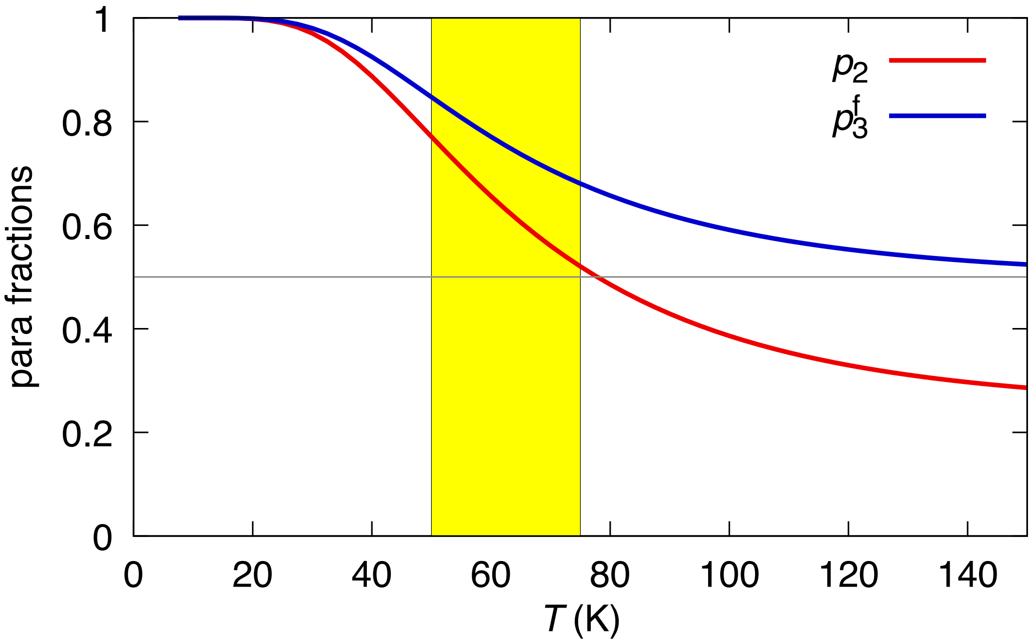
- Branching ratio $\mathrm{H}_2^+ + \mathrm{H}_2 \rightarrow \mathrm{H}_3^+ + \mathrm{H} + 20000\,\mathrm{K}$

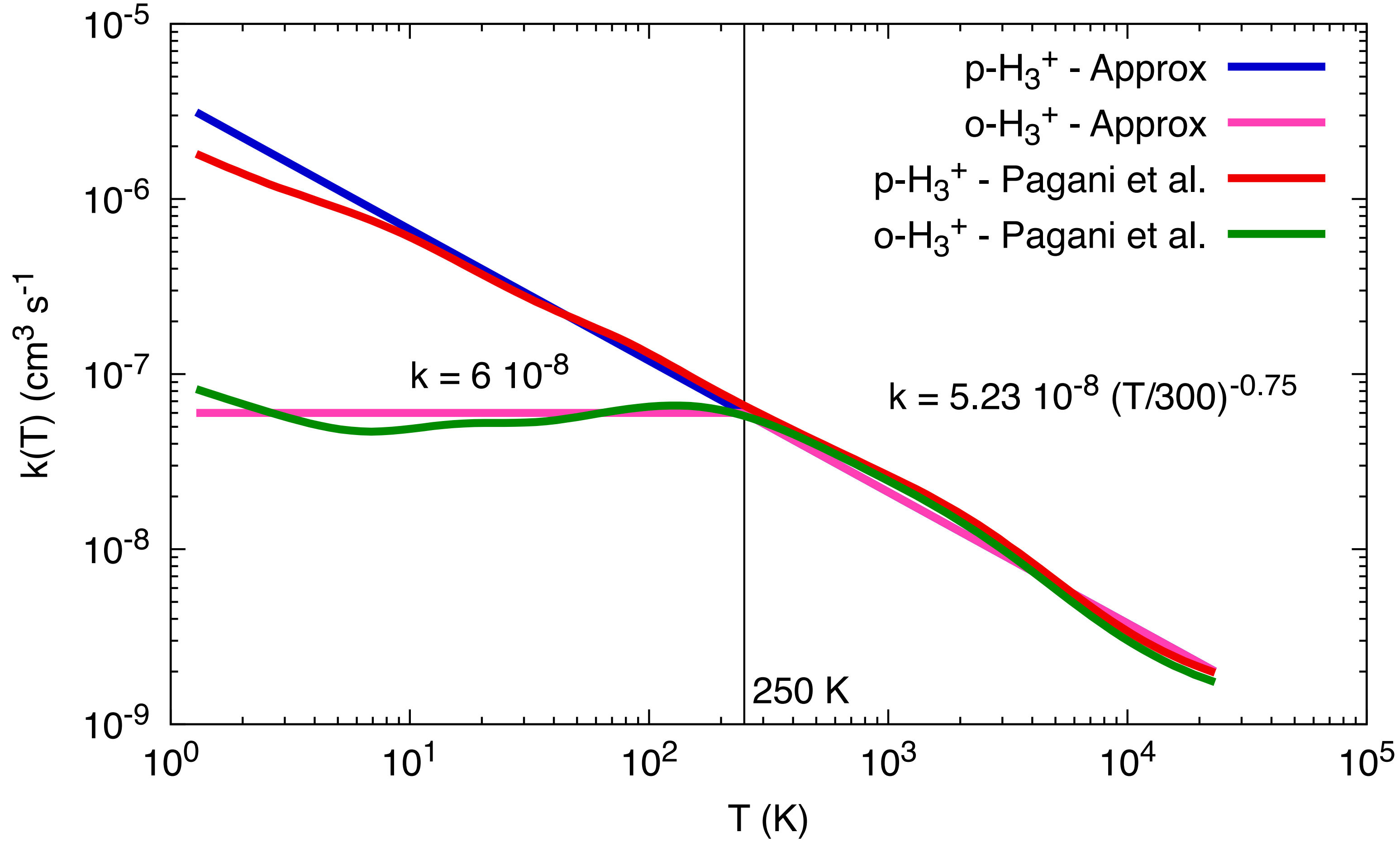


$$p_3^f = \frac{1+2\,p_2}{3}$$

$$x_{J,G} \propto g_{J,G}$$

Chemical destruction

- Dissociative recombination, Pagani et al. (2009):



Detailed balance

- 24 levels included.
- State specific formation / destruction included.
- State specific $\mathrm{H_2}$ collision rates included.
- Explore T, ζ, n_H.

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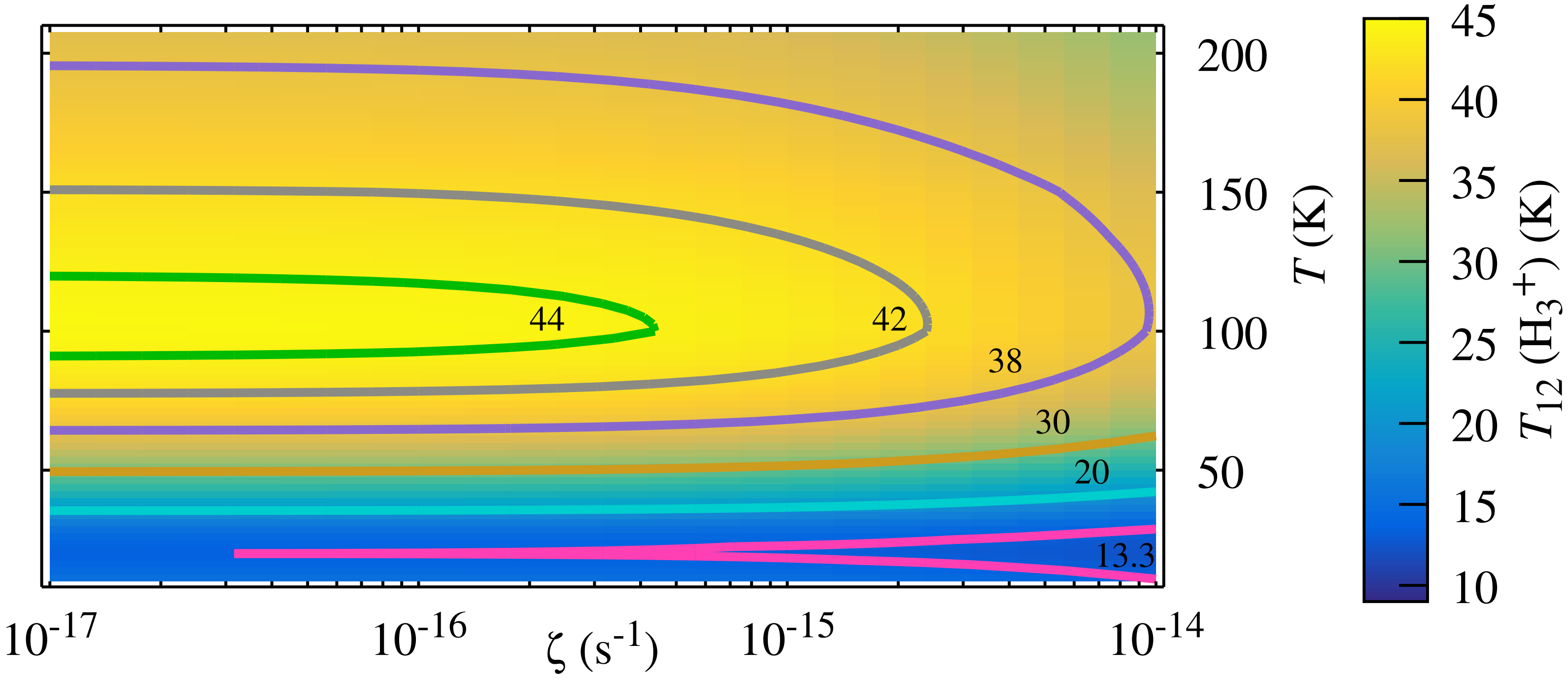
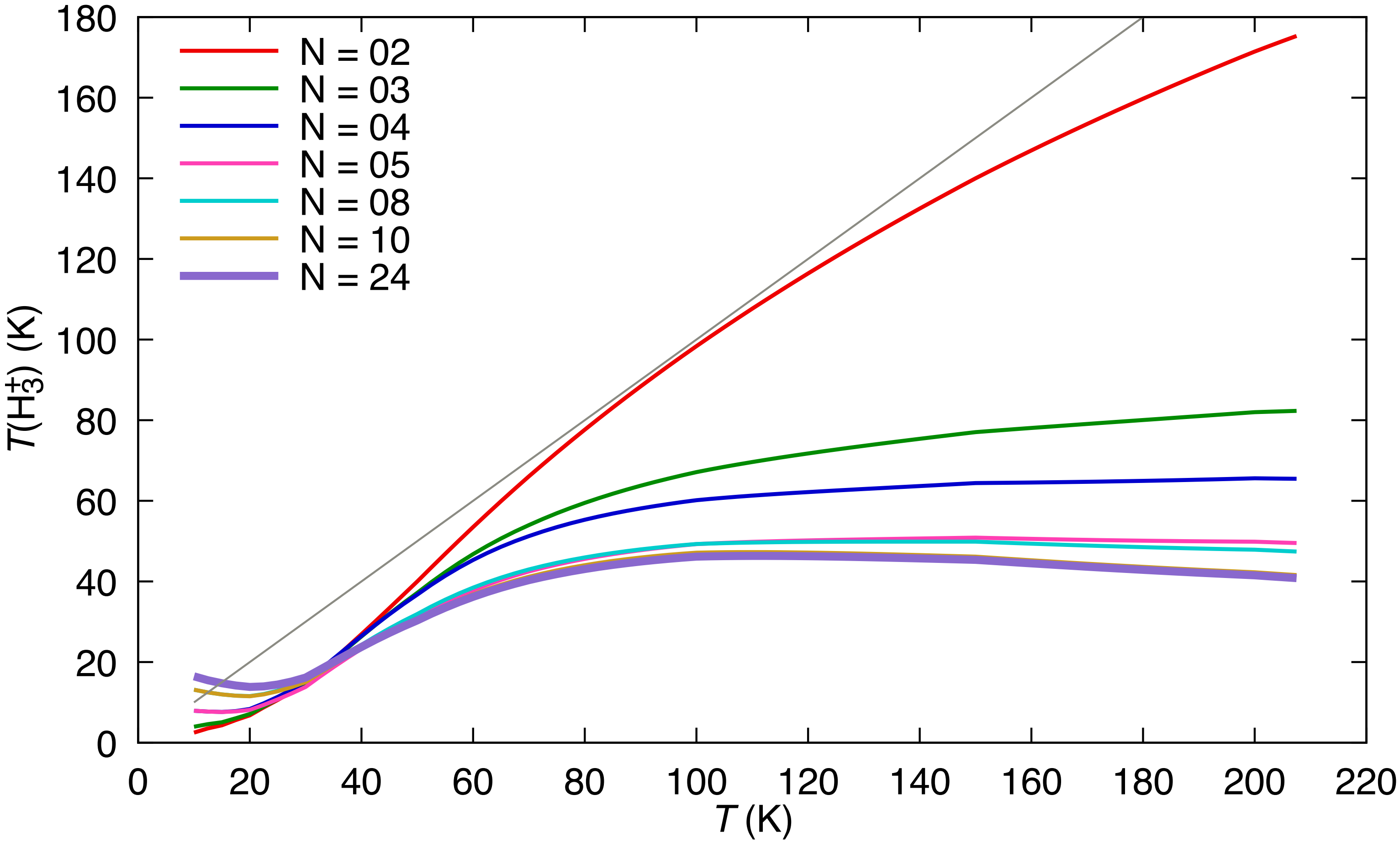
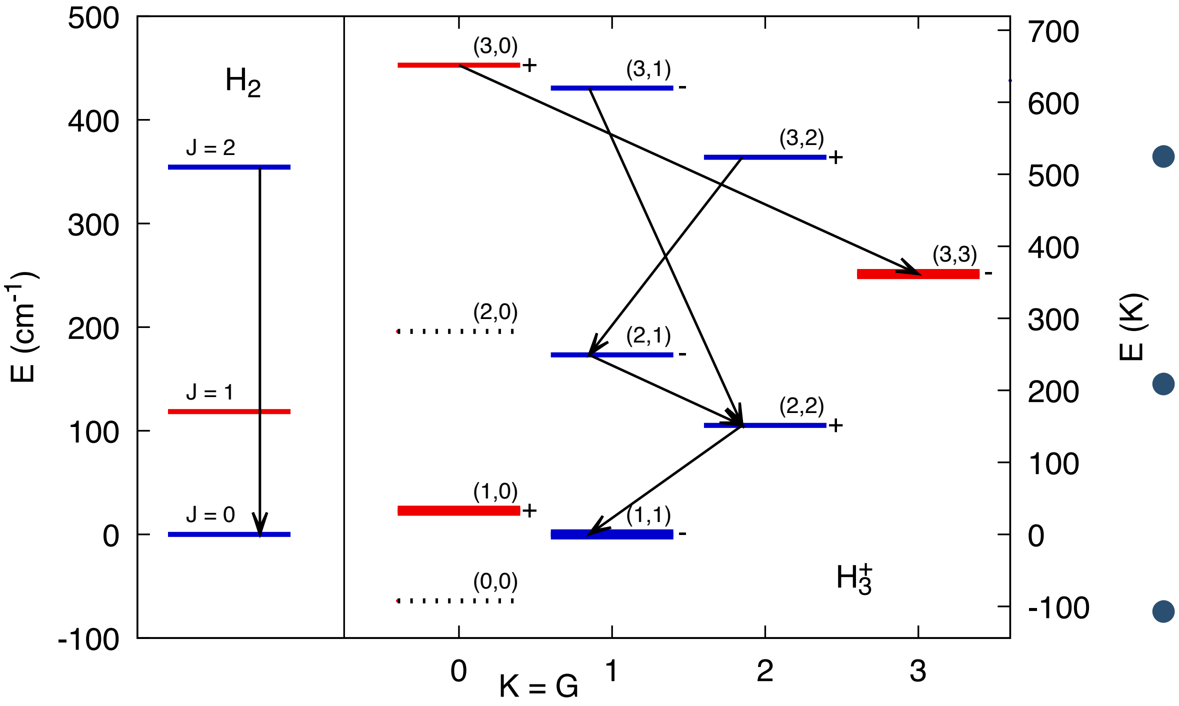


Impact of N, number of levels included



Use **at least** $N = 5$ (Number of levels in computation)

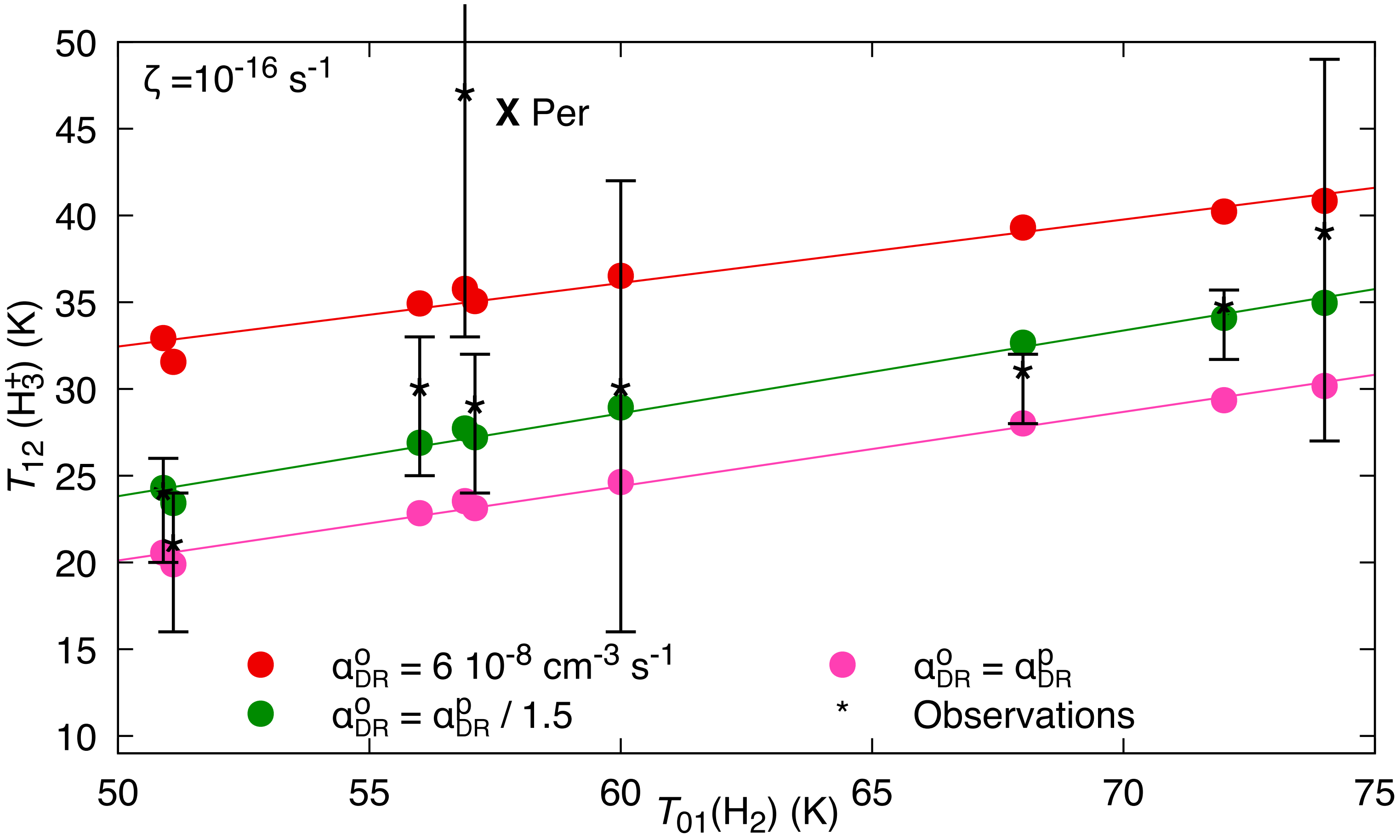
Why?



- Formation on high (G, J)
- Radiative cascades to $(1,1)$ and $(3,3)$
- Slow collisional transfer to $(1,0)$
- Competitive destruction by e^-

$(1,0)$ is underpopulated $\Rightarrow$ low $T_{12}\left(H_3^+\right)$

Observations



Further work on dissociative recombination rate α_{DR} needed!

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- Acknowledge the work of physicists.
  - Experiences.
  - Computations.
  - Databases.

Thank you!