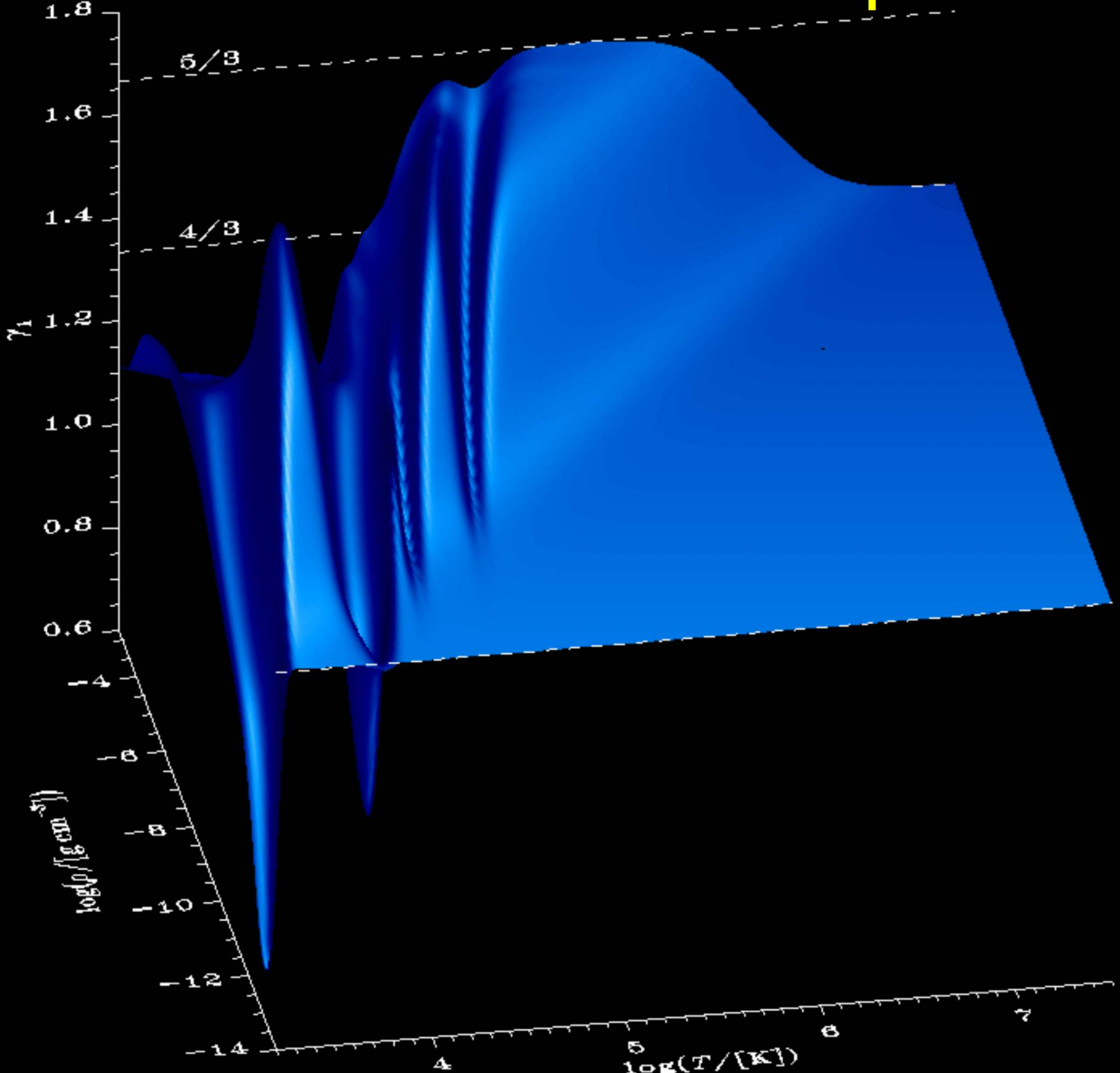
The T-MHD EOS
for stars - from atmospheres to cores



Equation of state (EOS)

Needed for **thermodynamics** and basis for **opacities**

Why do we need *updates* to the EOS?

- Physical processes missing from current ones.
- The so-called ‘Solar abundance problem’ could be an atomic physics problem instead.
- Opacity measurements at Z-pinch reveal problems!

Equation of state (EOS)

Two basic approaches (pictures):

- **Physical:** Assume only nuclei, e^- assemble to ions. Rigorous expansion in density – so far only to $\rho^{5/2}$: OPAL by Rogers+ (1996), Rogers & Nayfonov (2002).
- **Chemical:** Assume all species of ions/atoms, free energy minimization, ad-hoc but complex models for the various physical processes:
  MHD by Mihalas, Hummer & Däppen (1988), Free EOS by Irwin (2012), ChemEOS by Kilcrease (2015), etc.

Mihalas-Hummer-Däppen (MHD) EOS

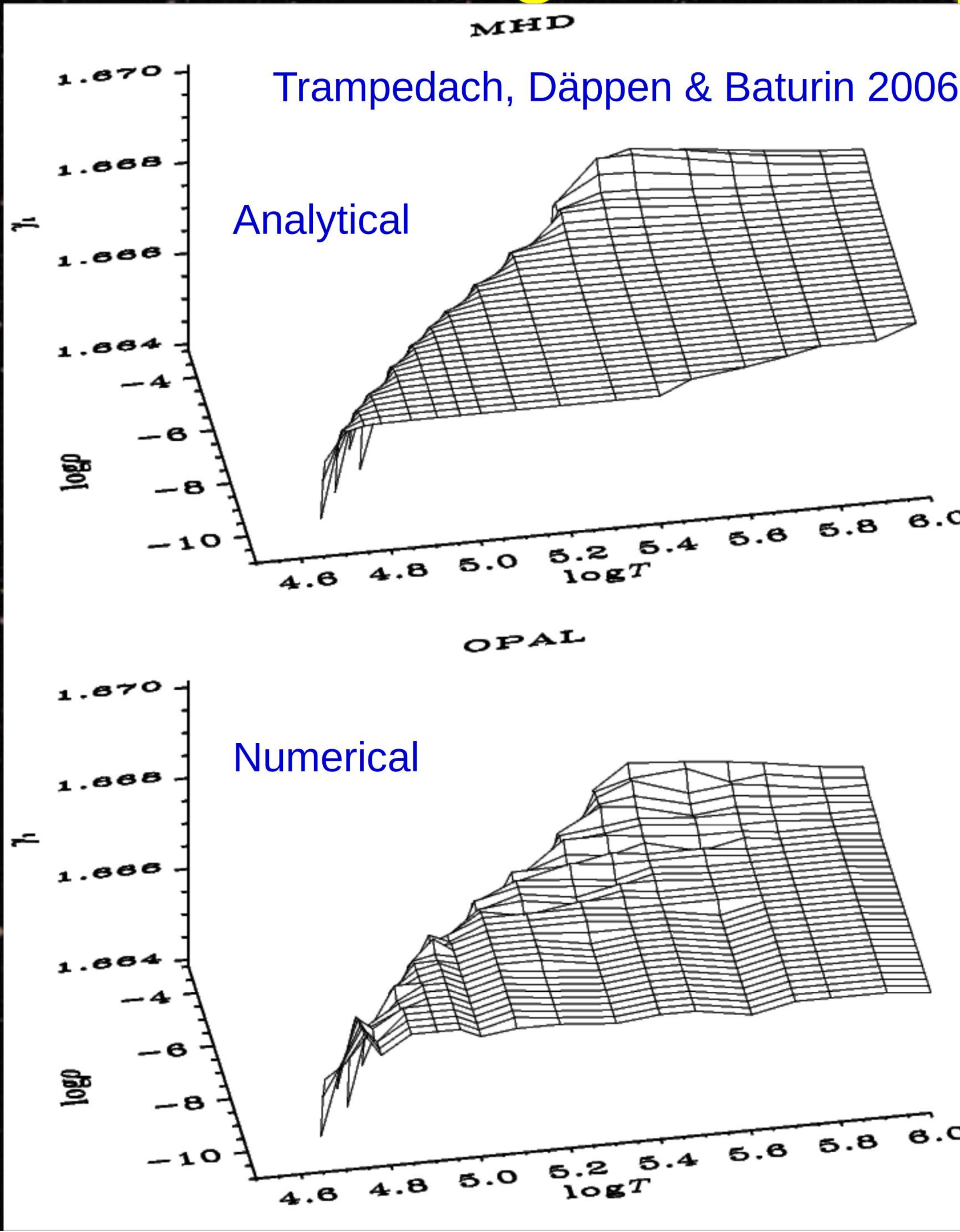
- Based on Helmholtz free energy, F.
- Minimize F w.r.t. number densities of each species
- $F = F_1 + F_2 + F_3 + F_4$
  - F_1: translational
  - F_2: Bound states
  - F_3: Free electrons
  - F_4: Coulomb forces
- Major strength of MHD: Analytical derivatives

$$p = -\left(\frac{\partial F}{\partial V}\right)_{T,\{N\}} , \quad S = -\left(\frac{\partial F}{\partial T}\right)_{V,\{N\}} \quad \text{and} \quad E = F - T\left(\frac{\partial F}{\partial T}\right)_{V,\{N\}} .$$

also need: $\frac{\partial F}{\partial N_\alpha}, \frac{\partial^2 F}{\partial N_\alpha \partial T}, \frac{\partial^2 F}{\partial N_\alpha \partial V}, \frac{\partial^2 F}{\partial N_\alpha \partial N_\beta}, \frac{\partial^2 F}{\partial T^2}, \frac{\partial^2 F}{\partial T \partial V}, \frac{\partial^2 F}{\partial V^2}$

- 15 elements and 2 molecules ⇒ 202 species!

Advantage of analytical derivatives



- Better interpolation
- $c_V, c_p, \chi_\rho, \chi_T, \gamma_1$ etc. are 2nd-order derivatives
- Safe to compute numerical derivatives for 3rd-order derivatives
- More robust minimization of F

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The trouble with analytical derivatives: more work for me!

$$
\begin{aligned}
\frac{\partial^2 F_2}{\partial N_\beta \partial N_\gamma} = & -k_{\rm B}T\frac{\partial \ln Z^*_\beta}{\partial N_\gamma} - k_{\rm B}T\frac{\partial \ln Z^*_\gamma}{\partial N_\beta} + k_{\rm B}T\sum_{\alpha\neq{\rm e}} N_\alpha \frac{\partial \ln Z^*_\alpha}{\partial N_\beta}\frac{\partial \ln Z^*_\alpha}{\partial N_\gamma} \\
& -\frac{\partial \ln\zeta}{\partial N_\beta}\frac{\partial \ln\zeta}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\left[\left(\frac{\partial \ln Q}{\partial \ln\beta_{i\alpha}}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}}\right)^2 + \frac{\partial^2 \ln Q}{\partial \ln\beta_{i\alpha}^2} + \frac{\partial^2 \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}^2}\right]\bar{w}_{i\alpha} \\
& -\frac{\partial \ln\zeta}{\partial N_\beta}\frac{\partial \ln s}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\left(\frac{\partial \ln Q}{\partial \ln\beta_{i\alpha}}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}}\right)\frac{\partial \ln Q}{\partial \ln s}\bar{w}_{i\alpha} - \frac{\partial \ln\zeta}{\partial N_\beta}\frac{\partial \ln s^{\rm b}_{i\alpha}}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\left(\frac{\partial \ln Q}{\partial \ln\beta_{i\alpha}}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}}\right)\frac{\partial \ln Q^{\rm b}}{\partial \ln s^{\rm b}_{i\alpha}}\bar{w}_{i\alpha} \\
& -\frac{\partial \ln\zeta}{\partial N_\beta}\frac{\partial \ln\Lambda}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\left(\frac{\partial \ln Q}{\partial \ln\beta_{i\alpha}}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}}\right)\left(\frac{\partial \ln Q}{\partial \ln\Lambda}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\Lambda}\right)\bar{w}_{i\alpha} \\
& -\frac{\partial \ln s}{\partial N_\beta}\frac{\partial \ln\zeta}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\frac{\partial \ln Q}{\partial \ln s}\left(\frac{\partial \ln Q}{\partial \ln\beta_{i\alpha}}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}}\right)\bar{w}_{i\alpha} - \frac{\partial \ln s}{\partial N_\beta}\frac{\partial \ln s}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\left[\left(\frac{\partial \ln Q}{\partial \ln s}\right)^2+\frac{\partial^2 \ln Q}{\partial \ln s^2}\right]\bar{w}_{i\alpha} \\
& -\frac{\partial \ln s}{\partial N_\beta}\frac{\partial \ln s^{\rm b}_{i\alpha}}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\frac{\partial \ln Q}{\partial \ln s}\frac{\partial \ln Q^{\rm b}}{\partial \ln s^{\rm b}_{i\alpha}}\bar{w}_{i\alpha} - \frac{\partial \ln s}{\partial N_\beta}\frac{\partial \ln\Lambda}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\frac{\partial \ln Q}{\partial \ln s}\left(\frac{\partial \ln Q}{\partial \ln\Lambda}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\Lambda}\right)\bar{w}_{i\alpha} \qquad (233) \\
& -\frac{\partial \ln s^{\rm b}_{i\alpha}}{\partial N_\beta}\frac{\partial \ln\zeta}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\frac{\partial \ln Q^{\rm b}}{\partial \ln s^{\rm b}_{i\alpha}}\left(\frac{\partial \ln Q}{\partial \ln\beta_{i\alpha}}+\frac{\partial \ln Q^{\rm b}}{\partial \ln\beta_{i\alpha}}\right)\bar{w}_{i\alpha} - \frac{\partial \ln s^{\rm b}_{i\alpha}}{\partial N_\beta}\frac{\partial \ln s}{\partial N_\gamma} k_{\rm B}T\sum_{\alpha\neq{\rm e}}\frac{N_\alpha}{Z^*_\alpha}\sum_i\frac{\partial \ln Q^{\rm b}}{\partial \ln s^{\rm b}_{i\alpha}}\frac{\partial \ln Q}{\partial \ln s}\bar{w}_{i\alpha} \\
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\end{aligned}
$$

February 27, 2019 51

Updates MHD → MHD2020 EOS

Added (w.r.t. Hummer & Mihalas, 1988):

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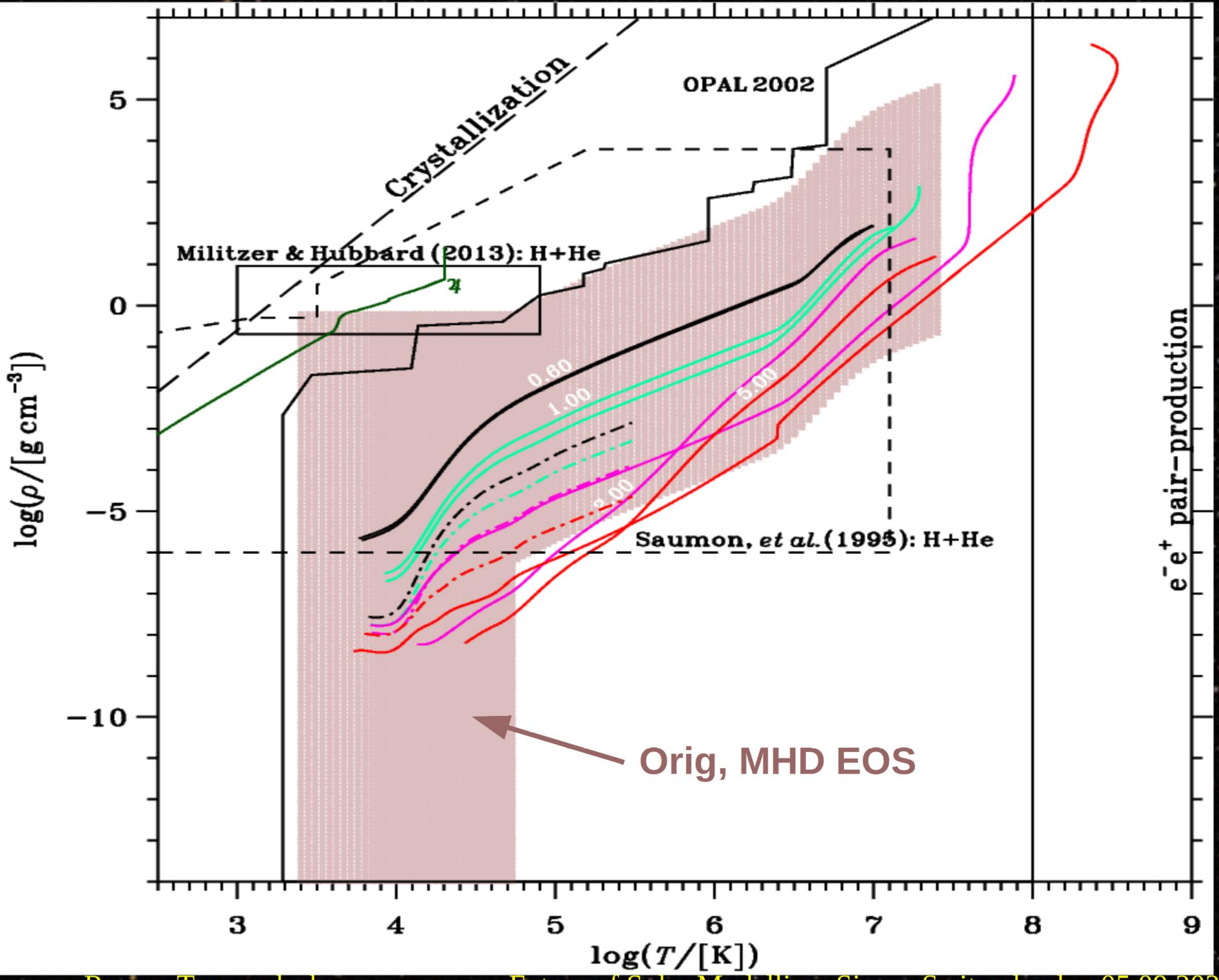
→ lower T

→ higher ρ

} → higher T

Updates MHD → MHD2020 EOS

Much larger range of validity



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More Elements

elem	Z	$\chi_1/[\mathrm{eV}]$	SGA[f]	OPAL[g]	OPAS[h]	Free[i]	OP[j]
H	1	13.5984	12.00	X	X	X	X
He	2	24.5874	10.93	X	X	X	X
Li	3	5.3917	1.05				
Be	4	9.3228	1.38				
B	5	8.2981	2.70				
C	6	11.2603	8.43	X	X	X	X
N	7	14.5341	7.83	X	X	X	X
O	8	13.6181	8.69	X	X	X	X
Ne	10	21.5646	7.93	X	X	X	X
Na	11	5.1391	6.21	X	X	X	X
Mg	12	7.6462	7.59	X	X	X	X
Al	13	5.9858	6.43	X	X	X	X
Si	14	8.1517	7.51	X	X	X	X
P	15	19.7695	5.41	X		X	
S	16	10.3599	7.12	X	X	X	X
Cl	17	23.8136	5.50	X		X	
Ar	18	15.7596	6.40	X	X	X	X
K	19	4.3407	5.04	X			
Ca	20	6.1132	6.32	X	X	X	X
Ti	22	13.5755	4.93	X		X	
V	23	29.3111	3.89				
Cr	24	16.4863	5.62	X	X	X	X
Mn	25	33.6679	5.42	X	X	X	X
Fe	26	7.8705	7.47	X	X	X	X
Co	27	33.5005	4.93				
Ni	28	54.9250	6.20	X	X	X	X
Zr	40	13.1299	1.75				

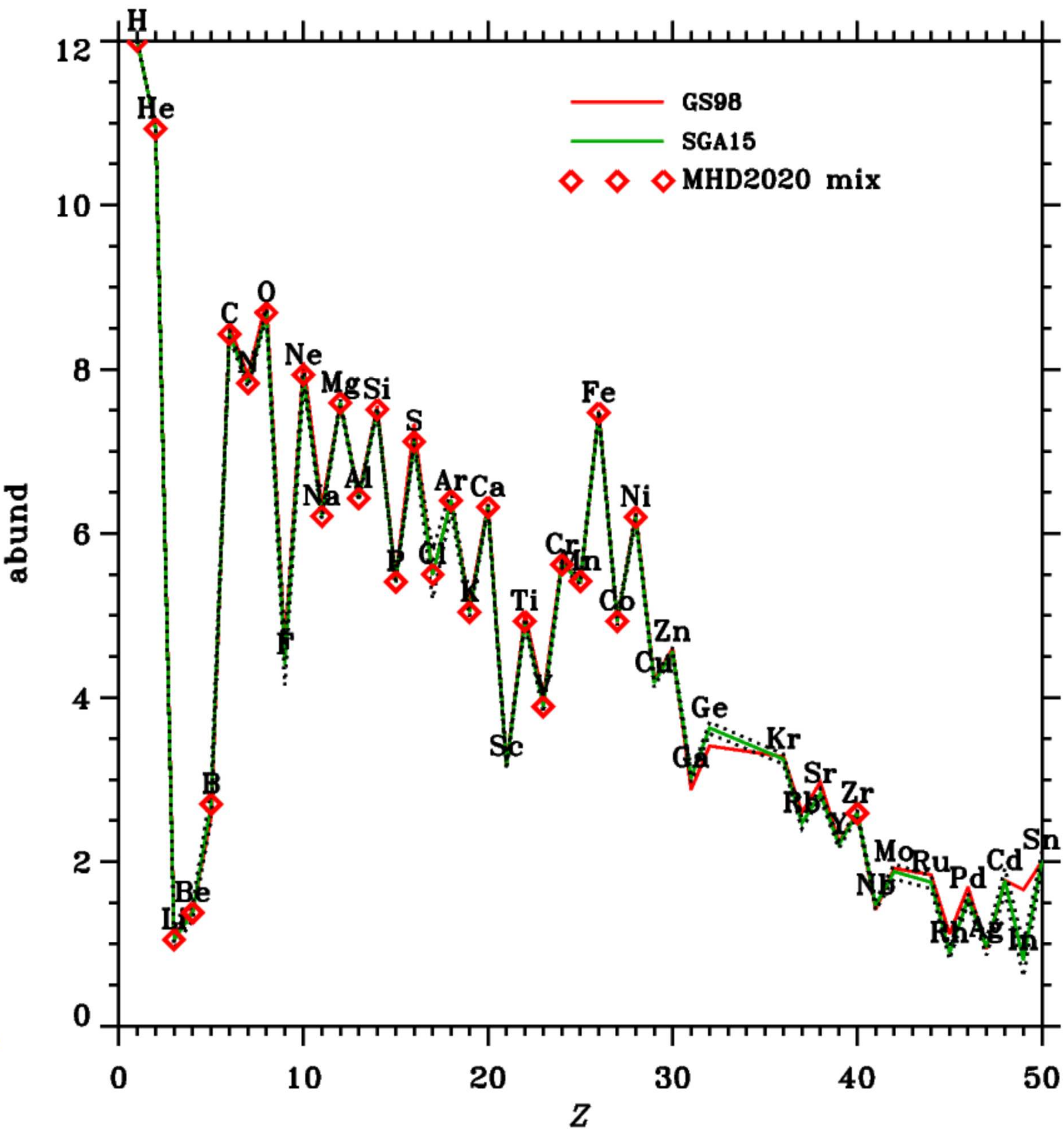
[f] The solar abundances by Scott et al. (2015b,a); Grevesse et al. (2015), supplemented by Asplund et al. (2009) for light elements.

[g] The OPAL EOS by Rogers & Nayfonov (2002)

[h] The OPAS opacities by Blancard et al. (2012)

[i] The FreeEOS by Irwin (2004).

[j] The OP opacities by Badnell et al. (2005)



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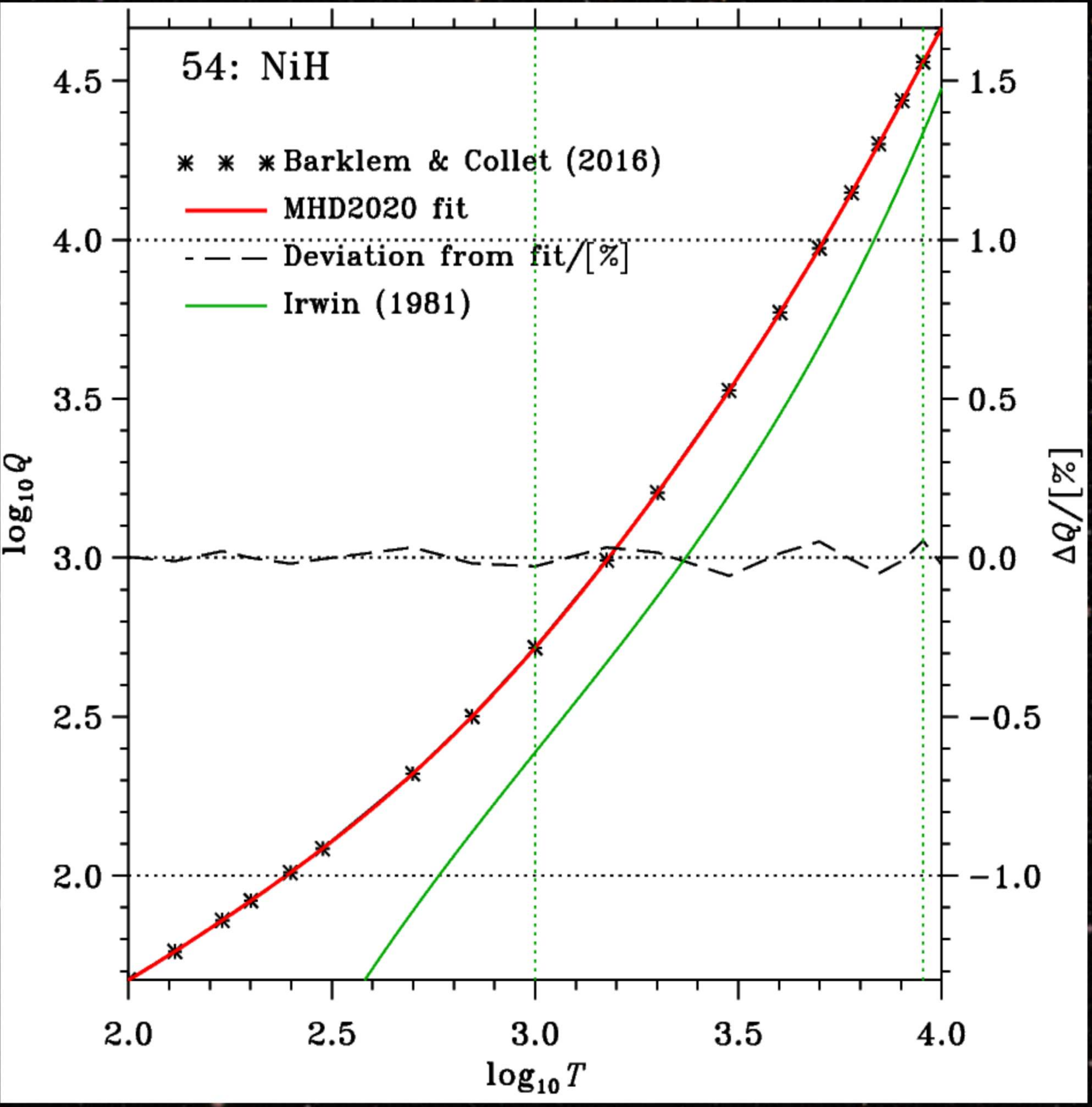
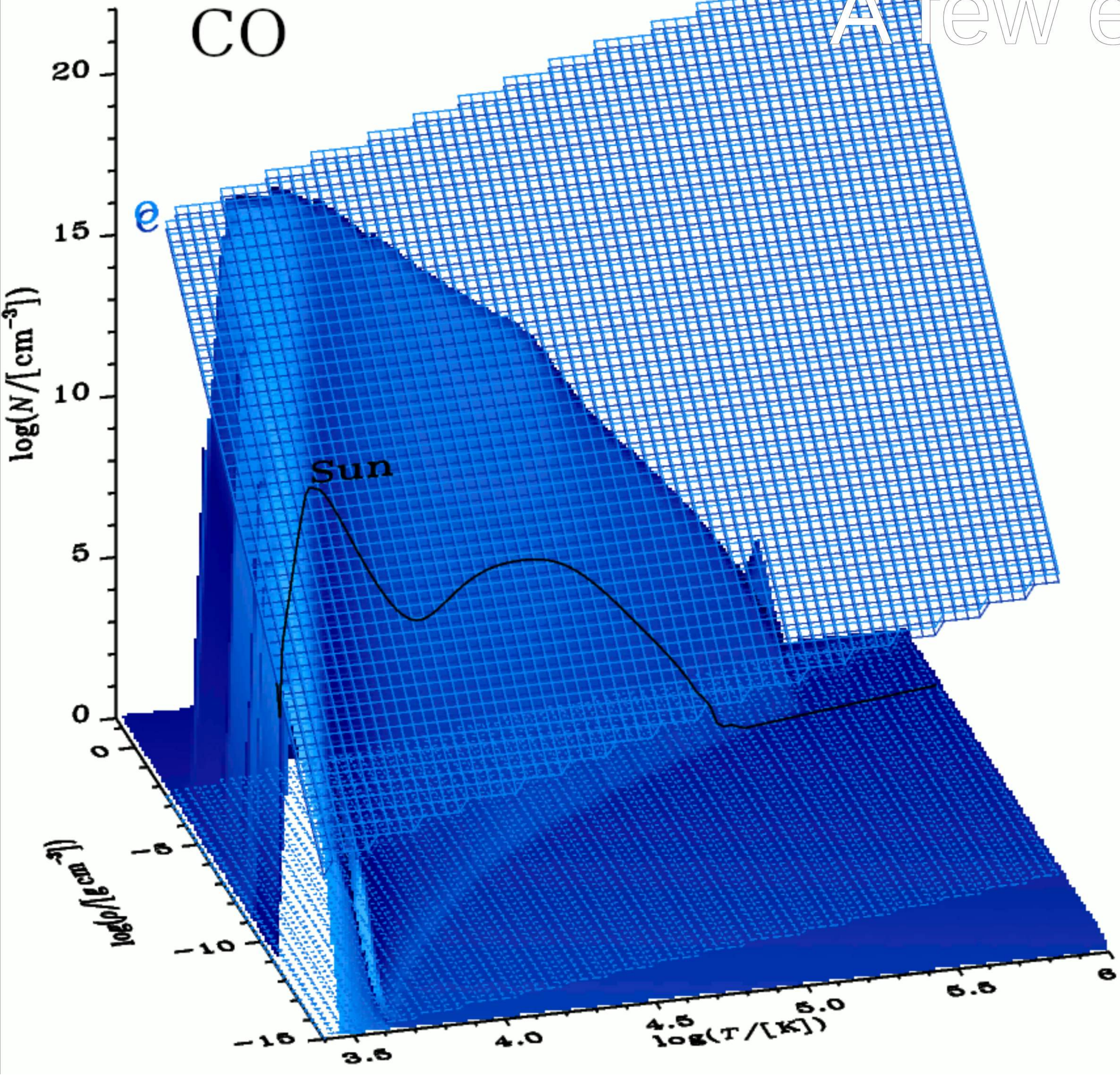
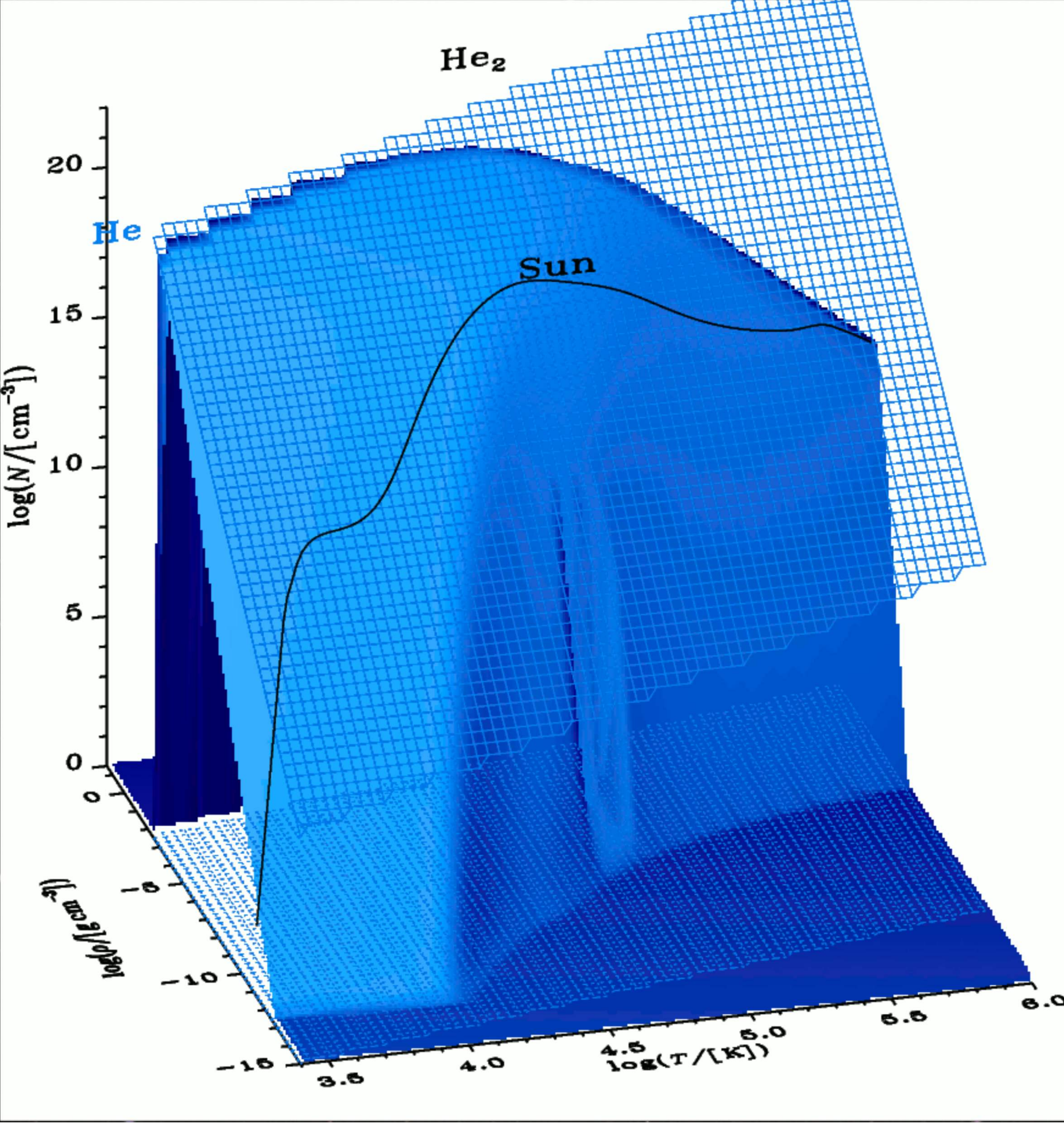
Molecules other than H_2 and H_2^+



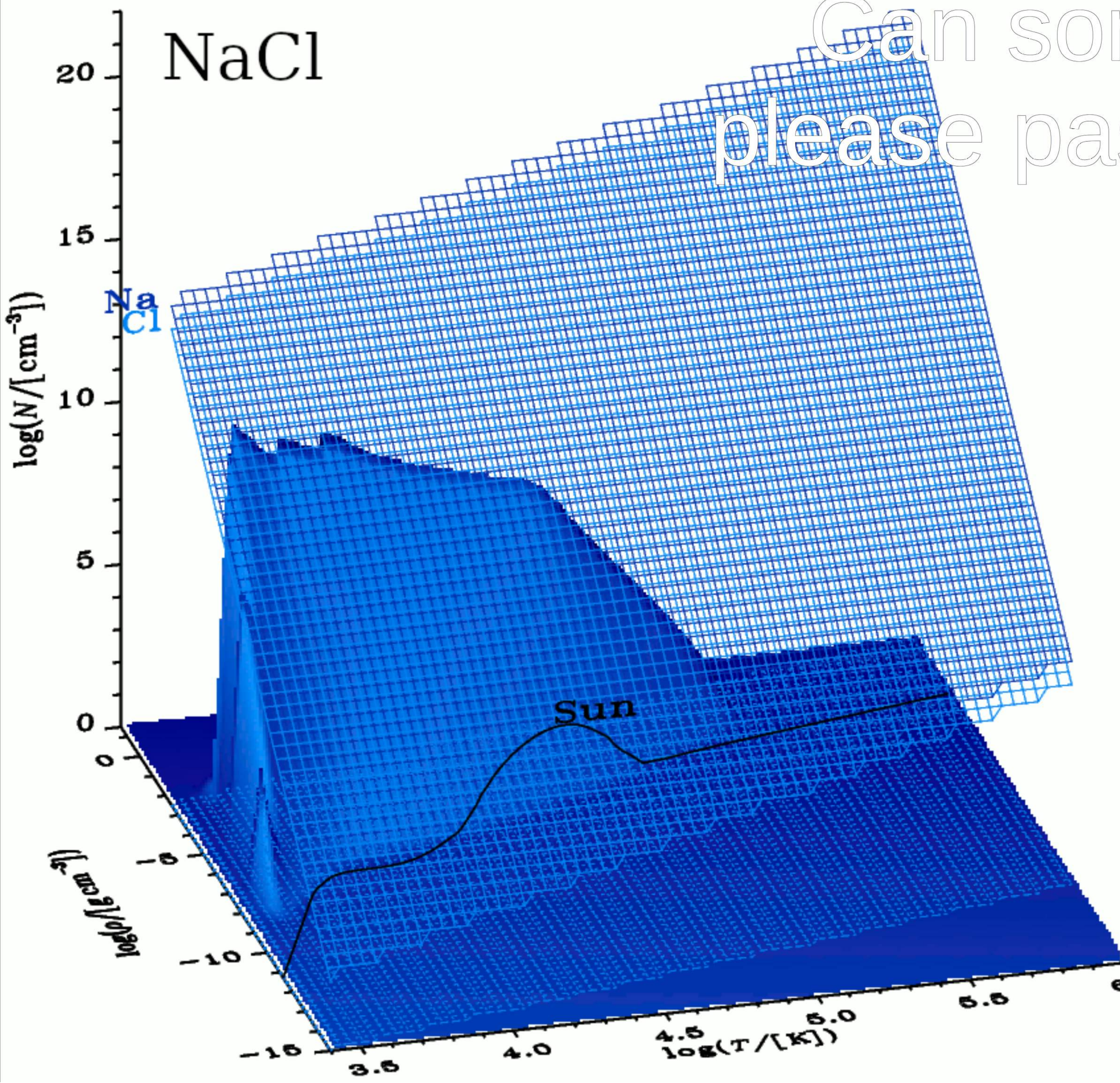
- 129 diatomic
- 58 polyatomic
- 35 molecular ions
- 10th-order part.func. fit to tabulated sums
- No ϱ/T-limits to where they can form
- Including pressure dissociation - 1st time!

A few examples:

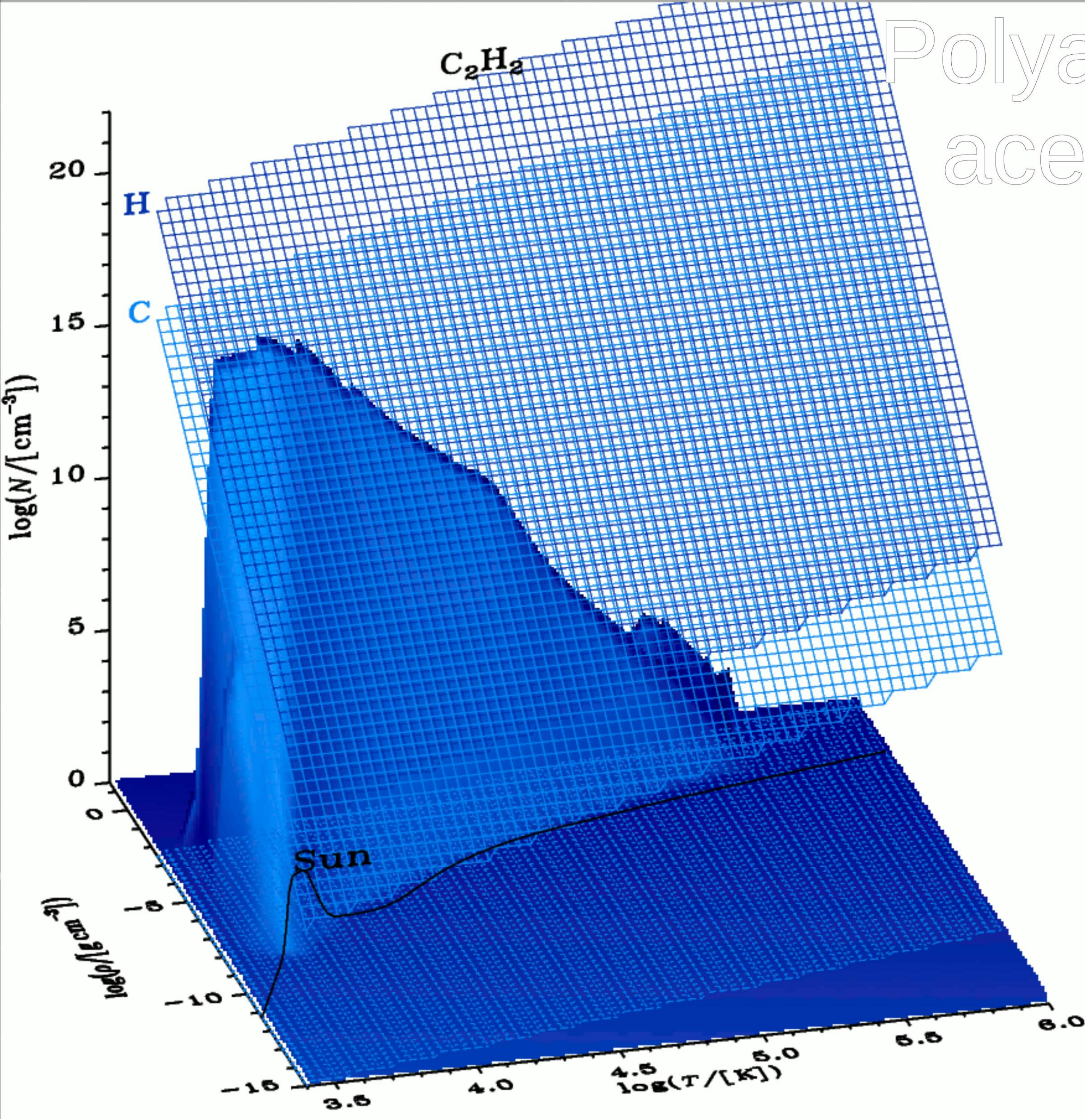



He₂
He
Sun
20
15
10
5
0
log(N/[cm^-3])
0
-5
-10
-15
log ρ/[g cm^-3])
3.5
4.0
4.5
5.0
5.5
6.0
log(T/[K])

Can somebody please pass the salt



Polyatomics, acetylene



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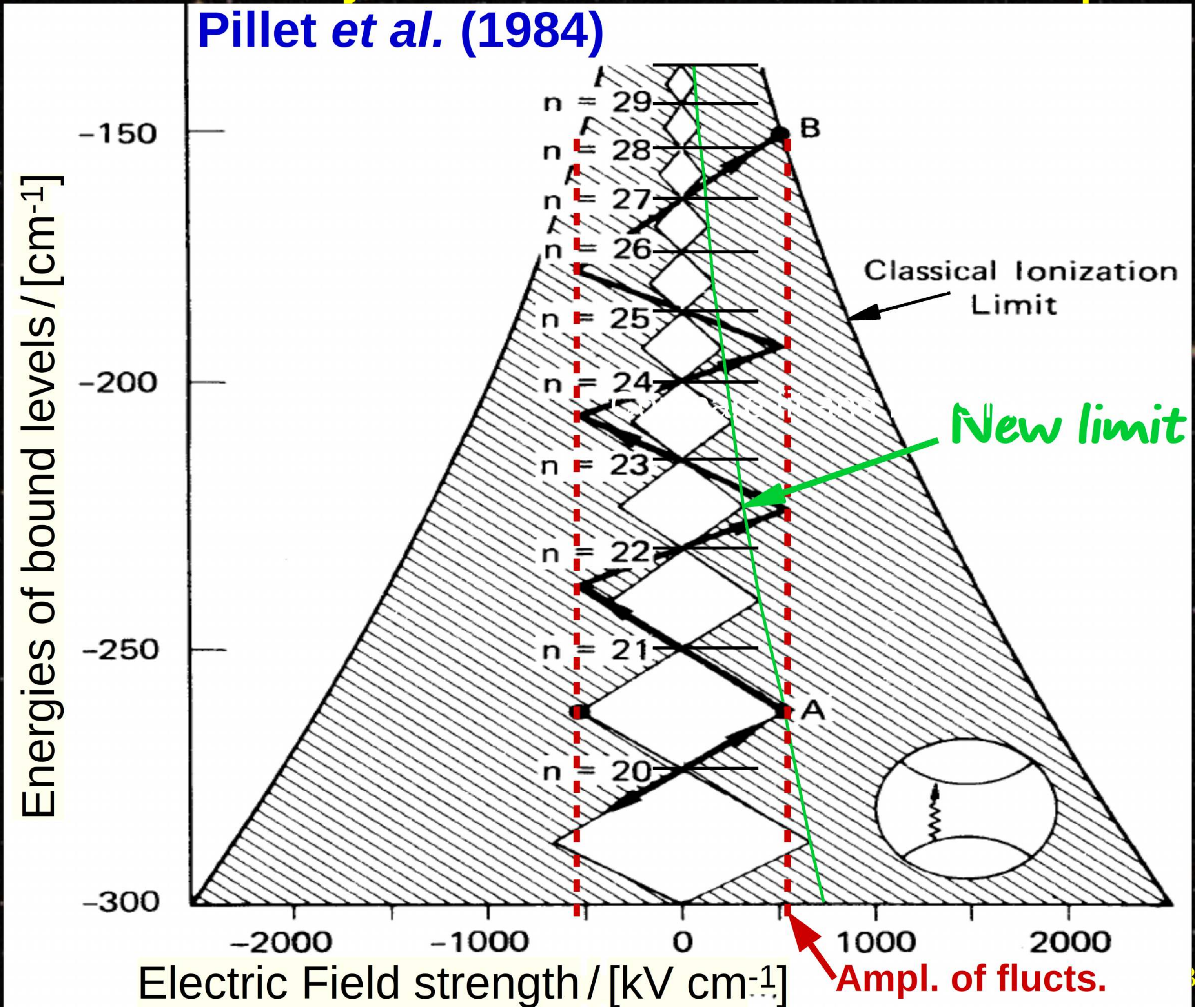
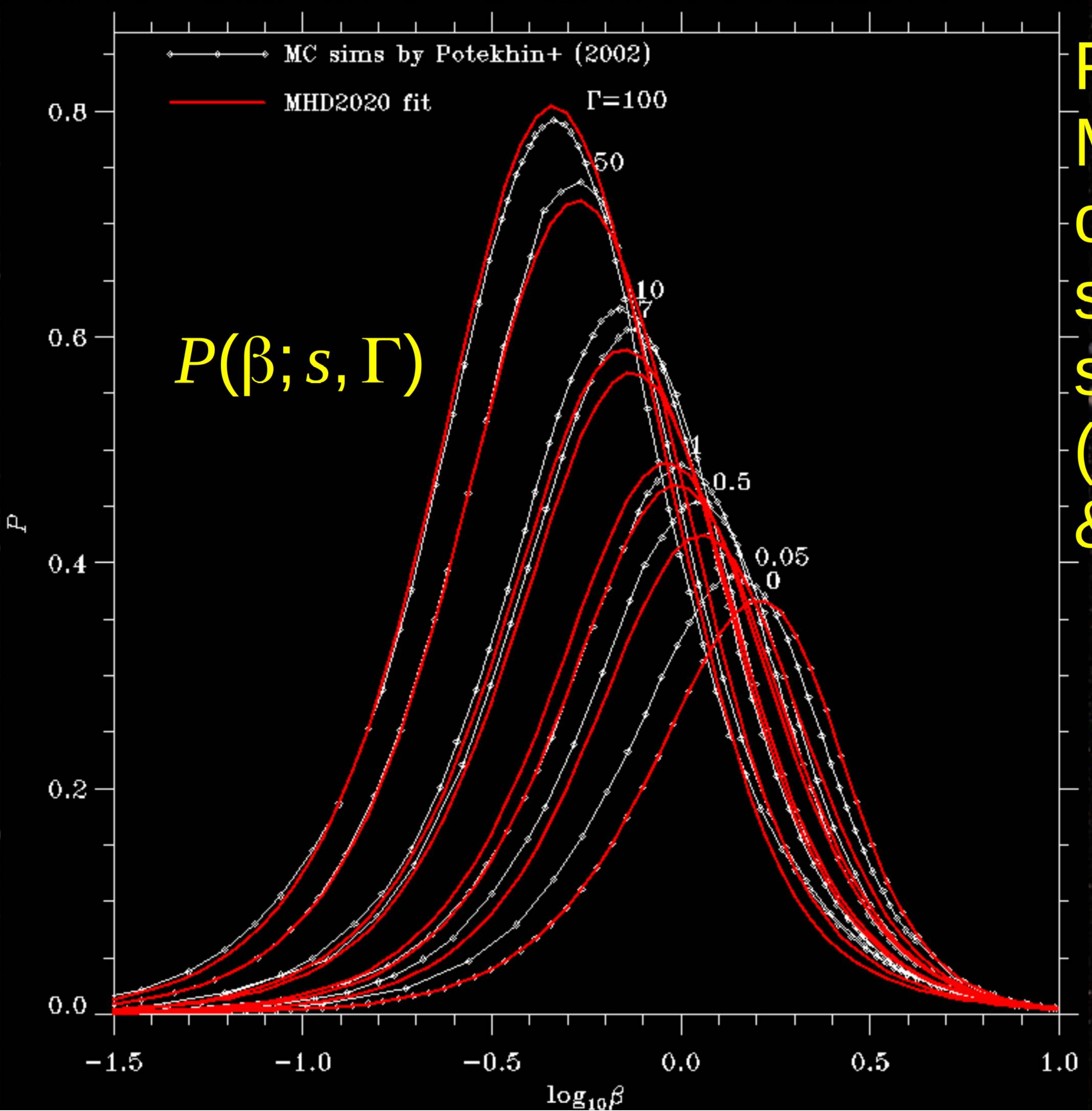
Micro-field distribution functions

Ionization by fluct. electric field from passing ions



Pressure-ionization

Micro-field distribution functions

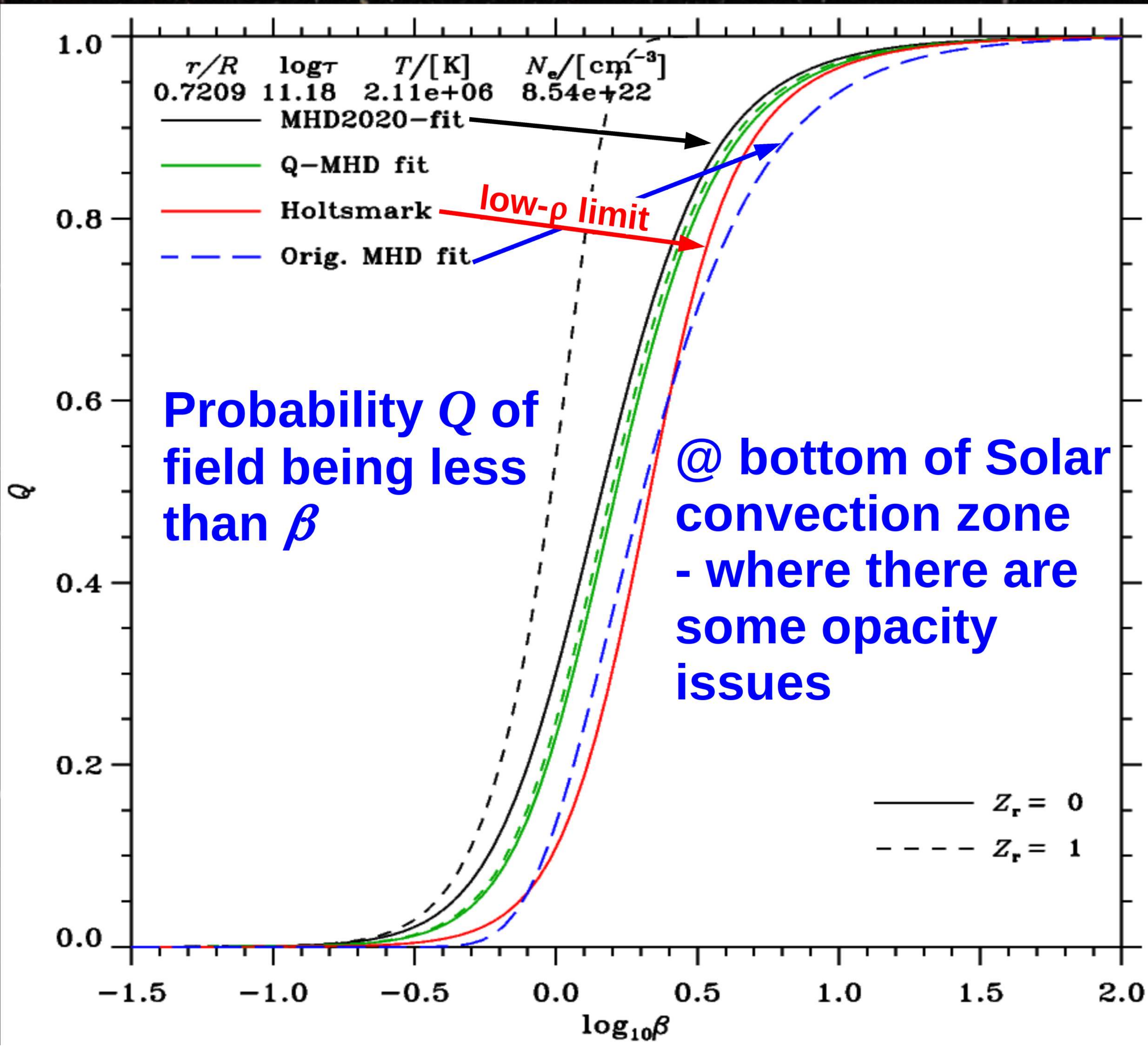


$P(\beta; s, \Gamma)$

Fitting to results of Monte-Carlo sims of gas composed of screened or un-screened charges (Potekhin, Chabrier & Gilles, 2002).

β: normalized field
s: screening length
Γ: plasma coupling

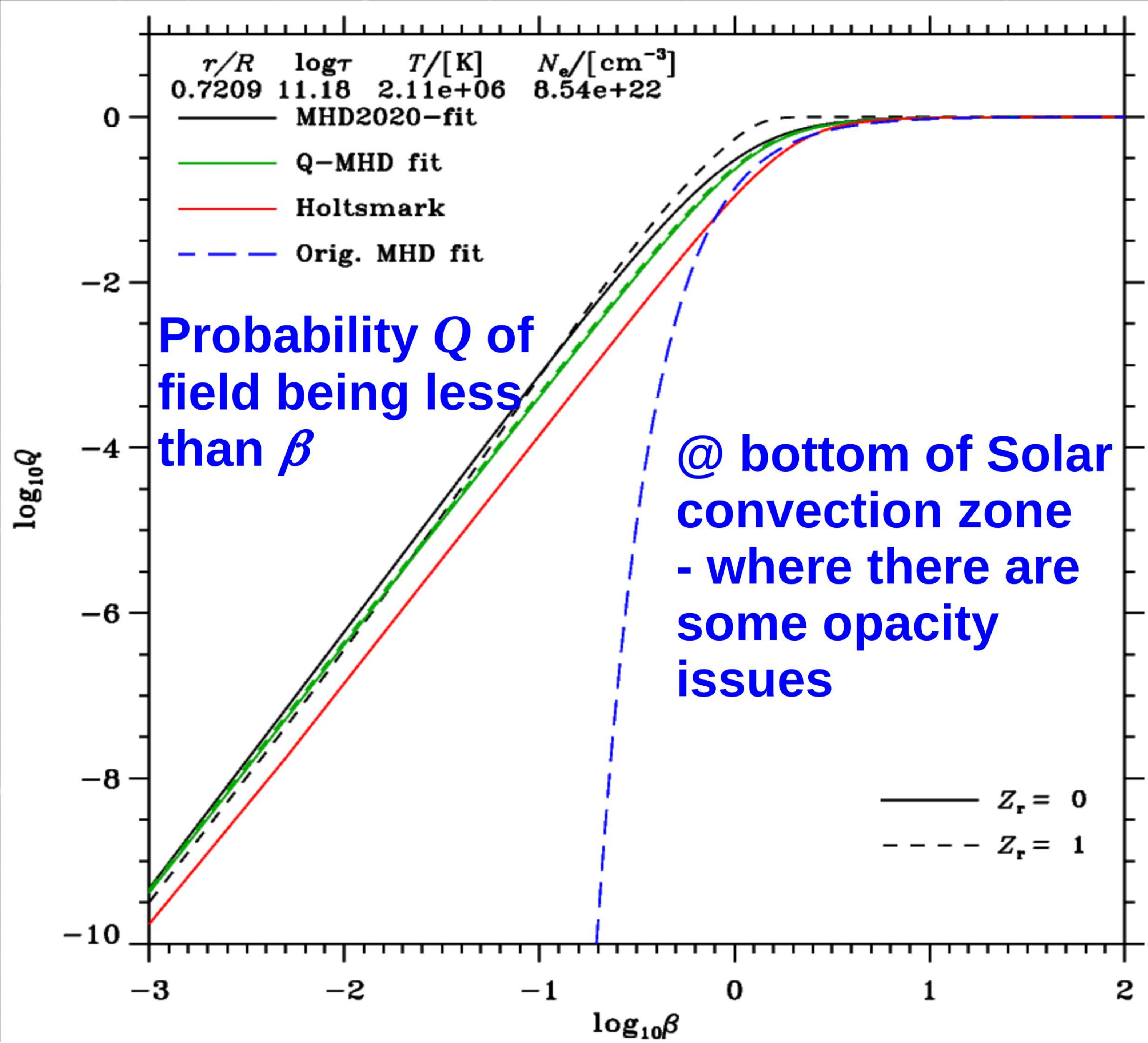
New micro-field distribution functions



Cumulative distribution

$$Q = \int P(\beta)\mathrm{d}\beta$$

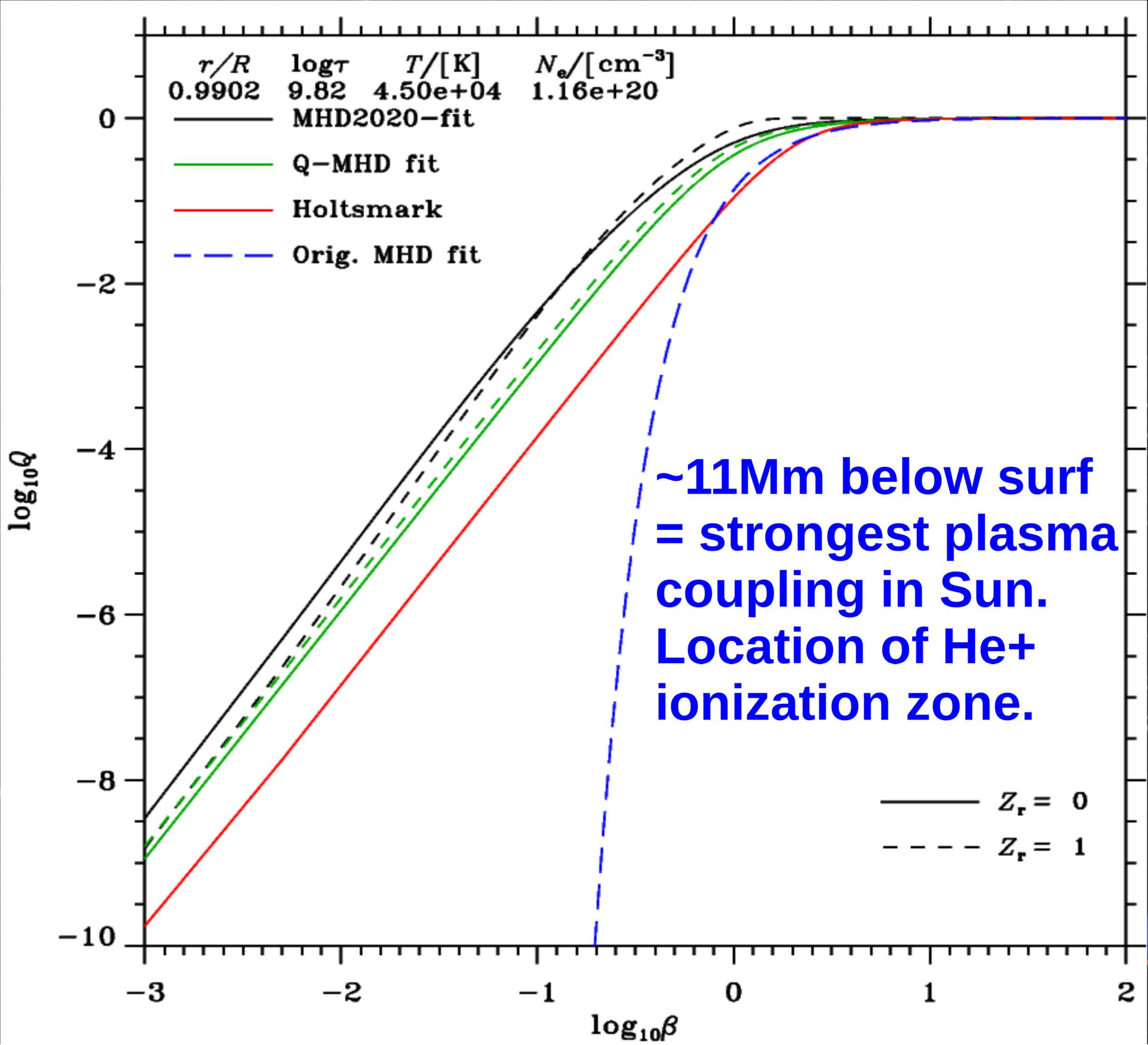
New micro-field distribution functions



Probability *Q* of field being less than *β*

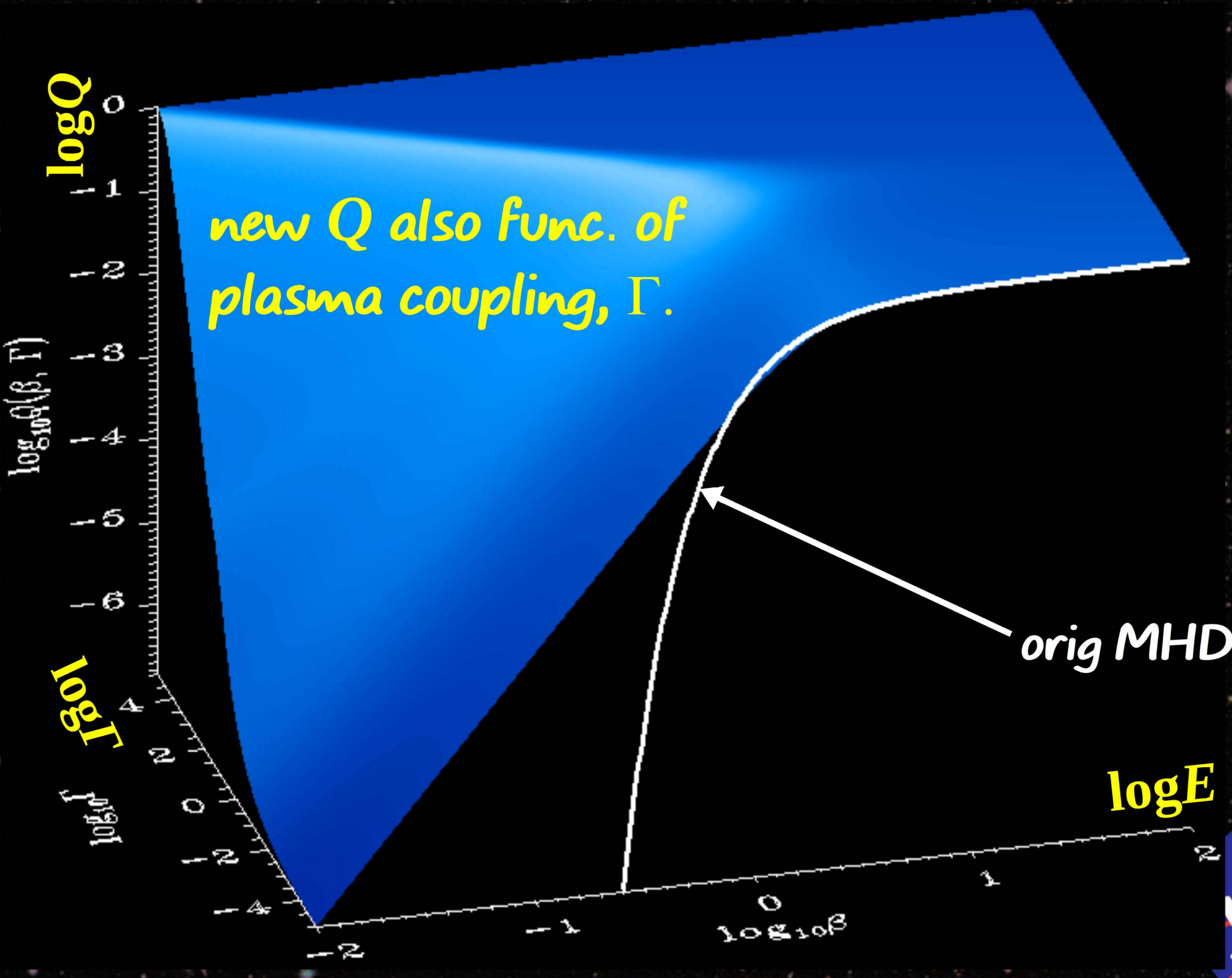
@ bottom of Solar convection zone - where there are some opacity issues

New micro-field distribution functions



~11Mm below surf = strongest plasma coupling in Sun. Location of He+ ionization zone.

New micro-field distribution functions



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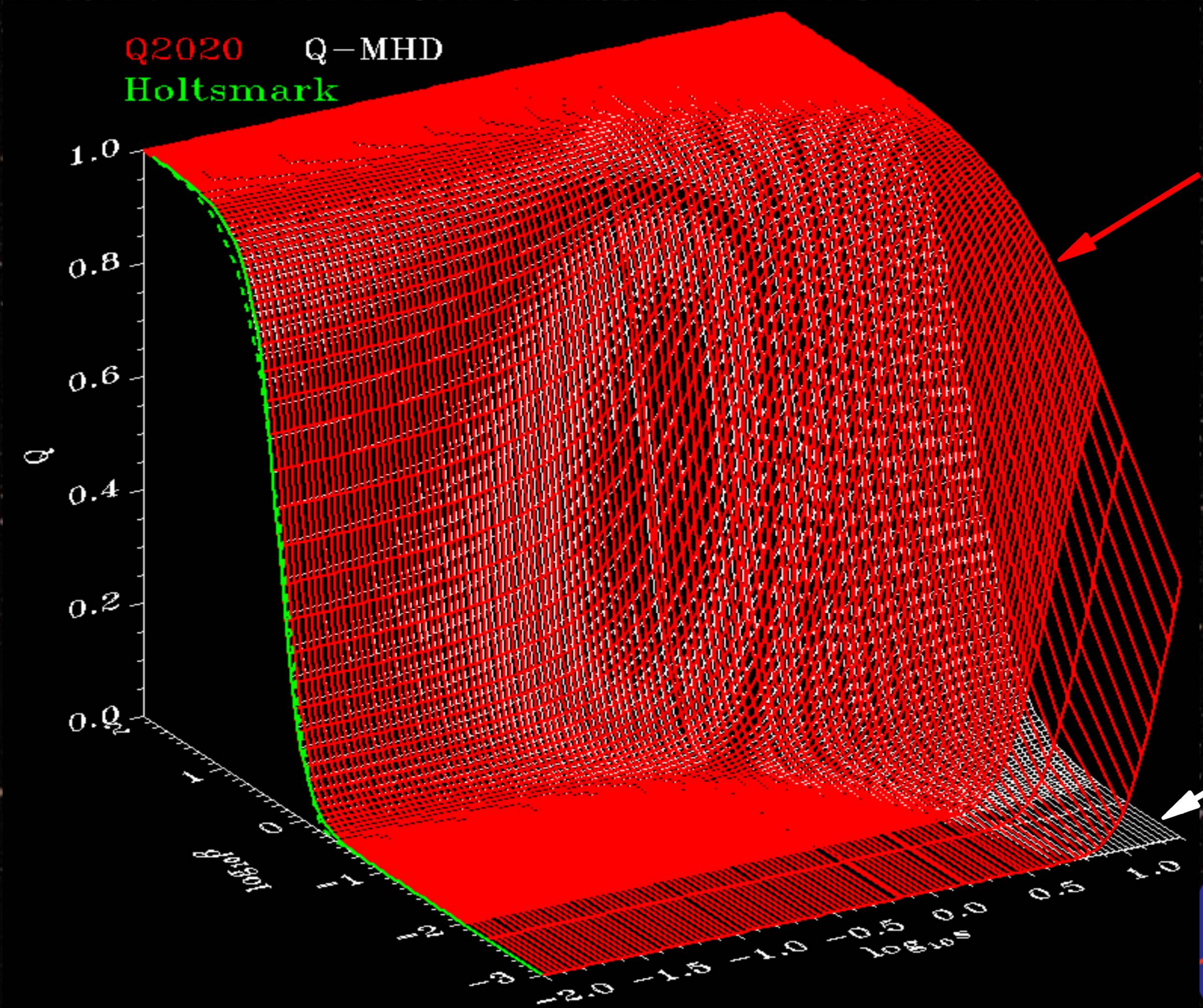
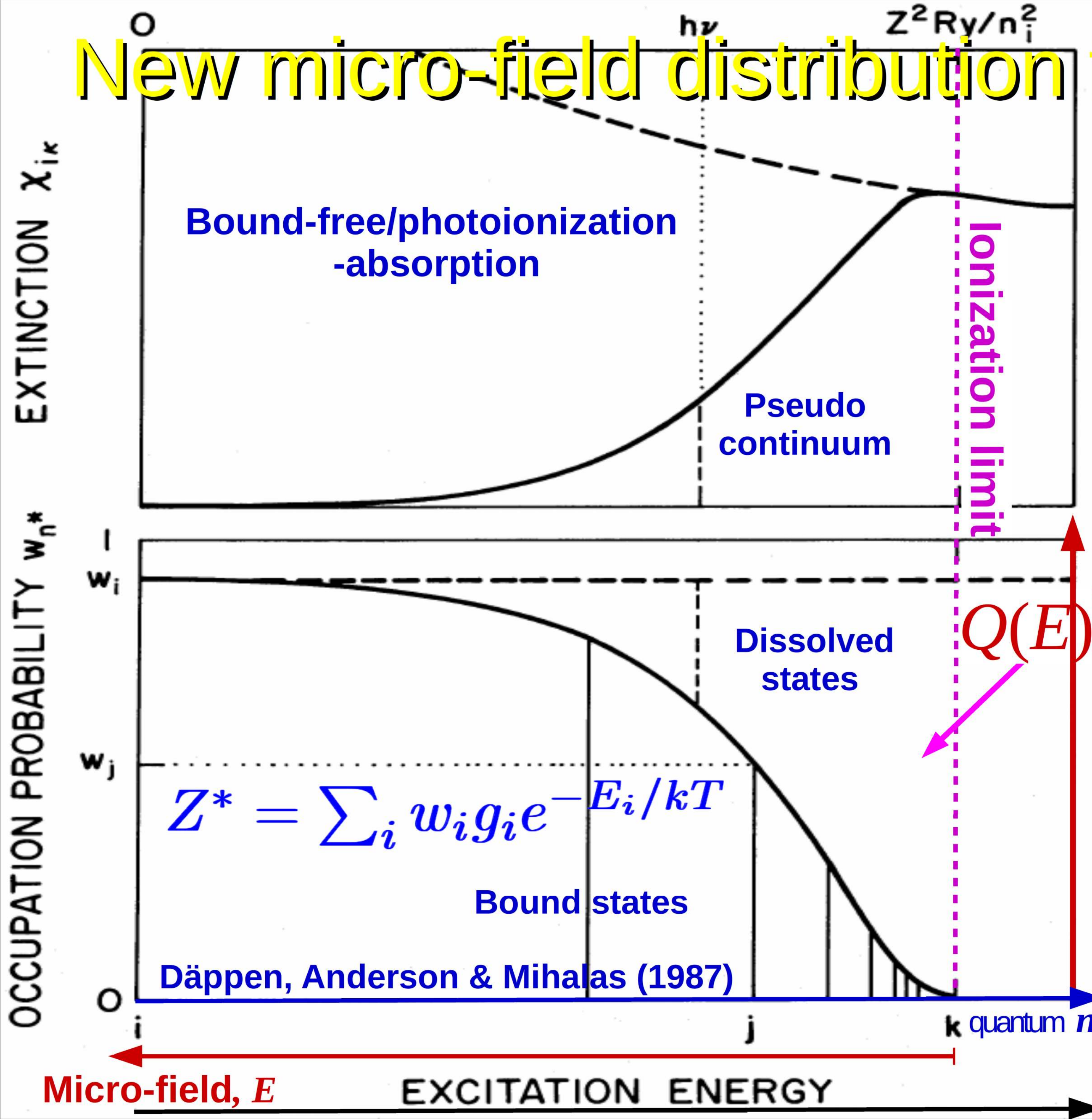
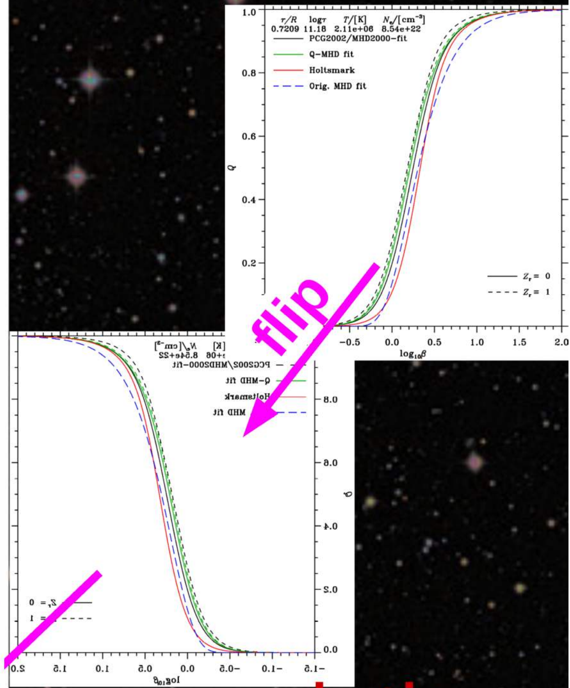


New Q also depends on e^--screening

Q-MHD by Nayfonov *et al.* (1999)

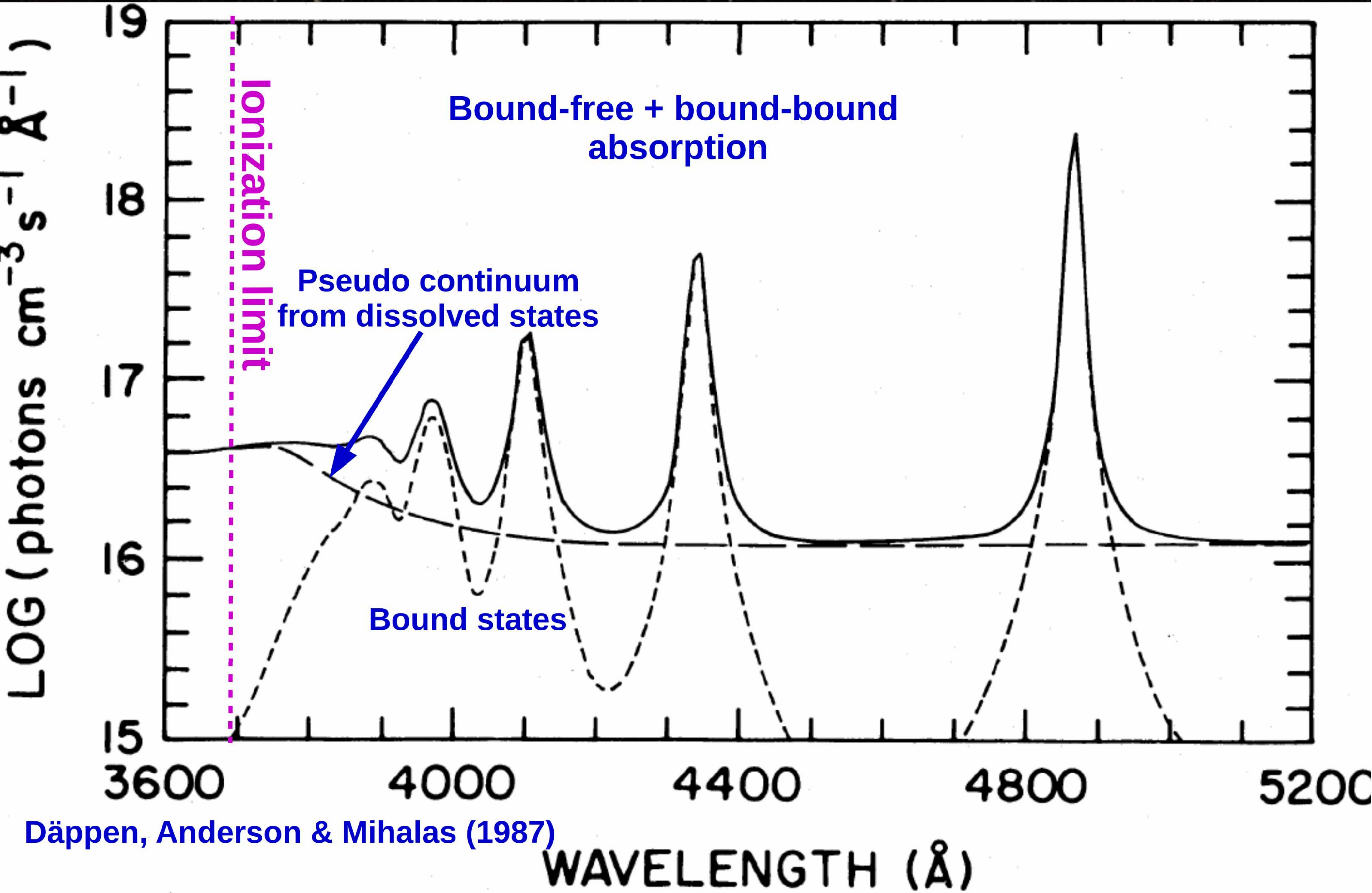
New micro-field distribution functions





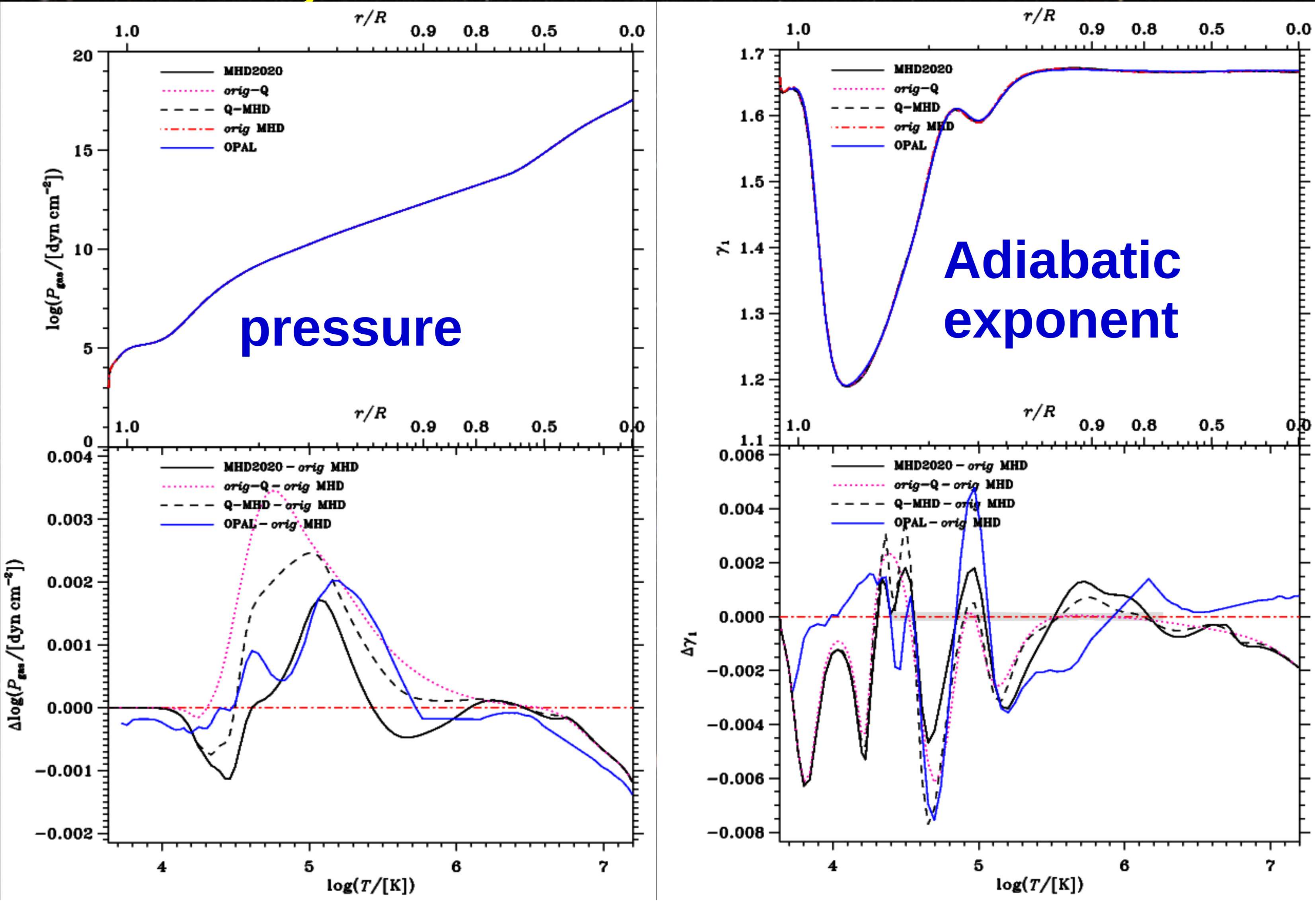
$Q(E)$ = cumulative micro-field distribution function

New micro-field distribution functions

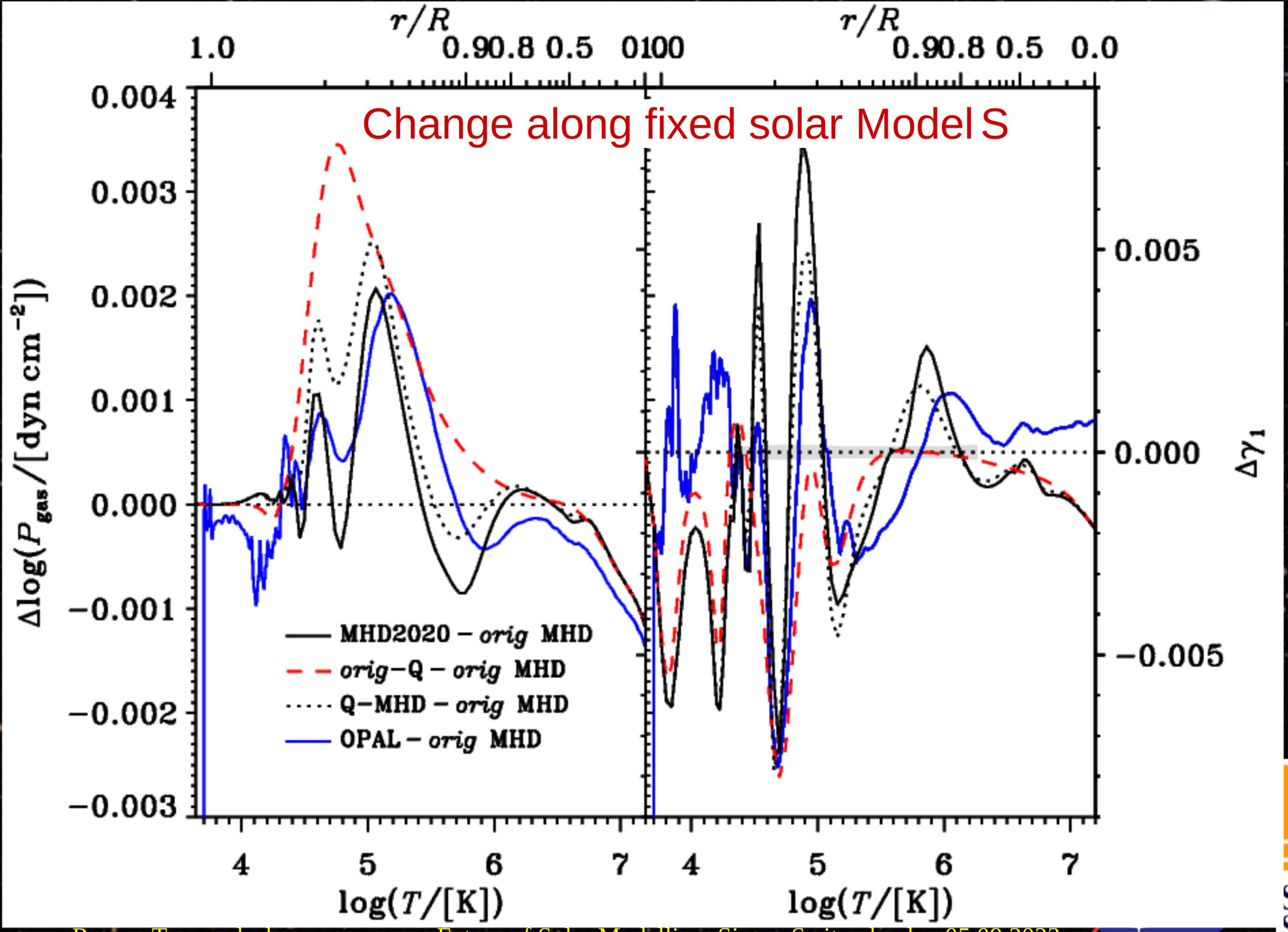


Däppen, Anderson & Mihalas (1987)

Thermodynamic effects on solar structure



New micro-field distribution functions



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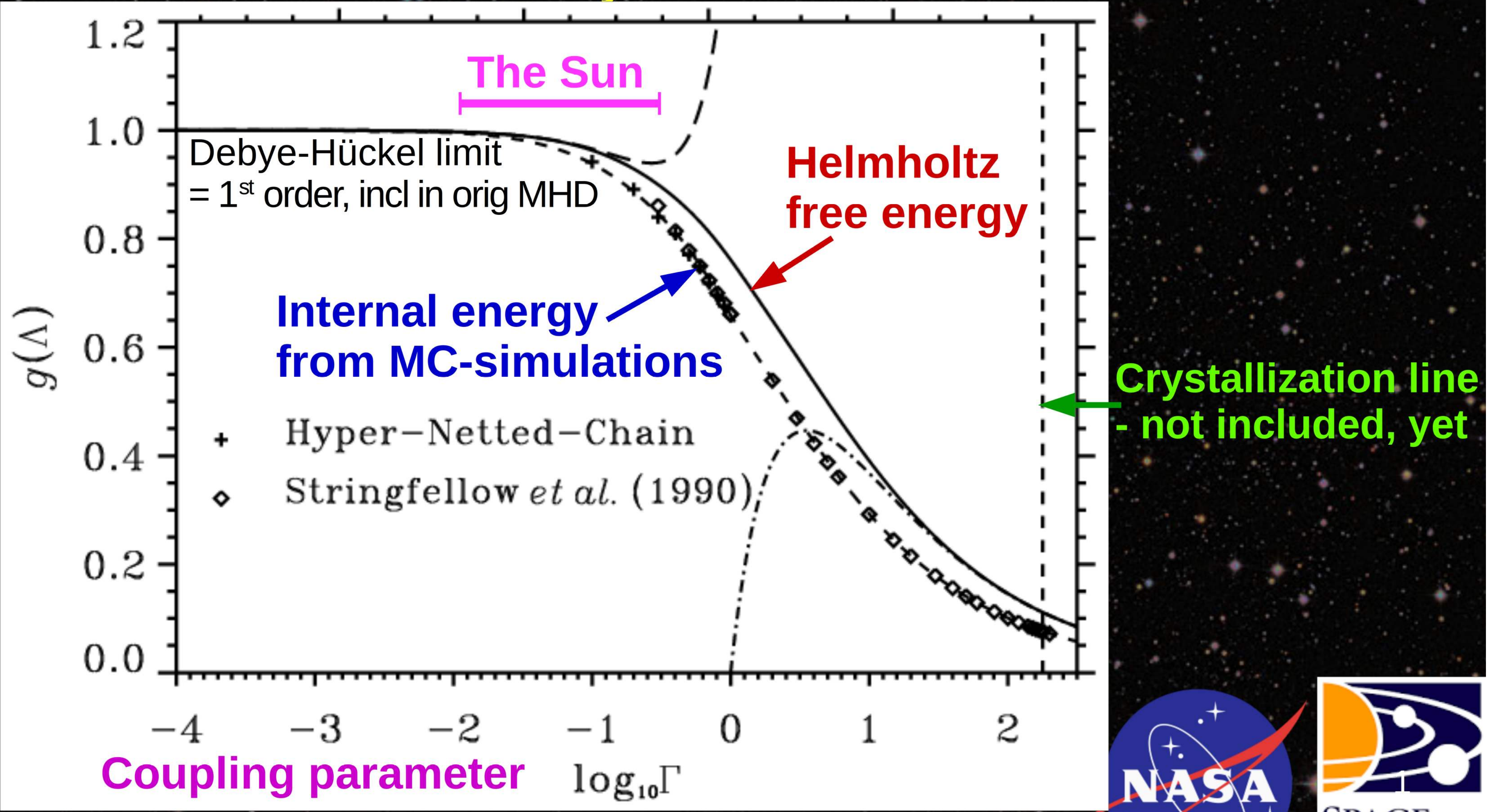
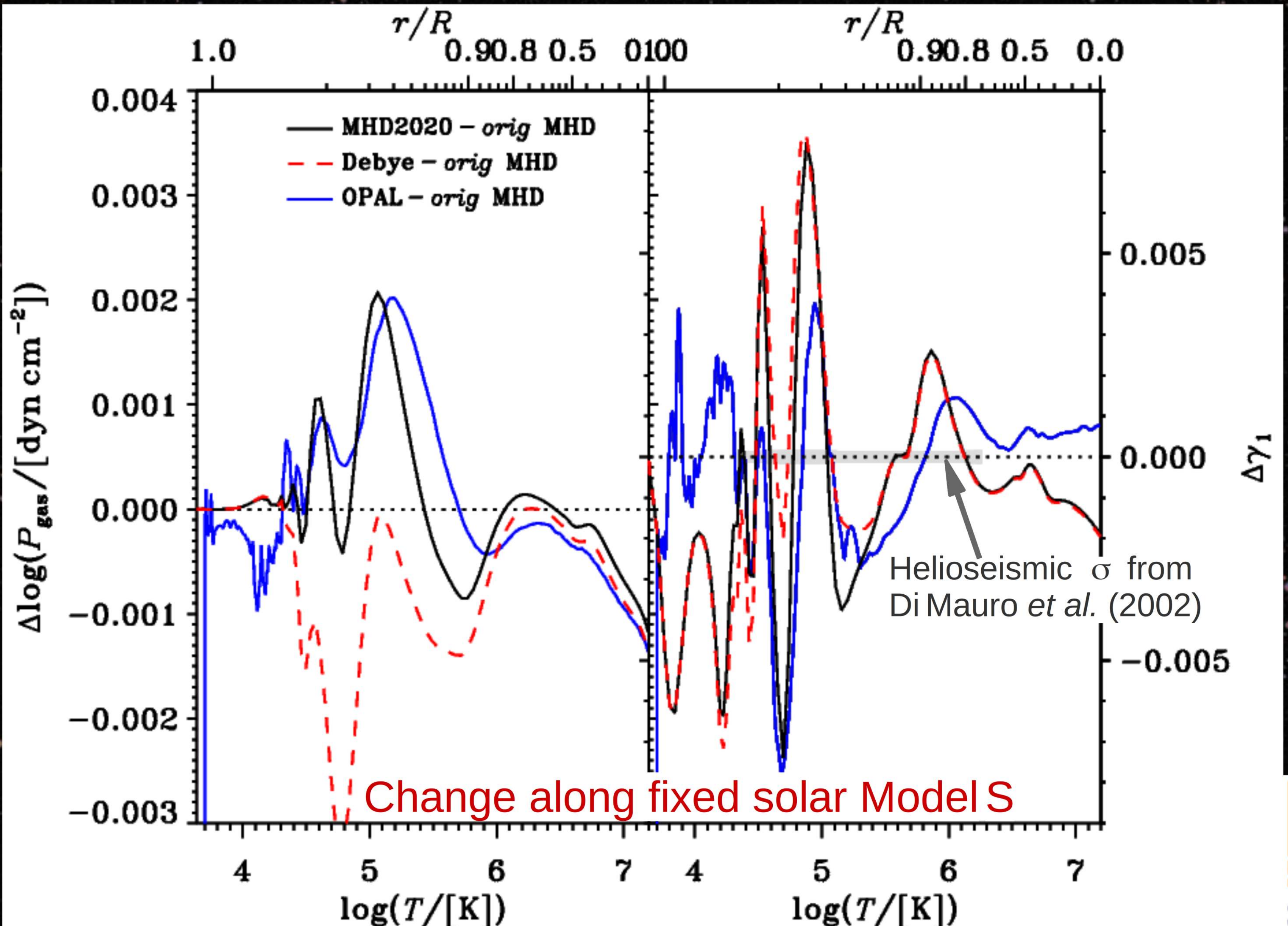
Coulomb effects beyond Debye-Hückel

Deviation from Debye-Hückel:



Coulomb effects beyond Debye-Hückel



Updates MHD → MHD2020 EOS

Added (w.r.t. Hummer & Mihalas, 1988):

- More elements: 6 → 27 ⇒ 447 atoms and ions
- All molecules of included elements (187 for 27 elems)
- New micro-field distribution functions (for occupation probabilities and Stark broadening)
- Coulomb effects beyond Debye-Hückel (1st order)
- Quantum effects – diffraction and exchange
- Abandoning hard-sphere approx. for neutrals
- Relativistic electrons
- More complete part.funcs/energy levels

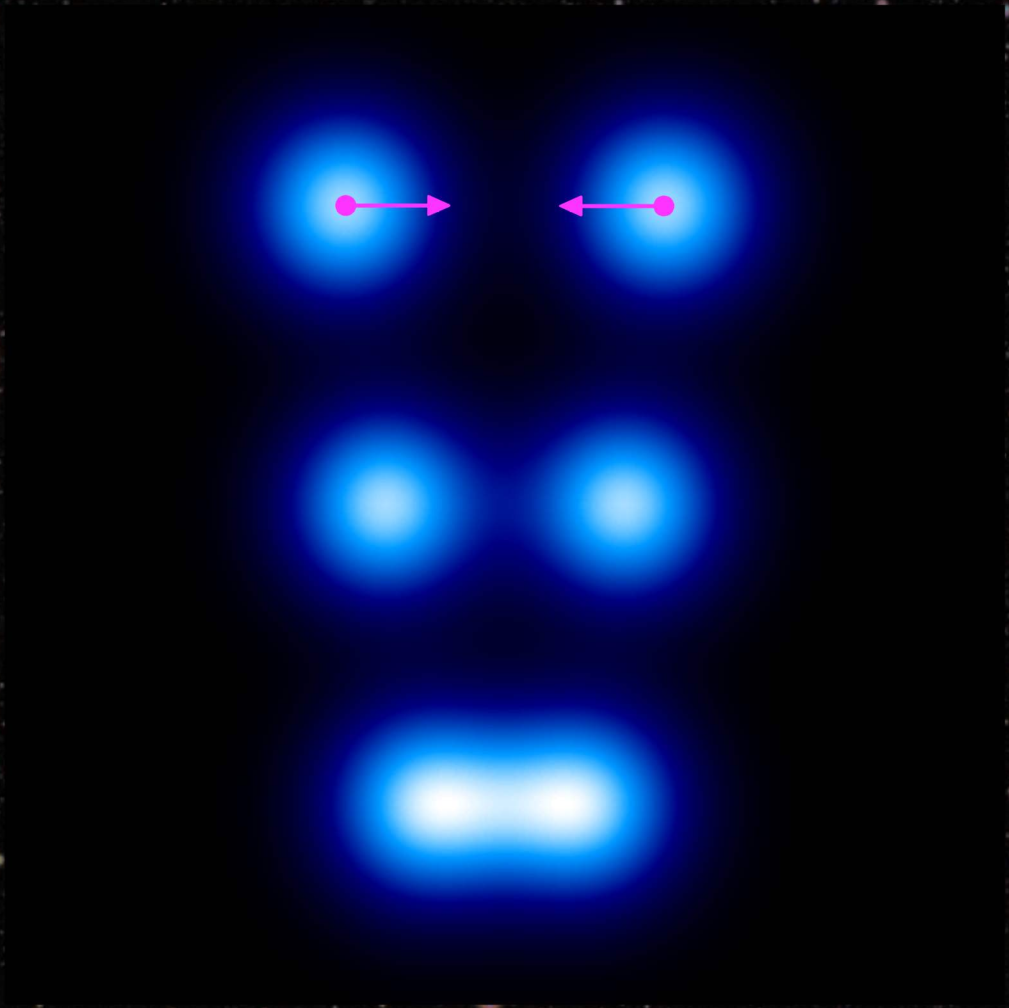
Neutral atoms = hard spheres?

orig MHD

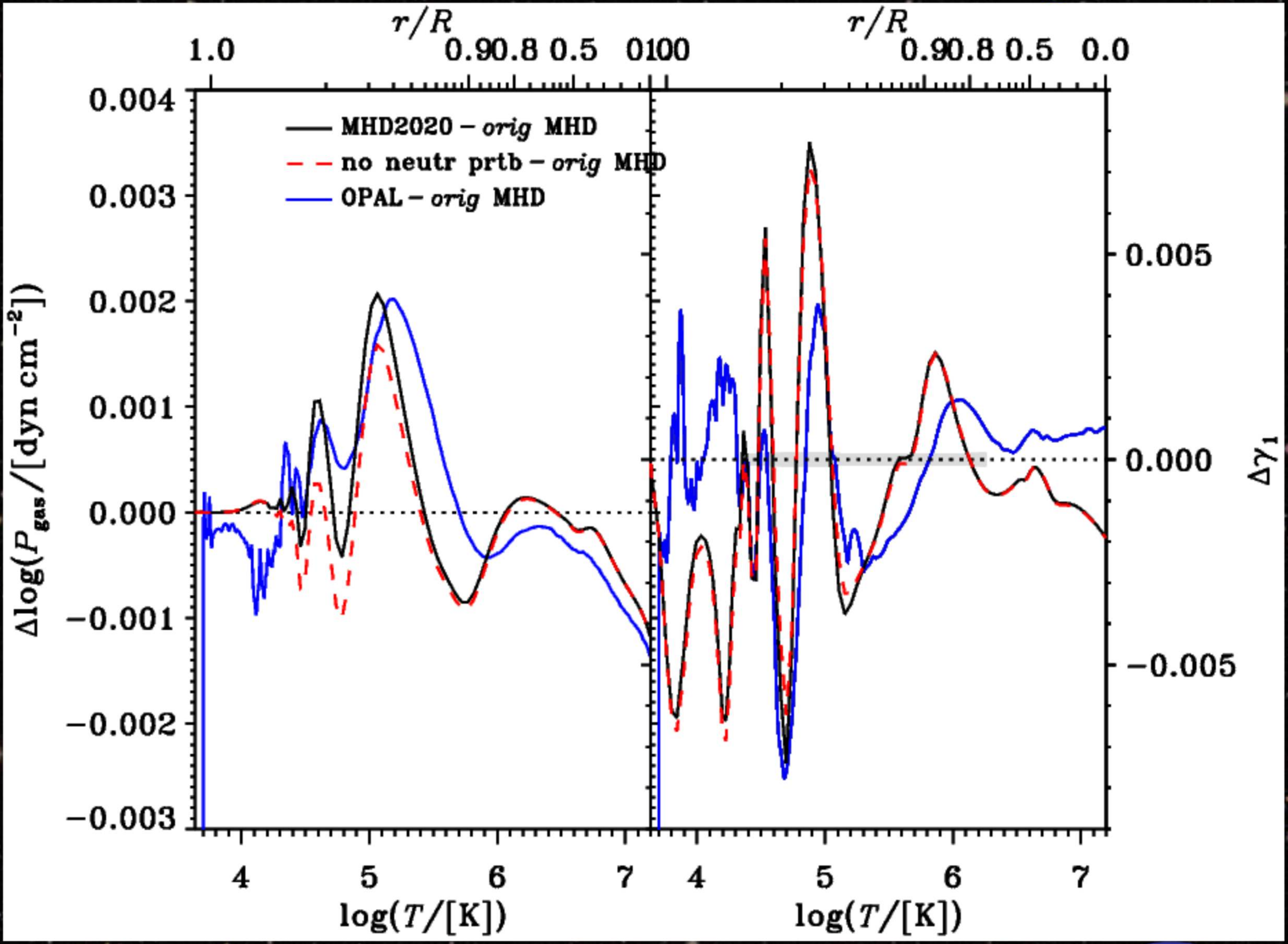
Is this what interacting neutral atoms look like?

Or is it more like this?

Neutral atoms = overlapping e^- clouds



Shielded nuclear charges



Microfield distribution with screening parameter from bound electrons – included for 1st time

Updates MHD → MHD2020 EOS

Added (w.r.t. Hummer & Mihalas, 1988):

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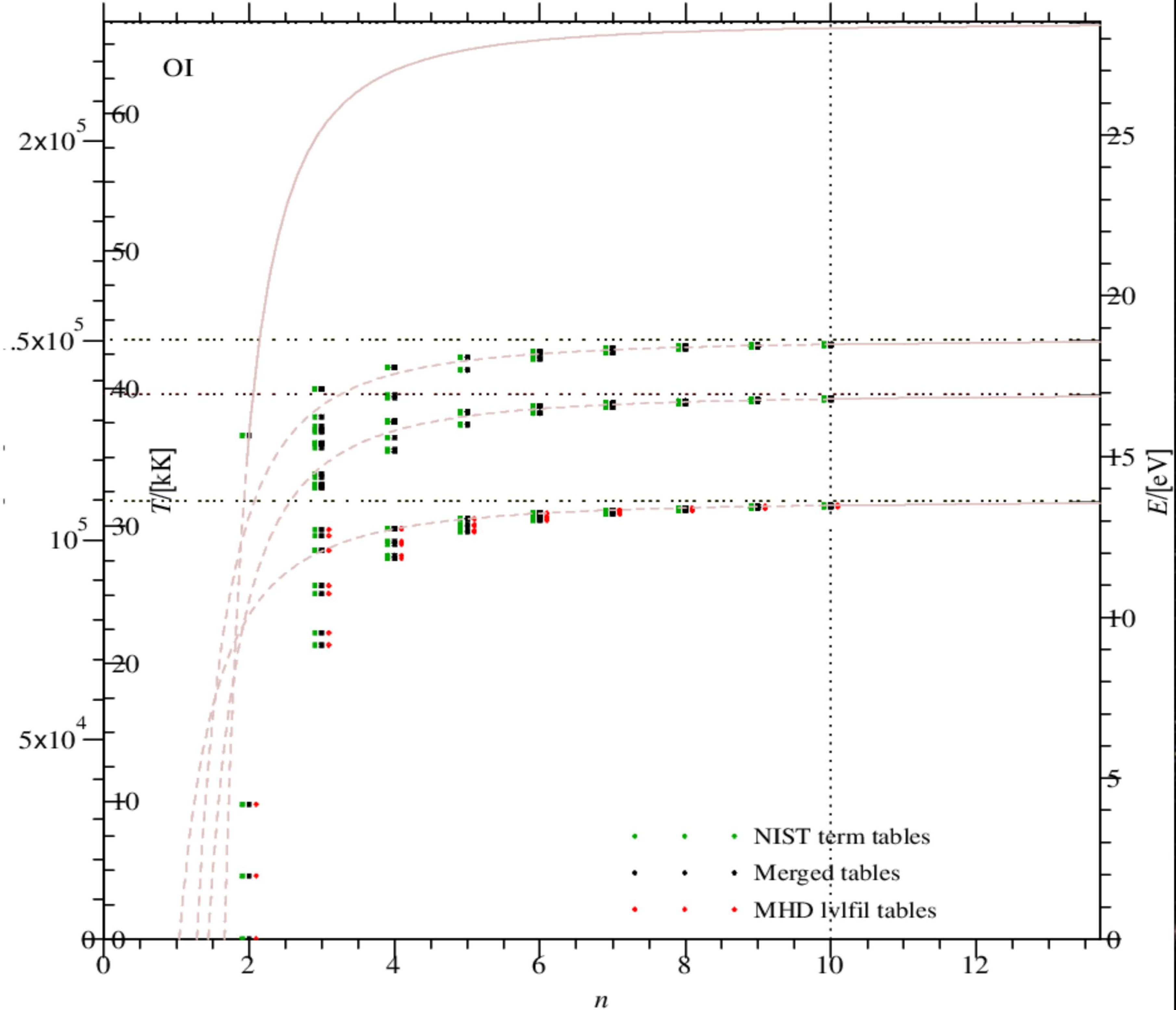

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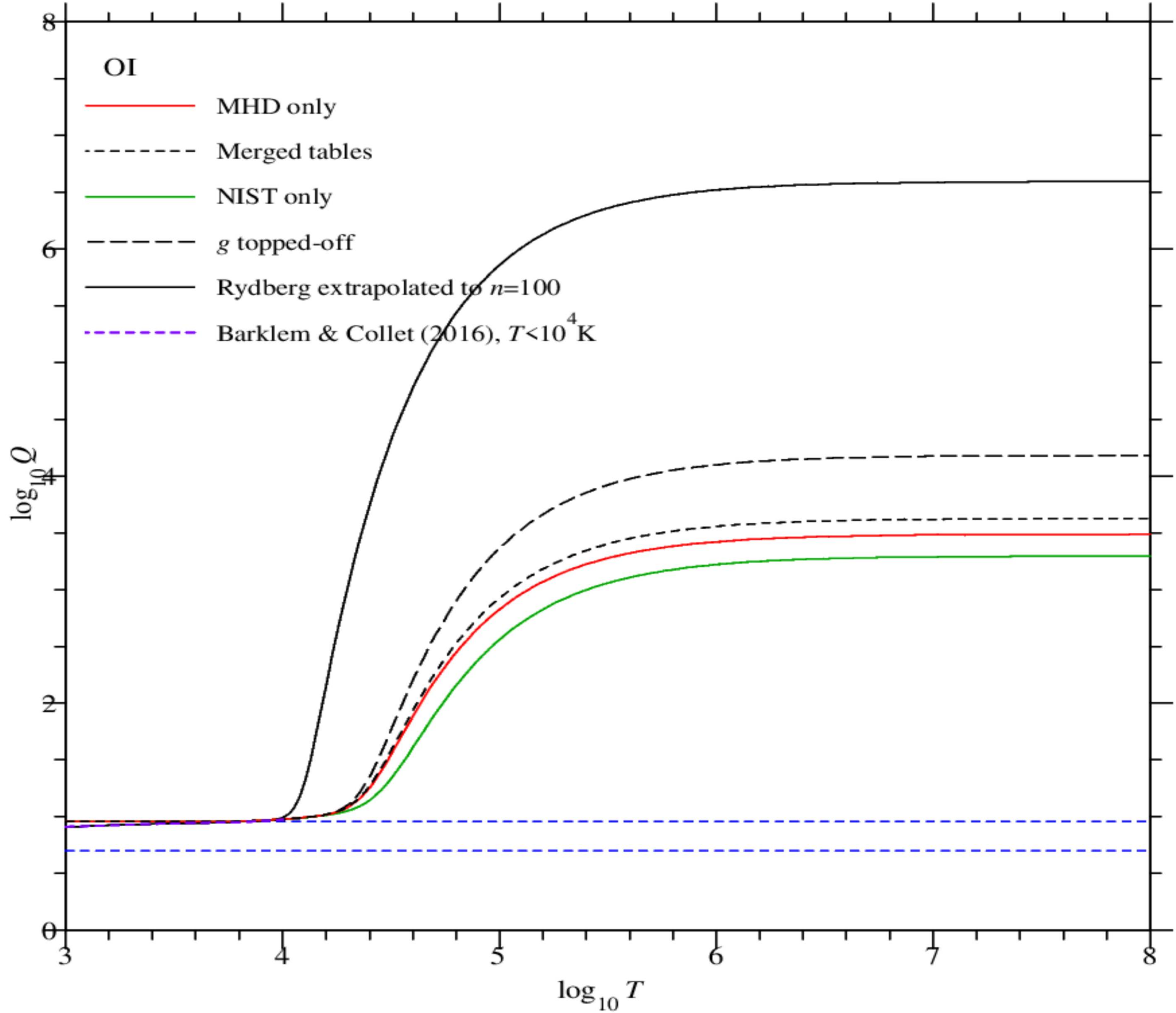

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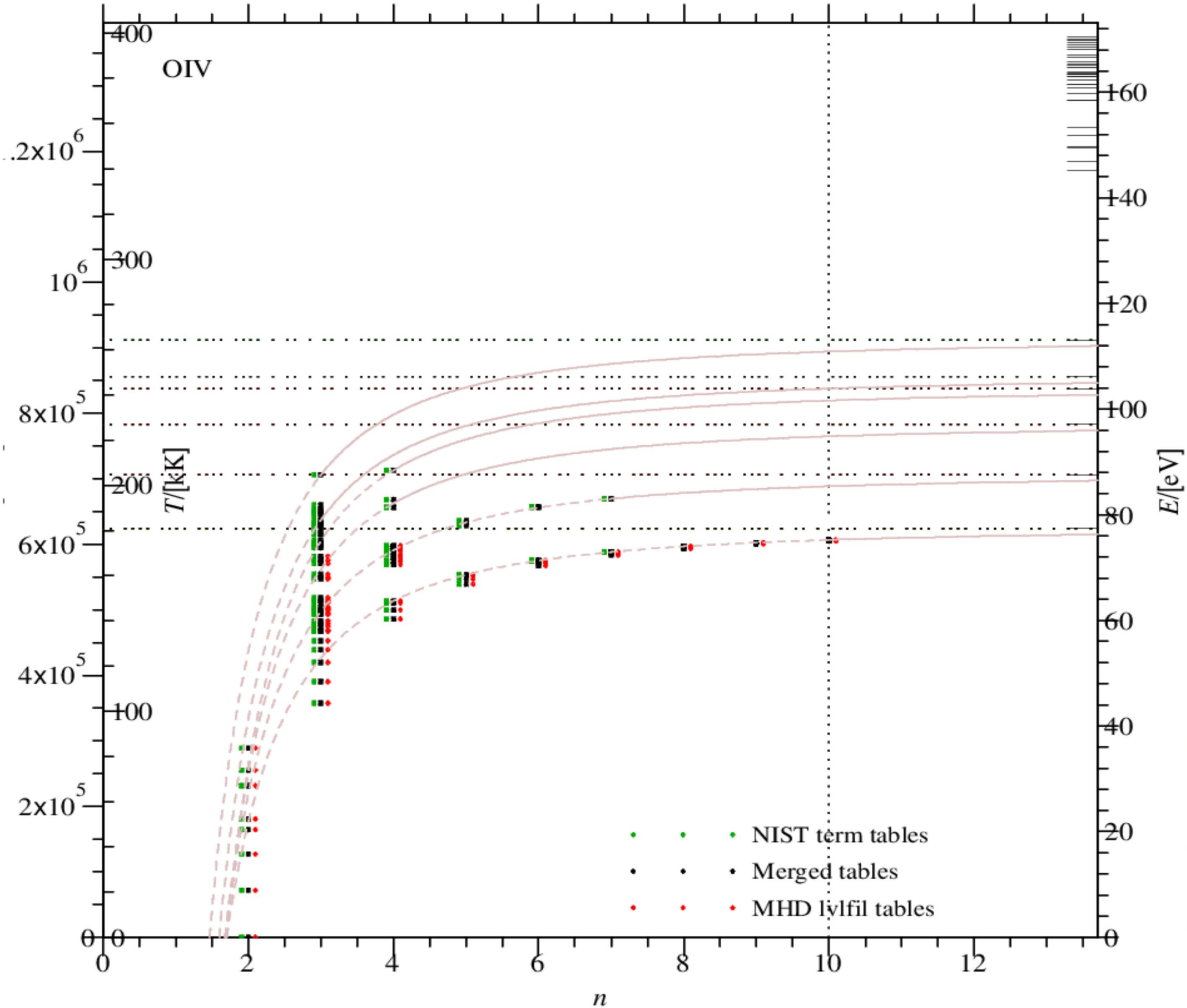

OIV
T/[kK]
E/[eV]
n
NIST term tables
Merged tables
MHD lvlfil tables
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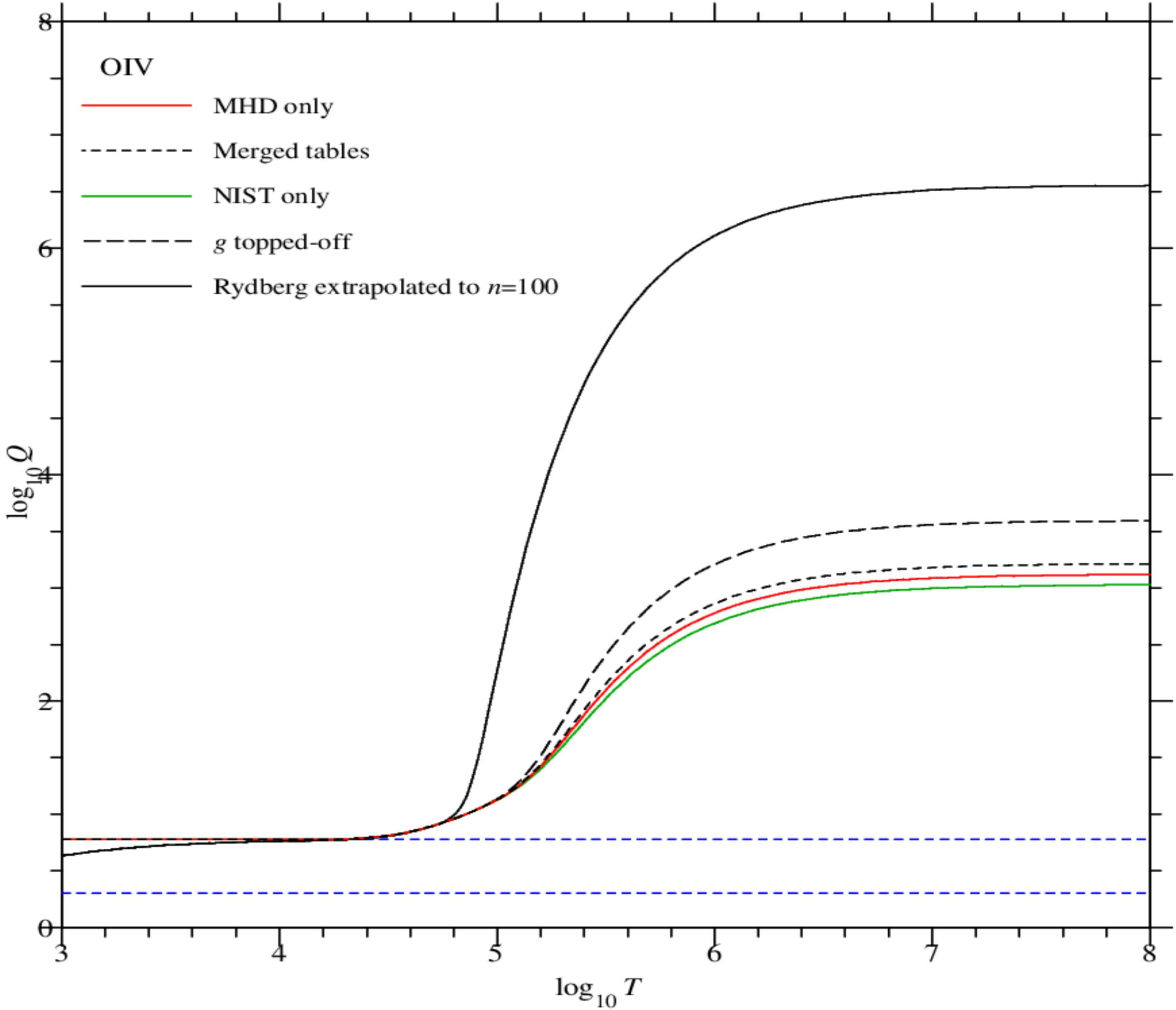

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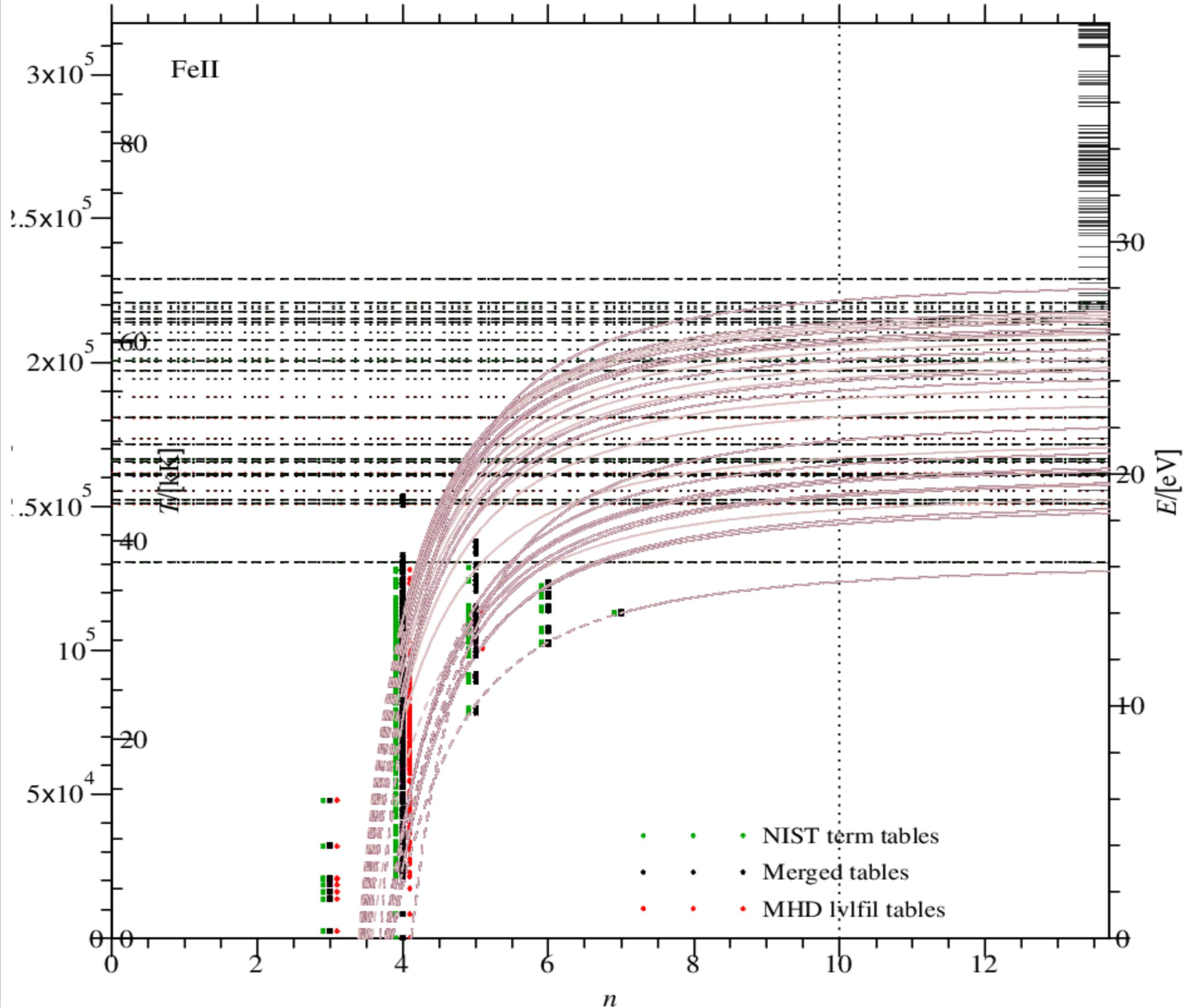

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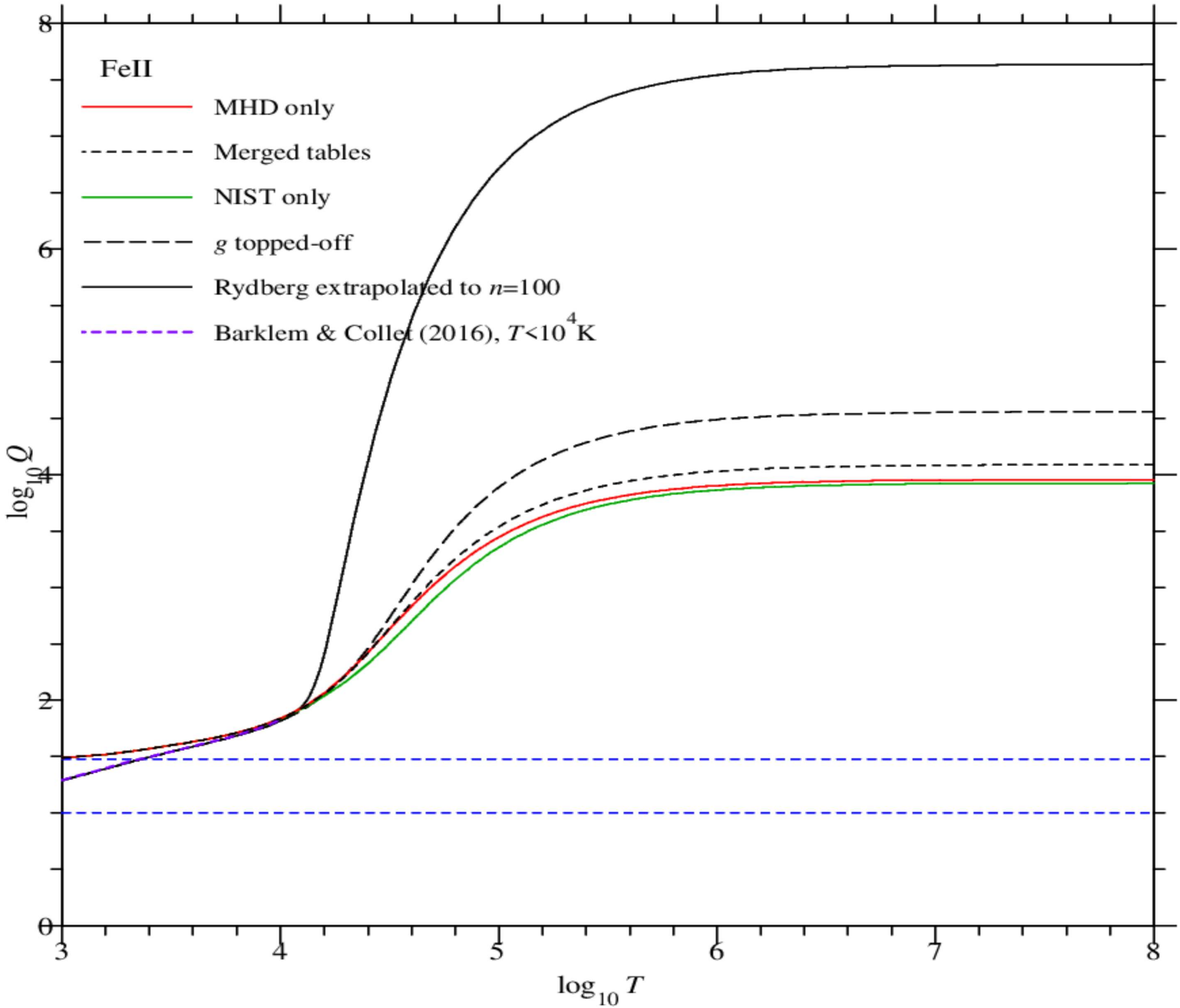

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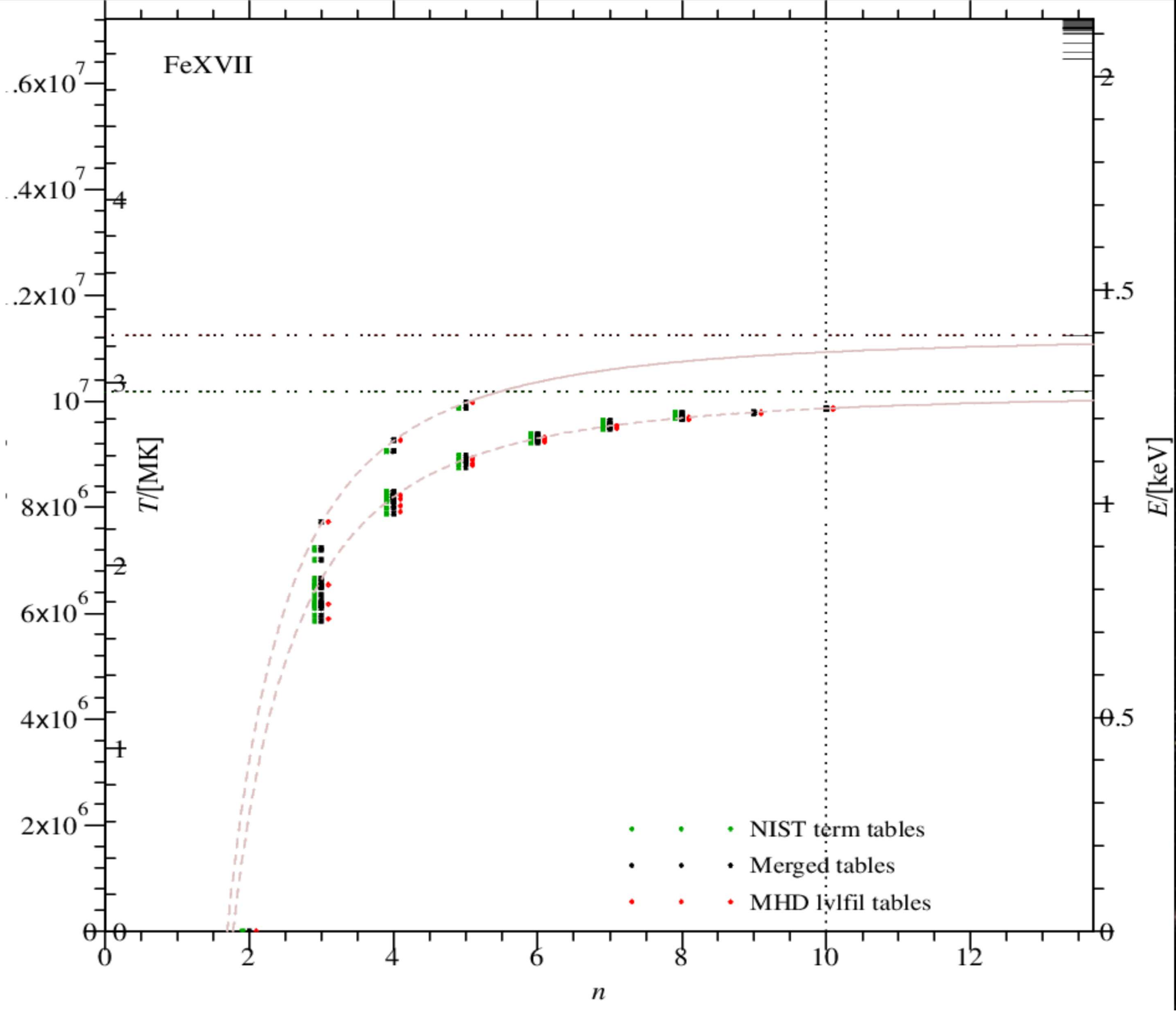
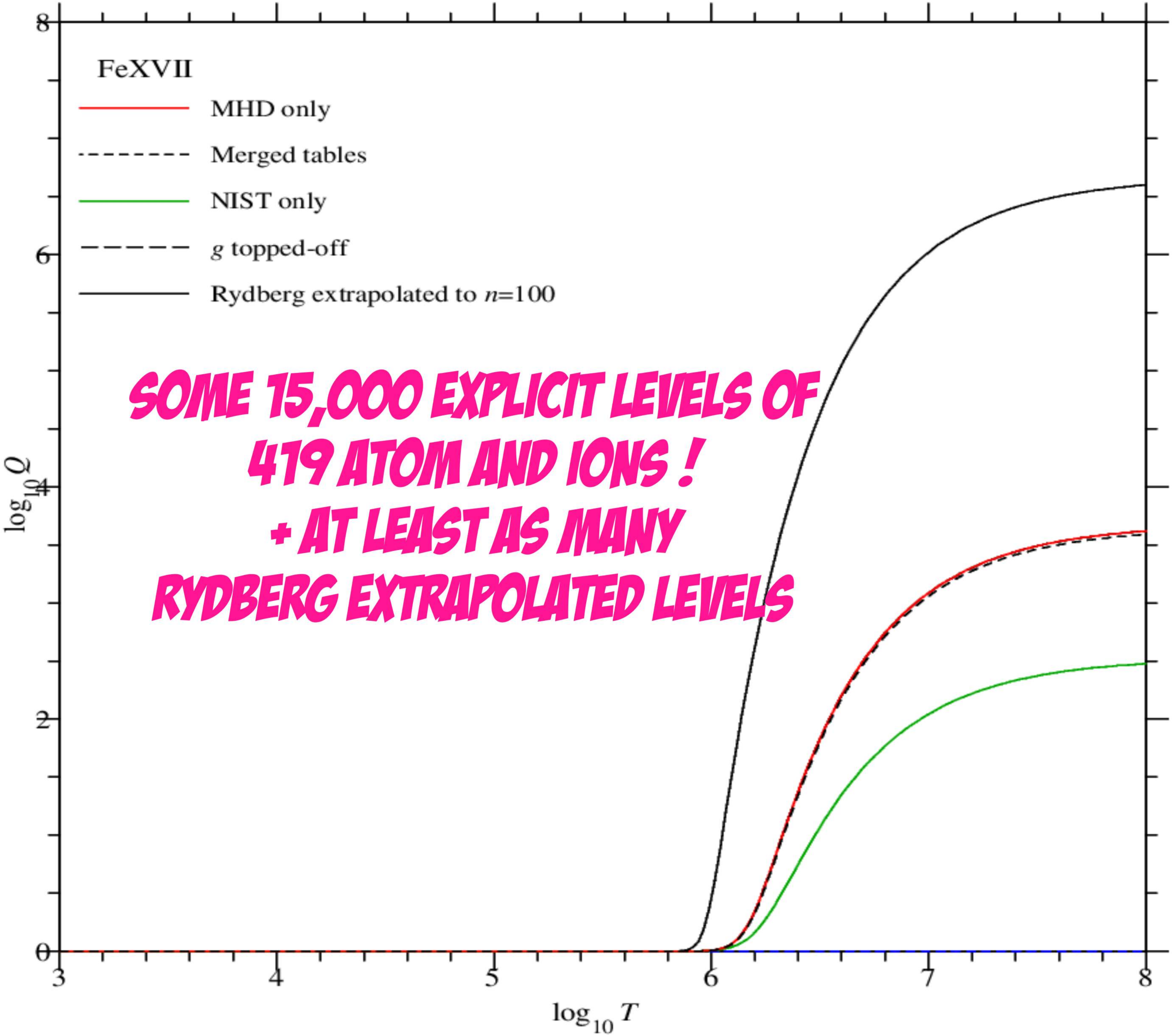


FeXVII
T/[MK]
E/[keV]
n
NIST term tables
Merged tables
MHD lvlfil tables



SOME 15,000 EXPLICIT LEVELS OF 419 ATOM AND IONS !
+ AT LEAST AS MANY RYDBERG EXTRAPOLATED LEVELS

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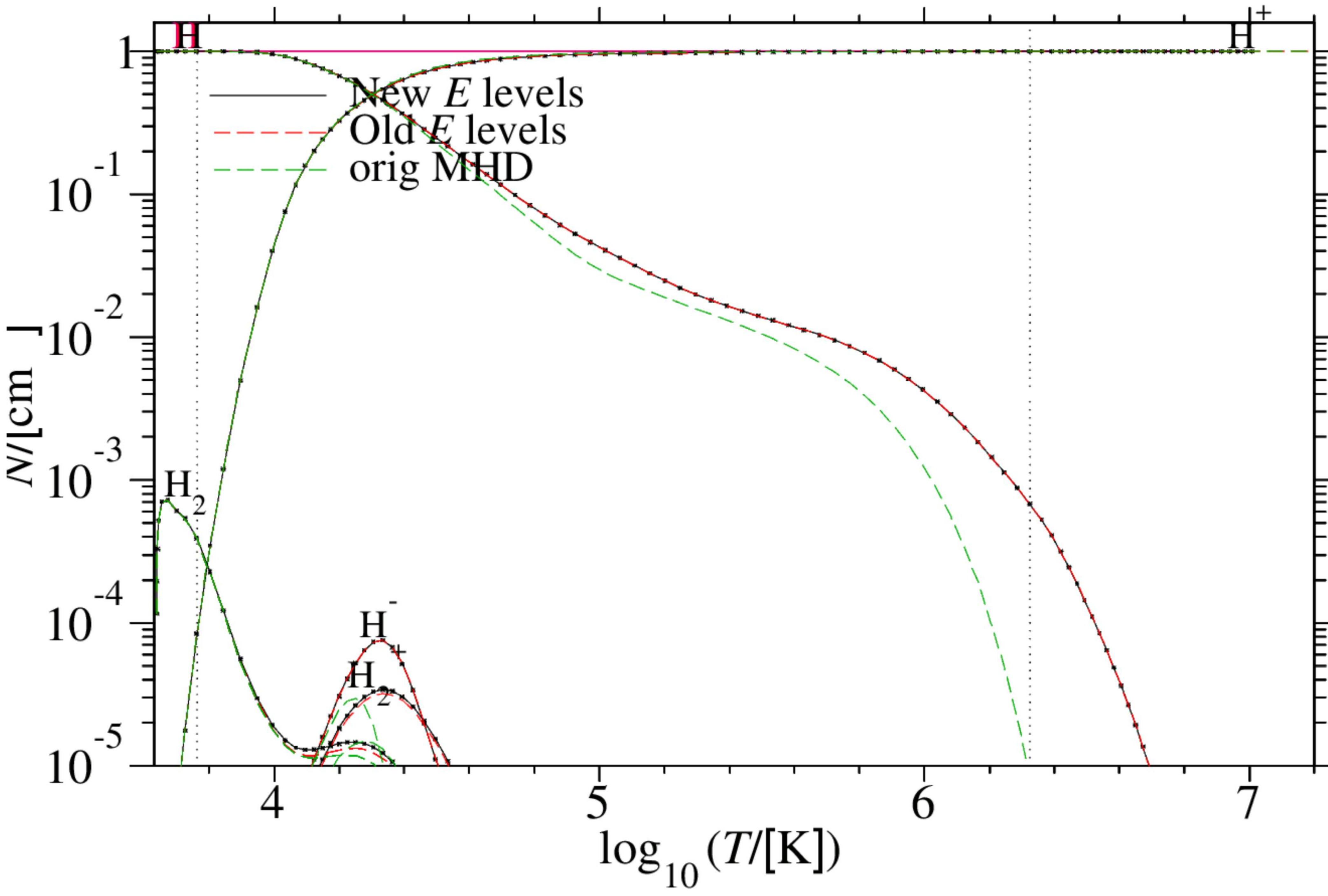
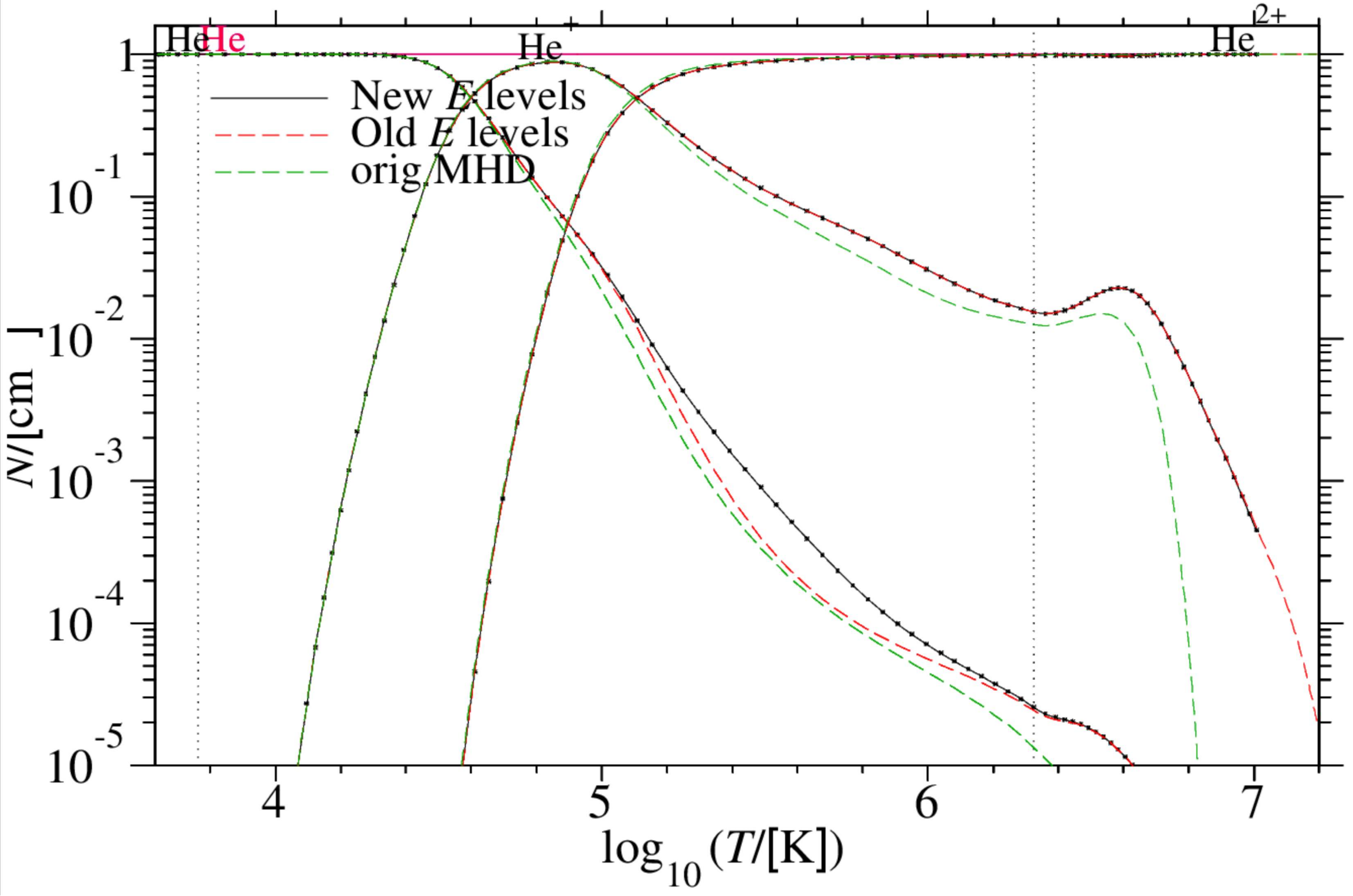
Some prelim. results of MHD2020

- Thermodynamics
- Helioseismic helium abundance
- Atmospheric opacities
- Interior opacities

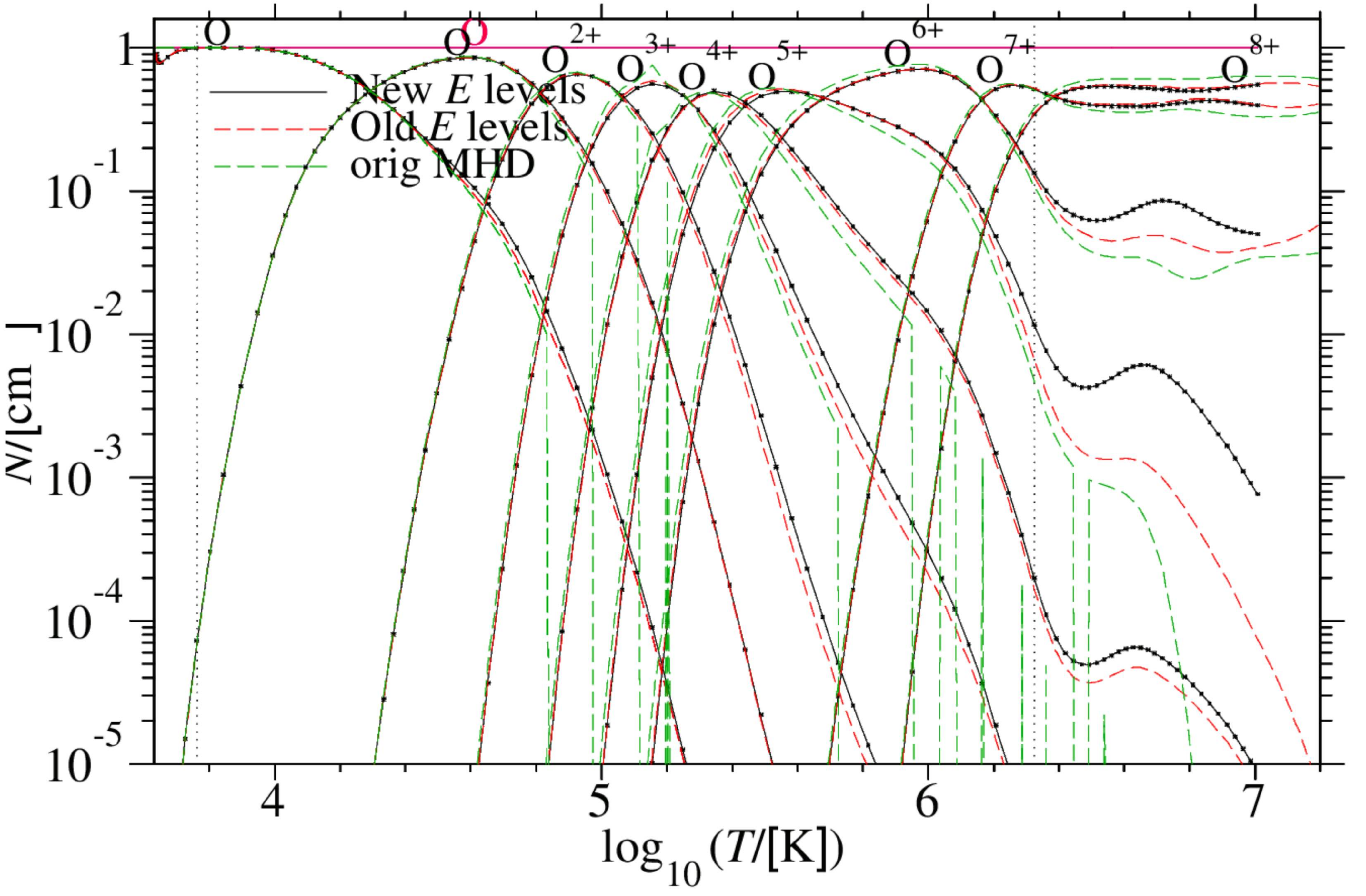
Consequences for ionization in the Sun



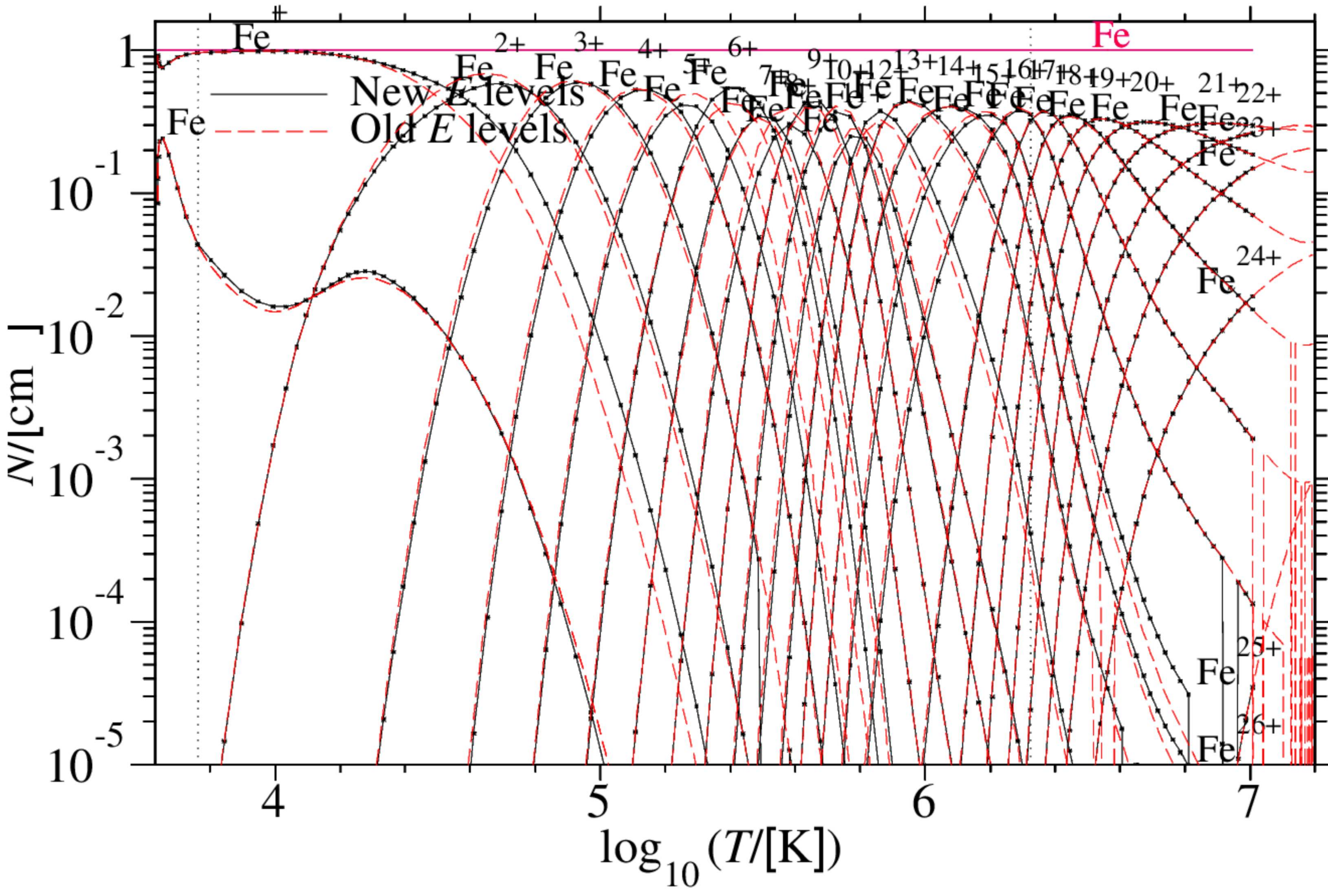
Consequences for ionization in the Sun



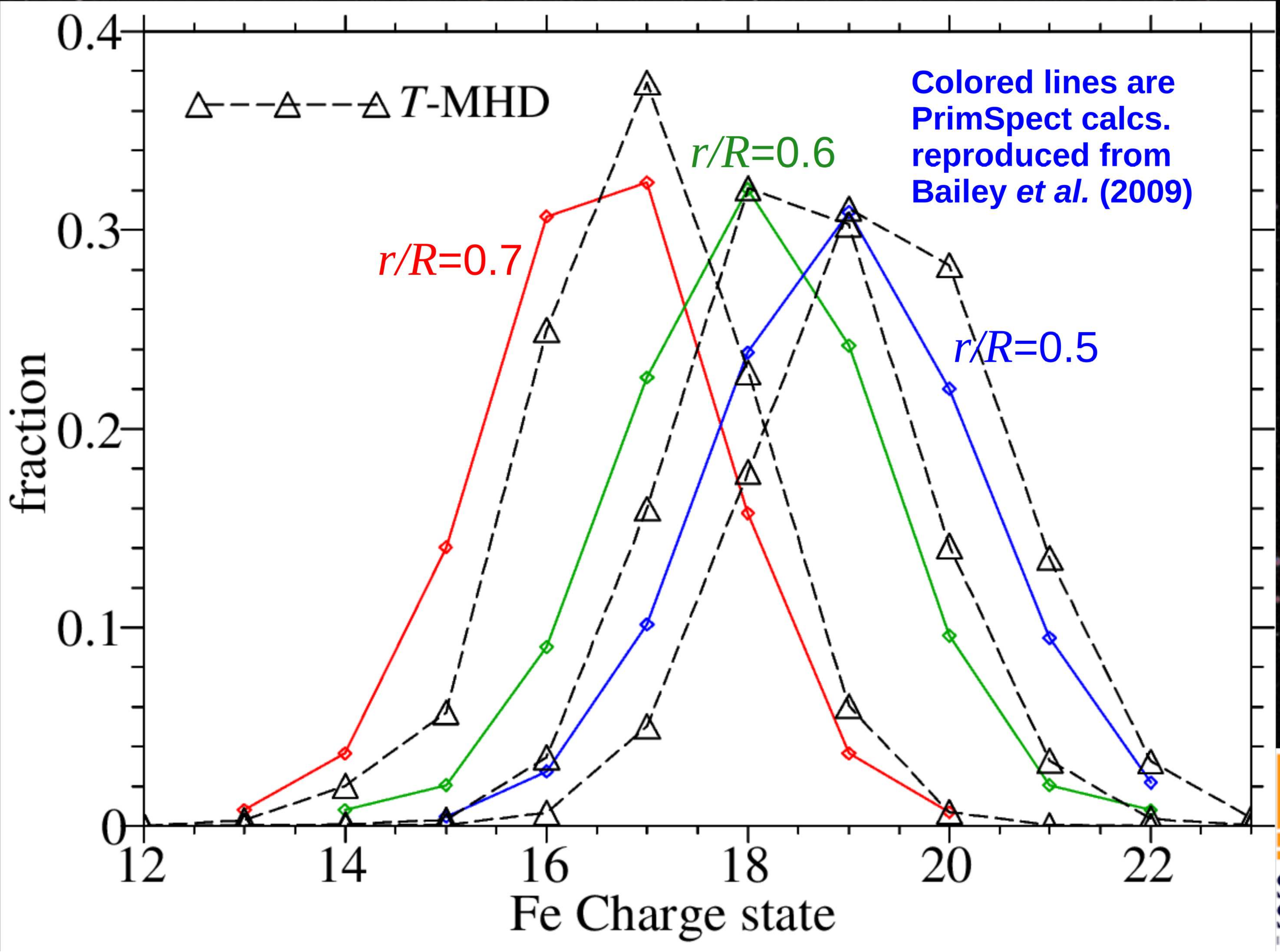
Consequences for ionization in the Sun



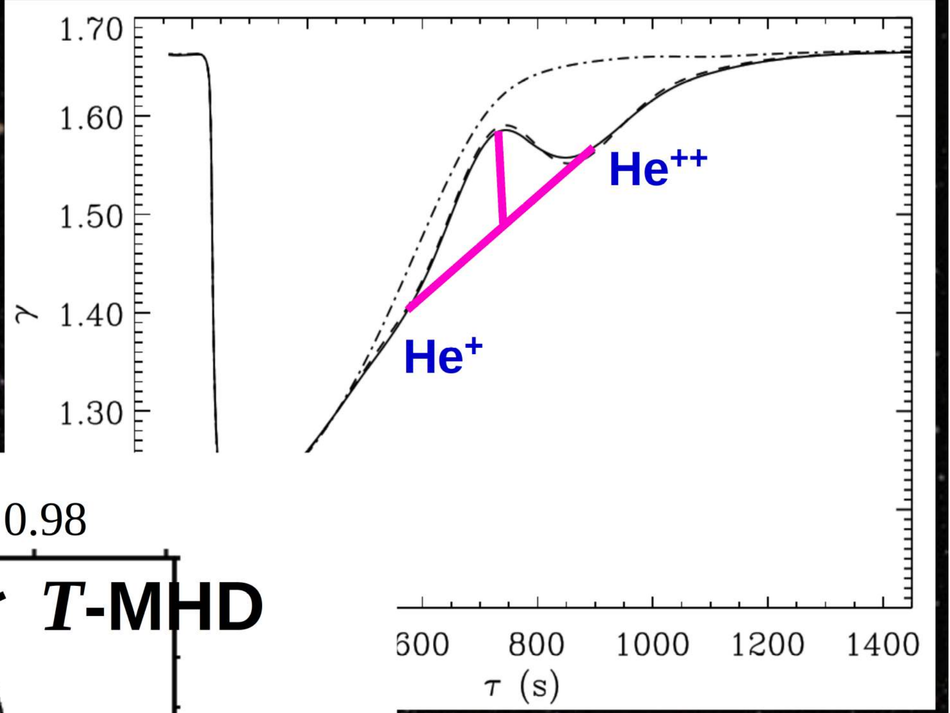
Consequences for ionization in the Sun

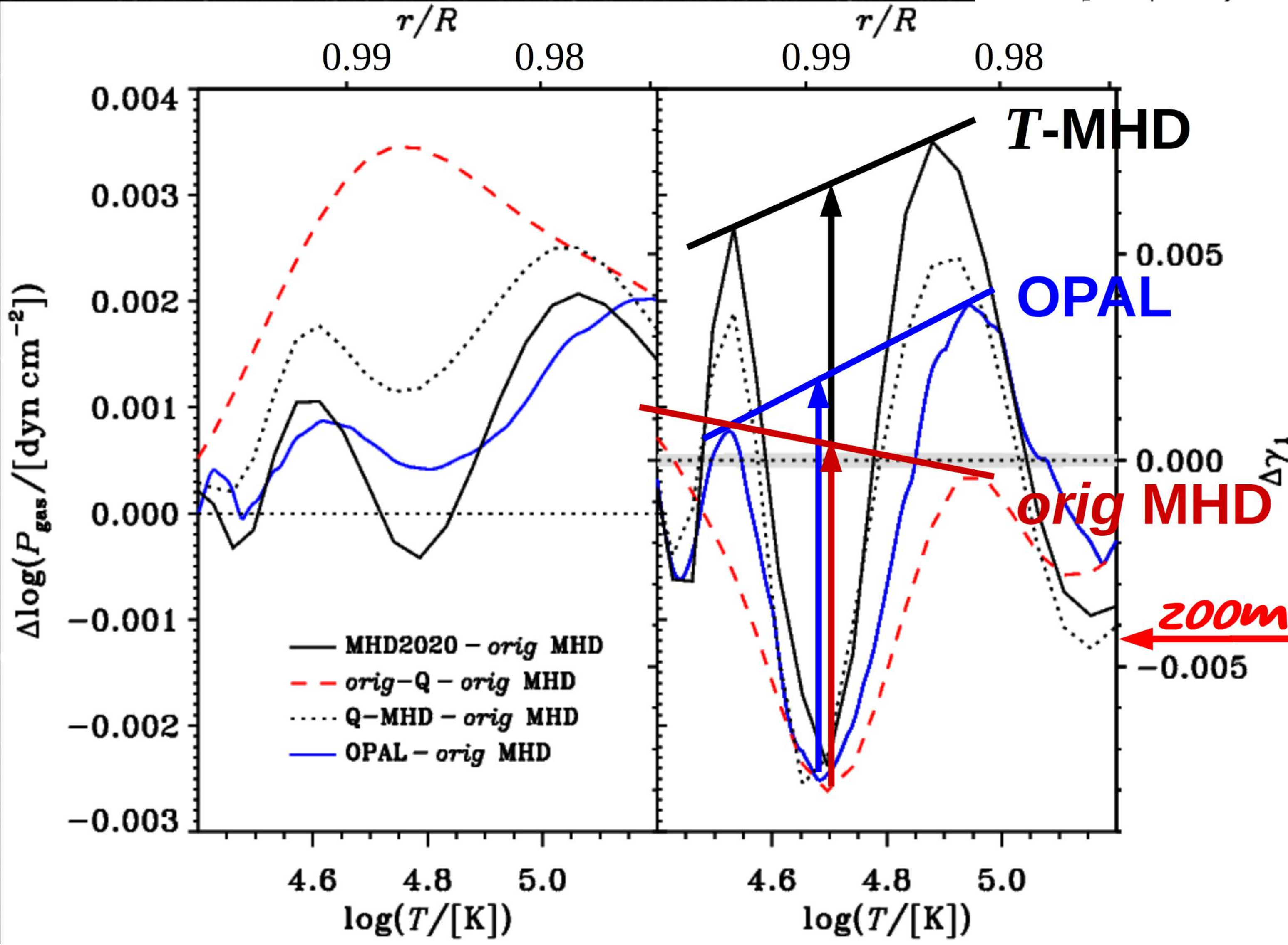


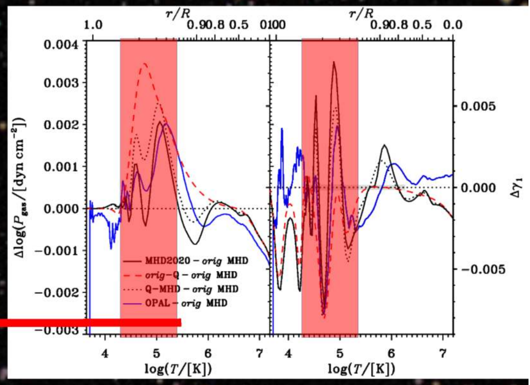
Consequences for ionization in the Sun



Consequences for He abundance? Hard to say yet.

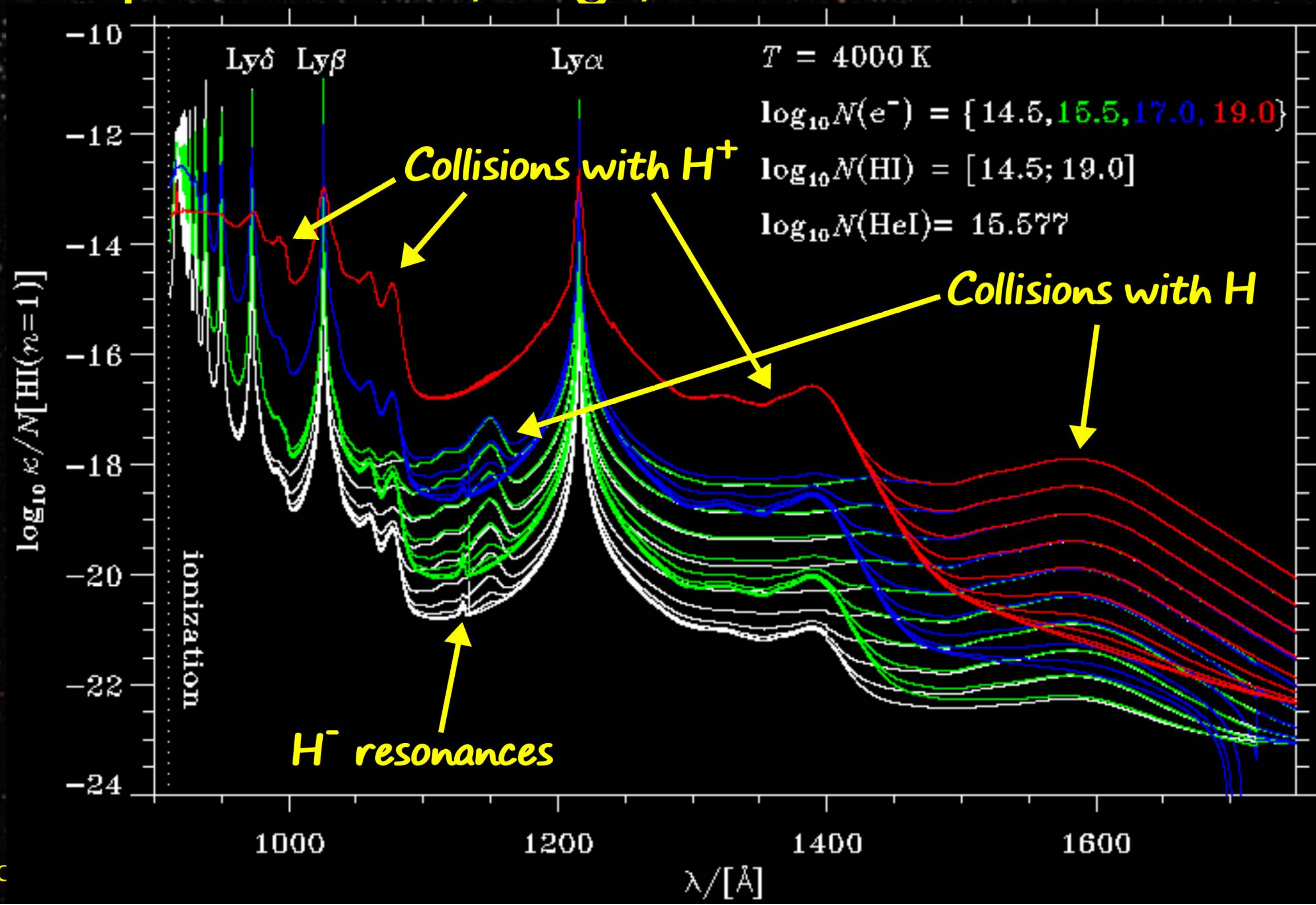


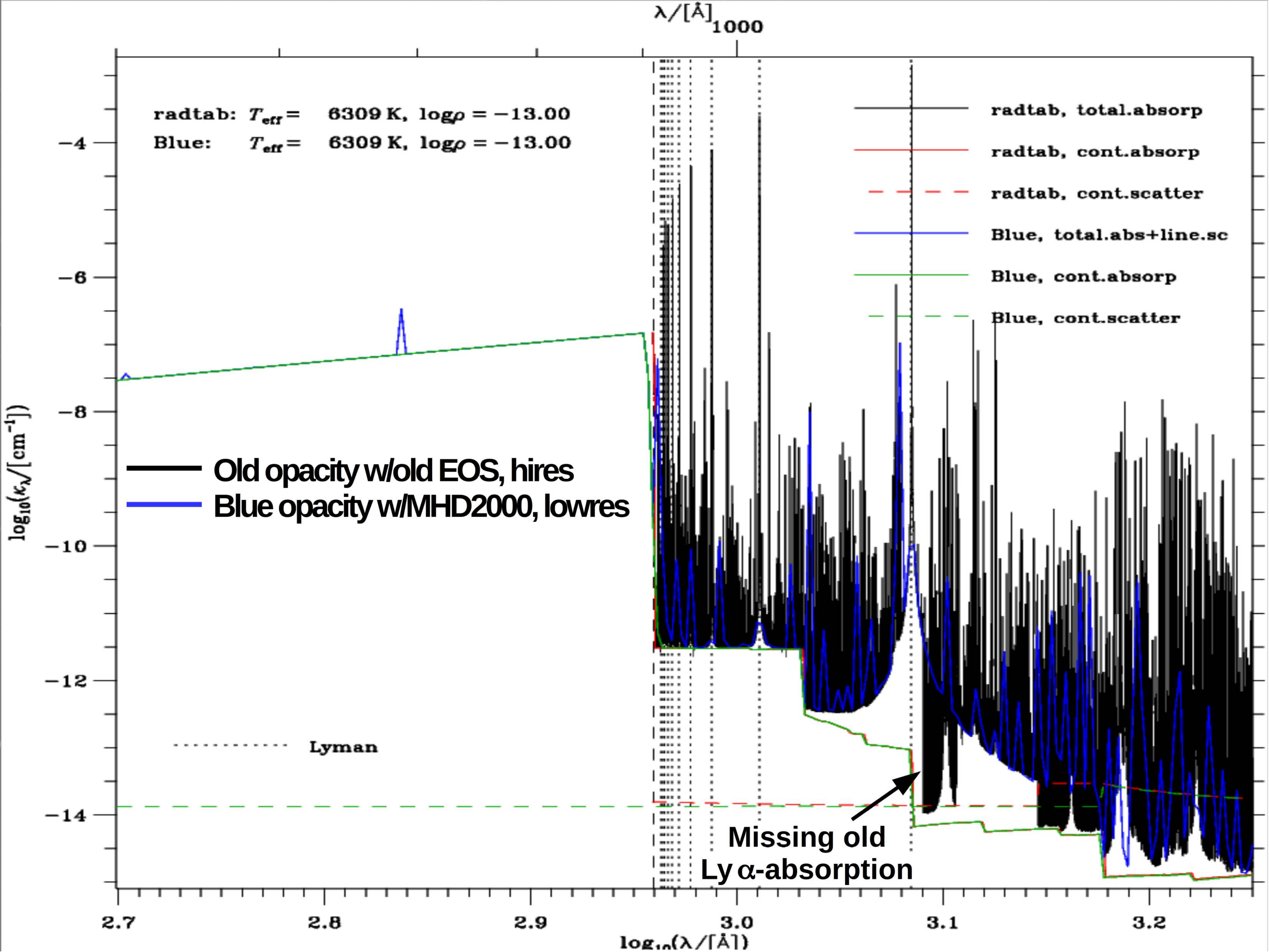




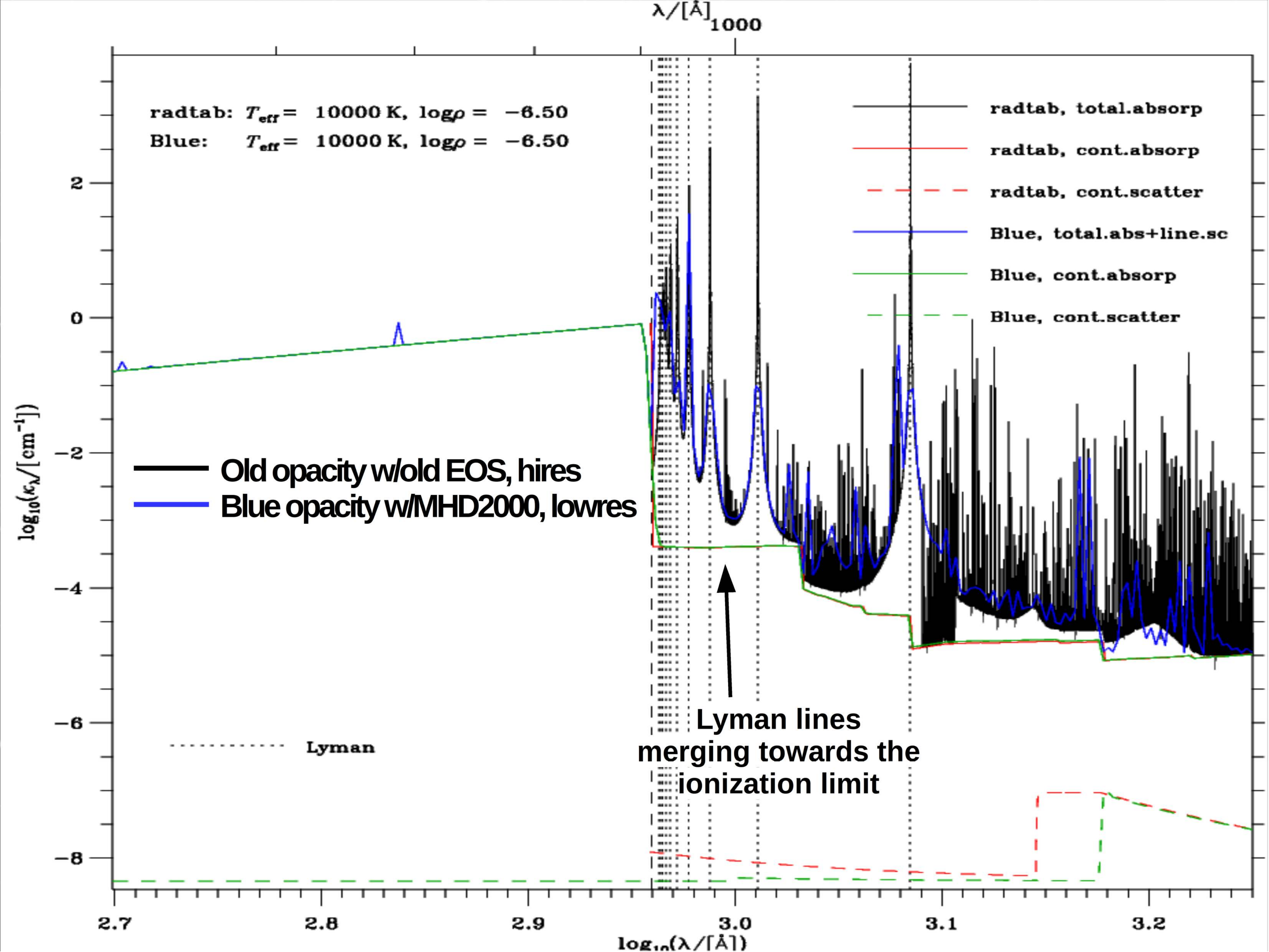
New atmospheric opacity

- Opacity $= \sum_{\text{absorber}} N(\text{absorber}) \times \text{absorption}$
- Ionization + dissociation equilibria from new EOS
- Also new processes, e.g., satellites from collisions:

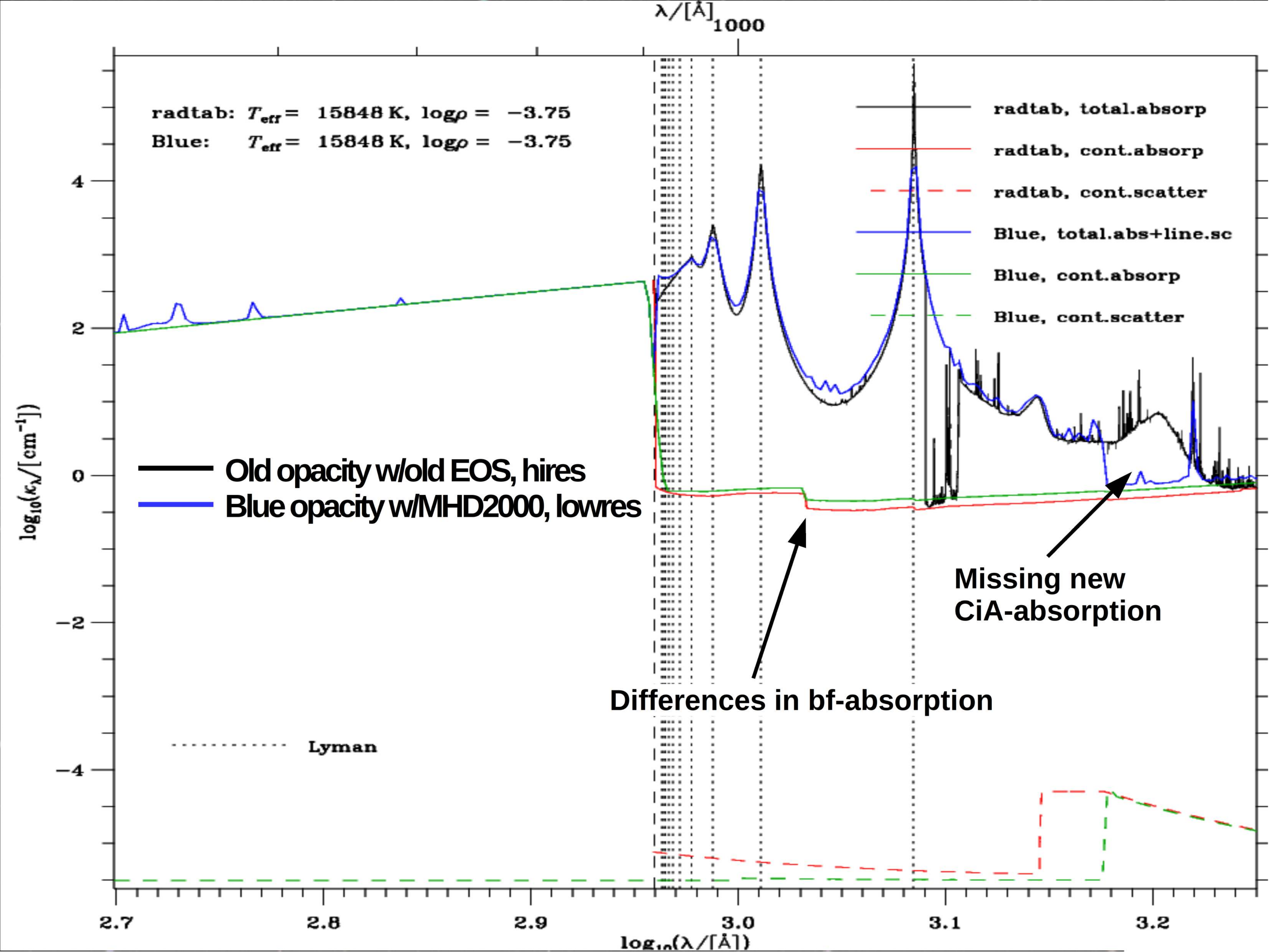


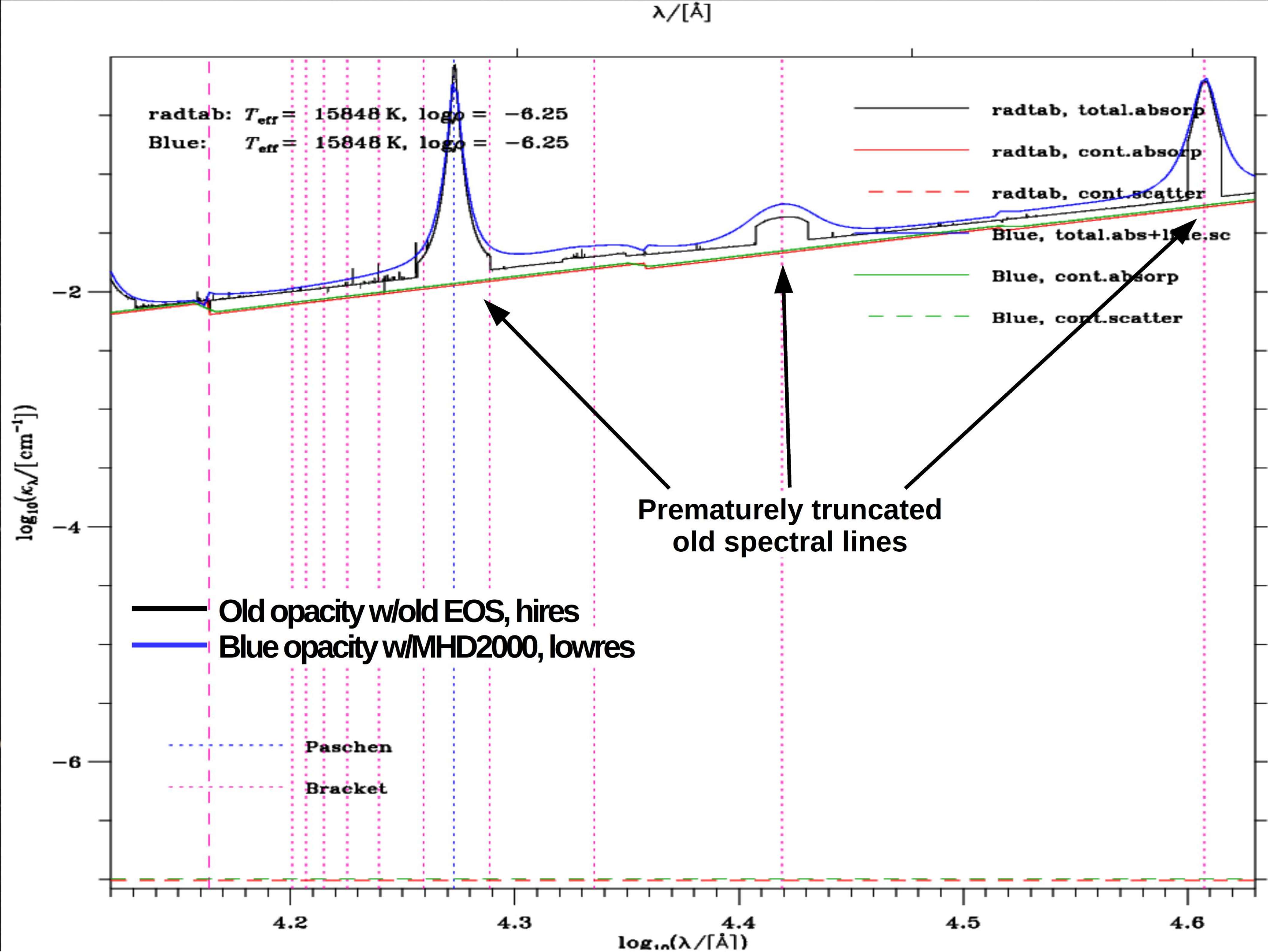


λ/[Å]
1000
radtab: $T_{\rm eff}$ = 6309 K, logρ = −13.00
Blue: $T_{\rm eff}$ = 6309 K, logρ = −13.00
radtab, total.absorp
radtab, cont.absorp
radtab, cont.scatter
Blue, total.abs+line.sc
Blue, cont.absorp
Blue, cont.scatter
Old opacity w/old EOS, hires
Blue opacity w/MHD2000, lowres
Lyman
Missing old
Ly α-absorption
$\log_{10}(\kappa_\lambda/[\rm cm^{-1}])$
−4
−6
−8
−10
−12
−14
2.7
2.8
2.9
3.0
3.1
3.2
$\log_{10}(\lambda/[\rm Å])$



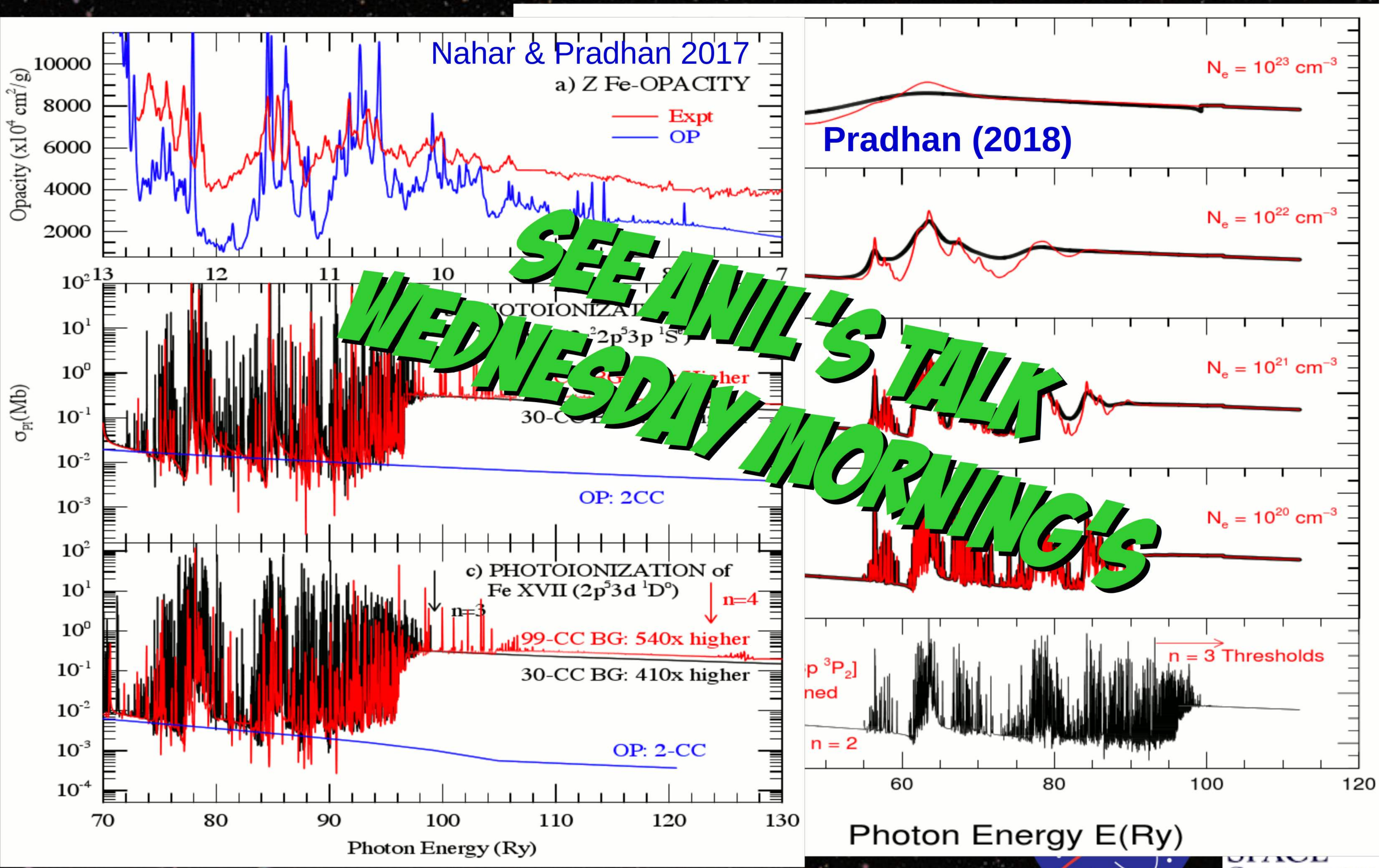
λ/[Å]
1000
radtab: T_{eff} = 10000 K, logρ = −6.50
Blue: T_{eff} = 10000 K, logρ = −6.50
radtab, total.absorp
radtab, cont.absorp
radtab, cont.scatter
Blue, total.abs+line.sc
Blue, cont.absorp
Blue, cont.scatter
Old opacity w/old EOS, hires
Blue opacity w/MHD2000, lowres
Lyman
Lyman lines merging towards the ionization limit
$\log_{10}(\kappa_\lambda/[\mathrm{cm}^{-1}])$
2
0
−2
−4
−6
−8
2.7
2.8
2.9
3.0
3.1
3.2
$\log_{10}(\lambda/[\mathrm{Å}])$


λ/[Å]
1000
radtab: T_{eff} = 15848 K, logρ = −3.75
Blue: T_{eff} = 15848 K, logρ = −3.75
radtab, total.absorp
radtab, cont.absorp
radtab, cont.scatter
Blue, total.abs+line.sc
Blue, cont.absorp
Blue, cont.scatter
Old opacity w/old EOS, hires
Blue opacity w/MHD2000, lowres
Missing new CiA-absorption
Differences in bf-absorption
Lyman
$\log_{10}(\kappa_\lambda/[\mathrm{cm}^{-1}])$
4
2
0
−2
−4
2.7
2.8
2.9
3.0
3.1
3.2
$\log_{10}(\lambda/[\text{Å}])$



λ/[Å]
radtab: T_{eff} = 15848 K, logρ = −6.25
Blue: T_{eff} = 15848 K, logρ = −6.25
radtab, total.absorp
radtab, cont.absorp
radtab, cont.scatter
Blue, total.abs+line.sc
Blue, cont.absorp
Blue, cont.scatter
Prematurely truncated
old spectral lines
Old opacity w/old EOS, hires
Blue opacity w/MHD2000, lowres
Paschen
Bracket
−2
−4
−6
4.2
4.3
4.4
4.5
4.6
$\log_{10}(\lambda/[Å])$
$\log_{10}(\kappa_\lambda/[\mathrm{cm}^{-1}])$

New Interior Opacity w/new EOS



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Conclusions

- First EOS valid for atmospheres, envelopes, cores, of hot stars, cool stars = just plain **stars!**
- Results in bound and more highly excited electrons, deeper in the Sun than both OPAL and orig MHD ⇒ more absorption.

To do list:

- New helio-seismic He abundance determination
- New atmospheric opacity tables based on new EOS
- New grid of 3D stellar atmosphere sim. Based on new EOS
- New interior opacity tables based on new EOS

Will test new EOS against:

- Helioseismology
- Lab experiments at stellar conditions

No atom or molecules were harmed during this project, although some Avogadro numbers of electrons were severely inconvenienced.

In memory of Dimitri Mihalas and David Hummer

Thanks to Werner Däppen for hosting many visits and for many stimulating discussions!