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A New Generation of Line Profile Calculations for Non-ideal Hydrogen Plasmas

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White Dwarf Stars

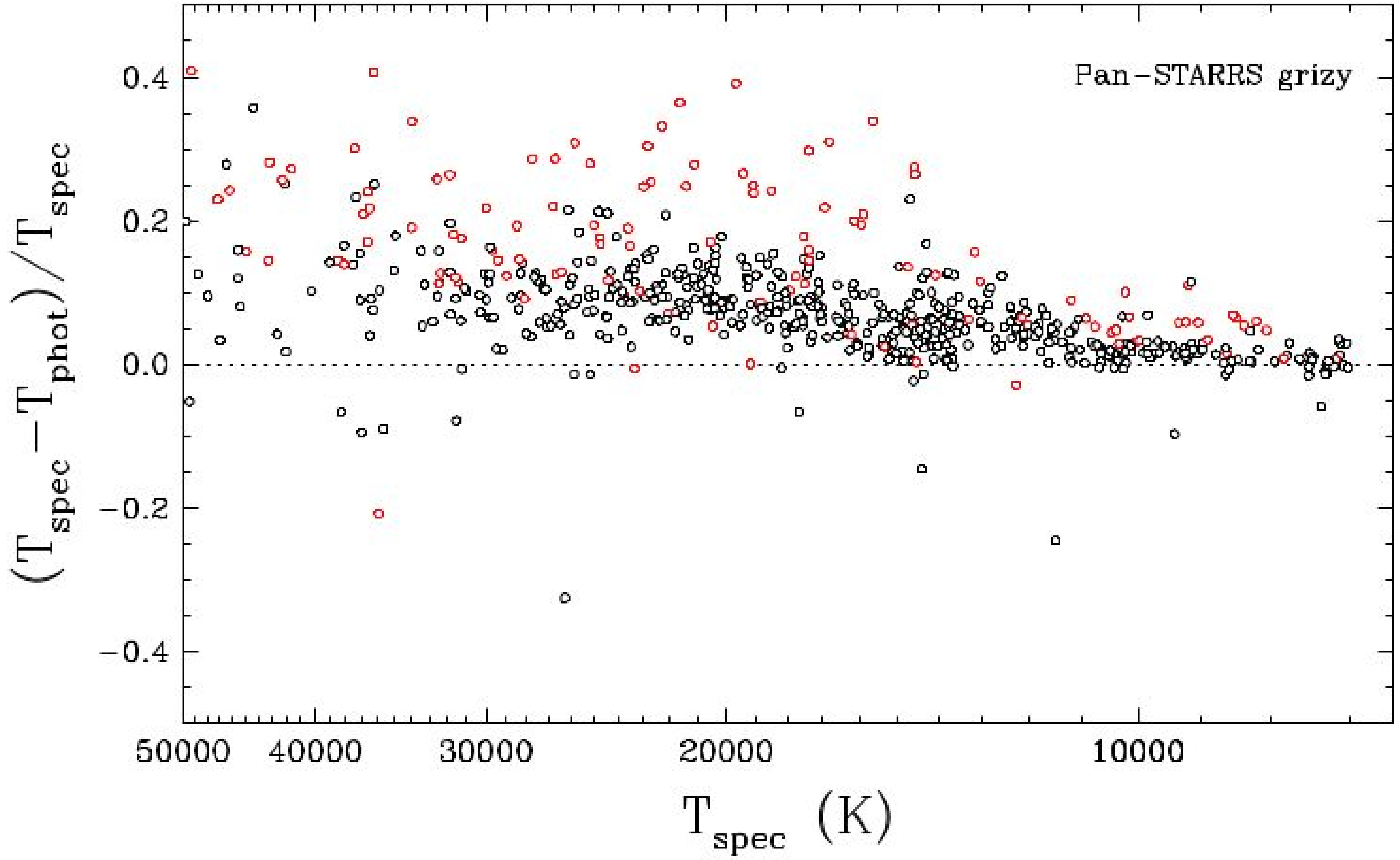
- Due to their high surface gravities ($g \sim 10^8 \, \mathrm{cm/s^2}$), the lightest chemical element rises to the surface
- 80% of all WDs have pure or nearly pure H atmospheres (20% are He, $<$ 1% are C/O)
- They are supported by electron degeneracy pressure, and nuclear reactions are negligible
  $\Rightarrow$ their evolution is a cooling problem
- Their temperatures can be used to deduce their ages, but *only if* we have accurate values for the masses ($M_\star$) and temperatures (T_{eff})

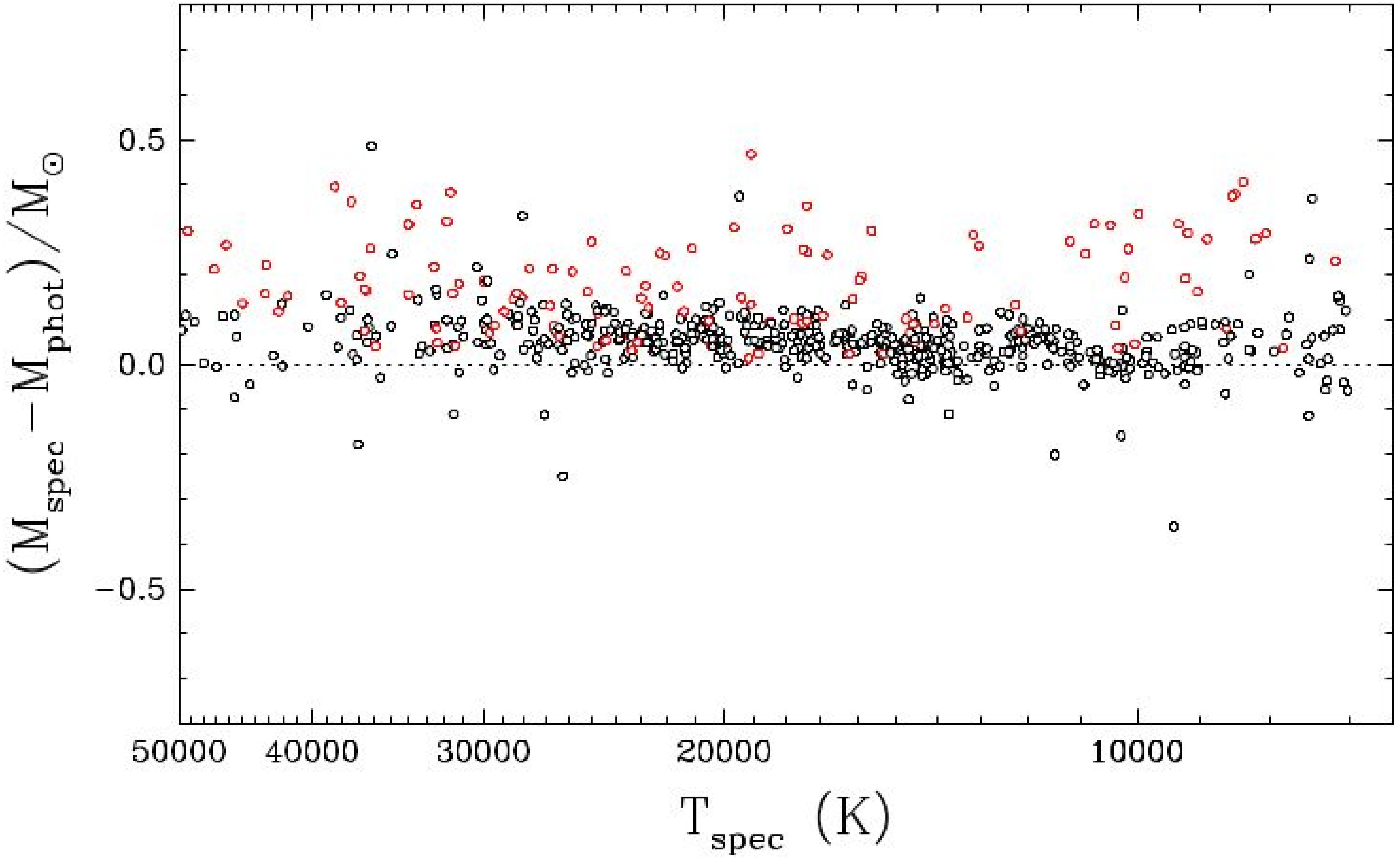
Systematic discrepancies indicate Stark broadening calculations may be inaccurate

- Temperatures inferred by the spectroscopic method are roughly 10% higher than those inferred using photometry.

- Masses also exhibit a similar, less dramatic systematic discrepancy.

Bergeron et al. (2019) *ApJ*

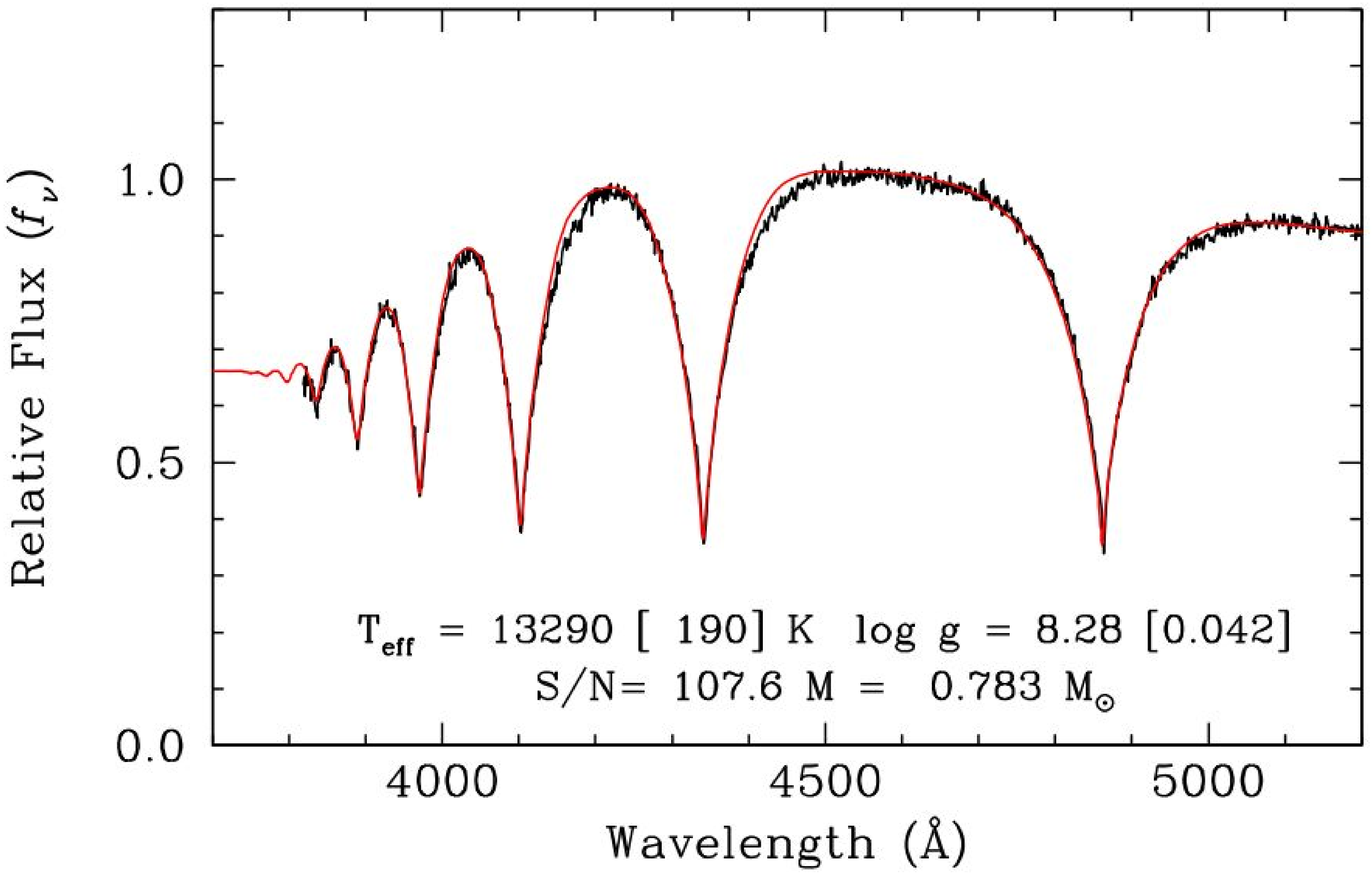




T_{eff} errors of 10%, Mass errors of 0.1 $M_{\odot}$

Systematic discrepancies indicate Stark broadening calculations may be inaccurate

- Fits to individual lines can give wildly discrepant parameters for the same star

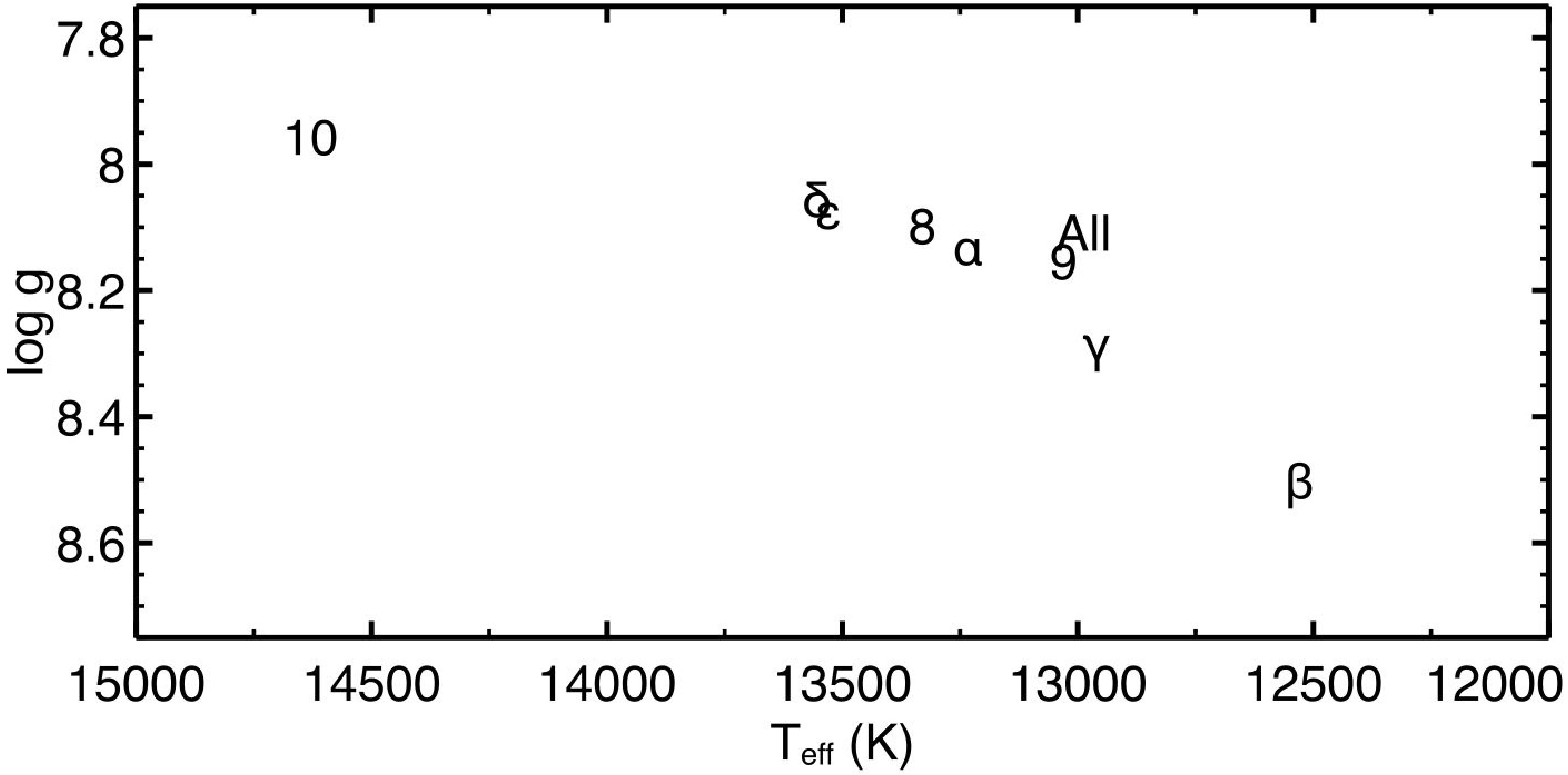


Genest-Beaulieu & Bergeron (2019)

Systematic discrepancies indicate Stark broadening calculations may be inaccurate

- Fits to individual lines can give wildly discrepant parameters for the same star
  - $H\beta$:
    $T_{\rm eff} = 12500{\rm K},\ \log {\rm g} = 8.5$
  - $H\gamma$:
    $T_{\rm eff} = 13000{\rm K},\ \log {\rm g} = 8.1$
  - $H\delta$:
    $T_{\rm eff} = 13500{\rm K},\ \log {\rm g} = 8.05$

Fuchs (2019) *Thesis*

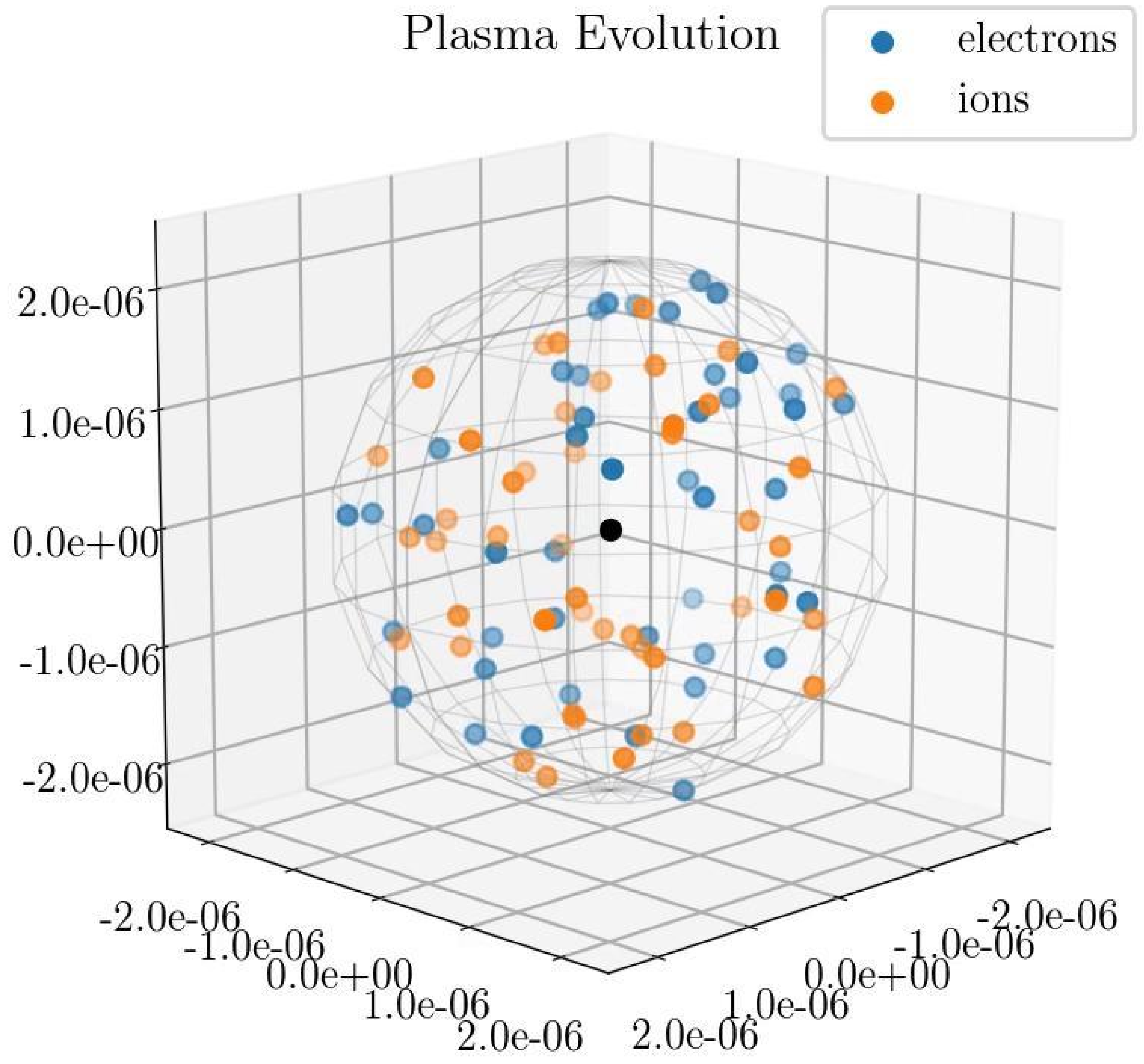


Systematic discrepancies indicate Stark broadening calculations may be inaccurate

Line shape Codes used for H-atmosphere WDs have not been updated since the 1970s

- Unified Theory: Vidal, Cooper, and Smith (VCS 1970)
- Large grid using VCS (Lemke 1997)
- Incorporation of an Occupation Probability (OP) Formalism: Tremblay & Bergeron (2009)
  - VCS profiles + Hummer & Mihalas (1988) OP for lines *and* pseudo-continuum

Our new code, *Xenomorph*, is a first attempt to go beyond this



Xenomorph: A Short Description

1. Place a radiator (neutral H atom) at the center
2. Construct the plasma (for a given T and n_e)
3. Evolve in time — straight line trajectories
4. Calculate net E field at radiator and construct full time-evolved Hamiltonian
   $$H(t) = H_0 + \sum_j V_j(t)$$
5. Solve the Schroedinger equation (Heisenberg picture) to get the time evolution operator:
   $$i\frac{d}{dt}\mathbf{U}_u(t) = \mathbf{H}_u(t)\mathbf{U}_u(t)$$
6. Time evolve the Dipole moment operator: $\mathbf{D}_{ul}(t) = \mathbf{U}_u(t)\mathbf{D}_{ul}\mathbf{U}^\dagger{}_l(t)$
7. Compute power spectrum of dipole moment: $I(\omega) = \Re\left[\int_0^\infty dt\, e^{i\omega t}\langle \mathbf{D}_{lu}(0)\cdot\mathbf{D}_{ul}(t)\rangle\right]$

Xenomorph

Simulation of Stark Broadened Hydrogen Balmer Line Shapes for DA White Dwarf Synthetic Spectra

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Submitted to ApJ

ABSTRACT

White Dwarfs (WD) are useful across a wide range of astrophysical contexts. For example, their cooling can be leveraged in cosmochronology, they are the progenitors of type Ia supernovae, their pulsations tell us about their interior structure and prior stages of stellar evolution, and they are used as spectrophotometric standards for many major astronomical observatories. In all of these contexts, the fidelity of the information we can extract relies on the accuracy of WD atmosphere models. One essential ingredient of atmosphere models is the theory used to calculated broadened spectral lines for bound-bound transitions, known as line shape calculations.

Xenomorph

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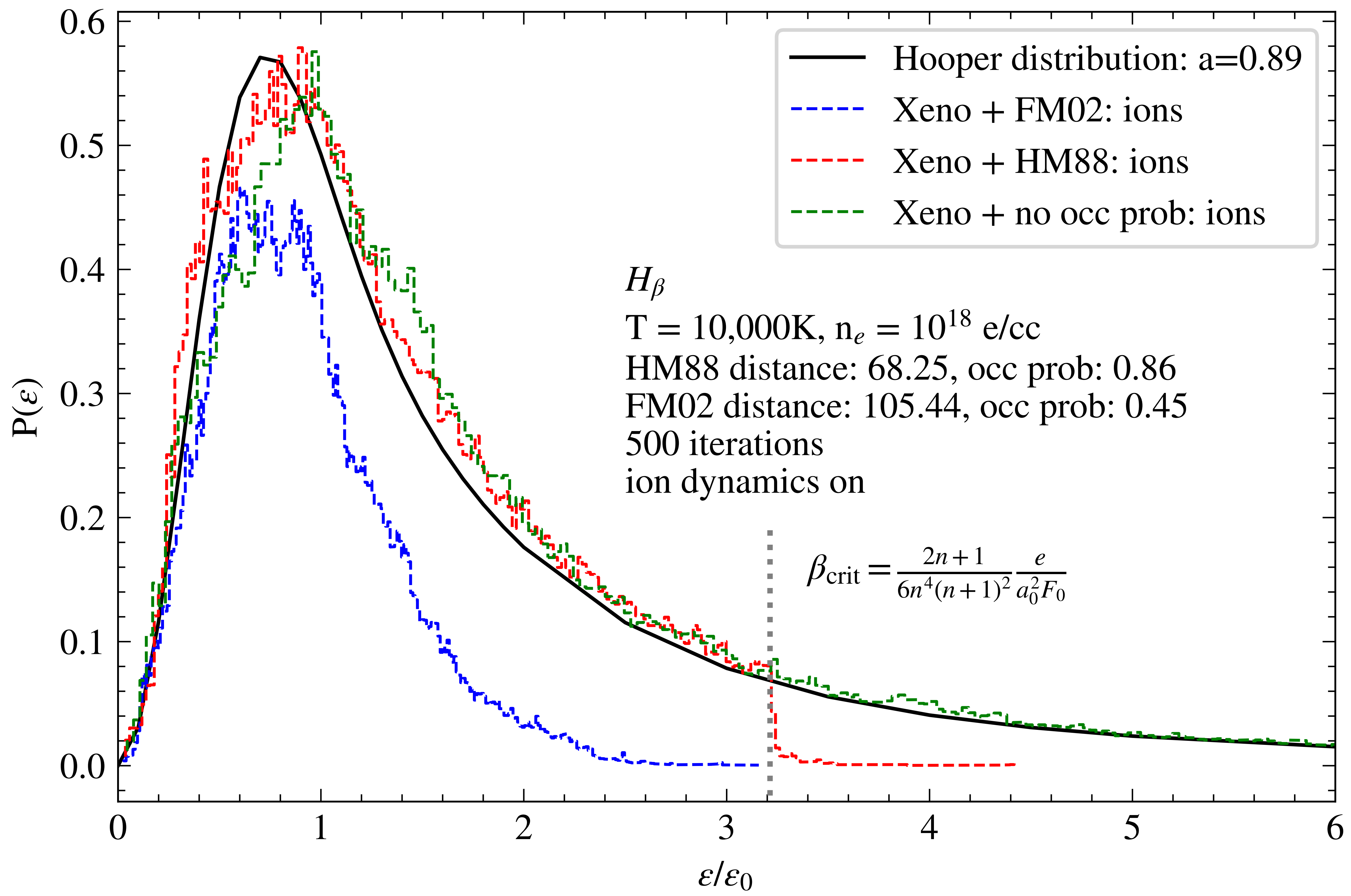
from higher principle quantum numbers will be explored in future work. We find that screening effects and occupation probability have the largest effects on the line shapes and the way they are calculated will likely have important consequences in stellar synthetic spectra. This paper presents a detailed description of these

Xenomorph physics improvements

- ion dynamics
  - ⇒ electrons *and* protons can move
- an expanded basis set
  - ⇒ more atomic states are included in the calculation
- higher-order multipole expansion
  - ⇒ gradients in the electric field are taken into account
- "time ordering" is implicitly included
- increased randomness in the simulations
  - ⇒ particle re-injection now allows for a change in both the velocity and impact parameter of particle



But, for the things that matter most:

- For the first time, an occupation probability/continuum lowering formalism was incorporated in simulation-based line profile calculations
- The "usual" screening prescription was used:
  - Debye screening with protons screened only by electrons:

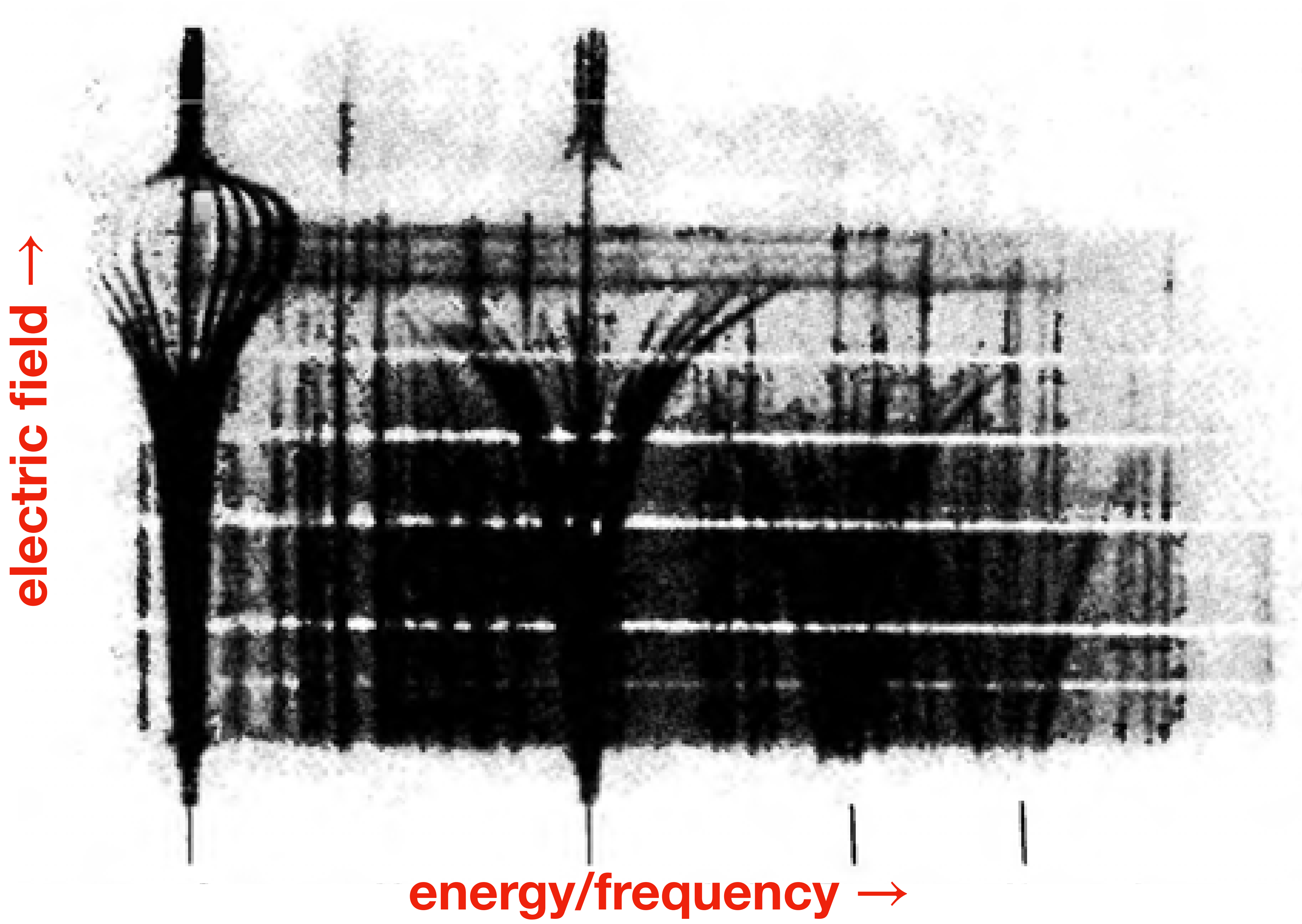
$$V(r) = \frac{q}{r} e^{-r/\lambda_D} \qquad \lambda_D = \left(\frac{k_B T}{4\pi n_e e^2}\right)^{1/2}$$

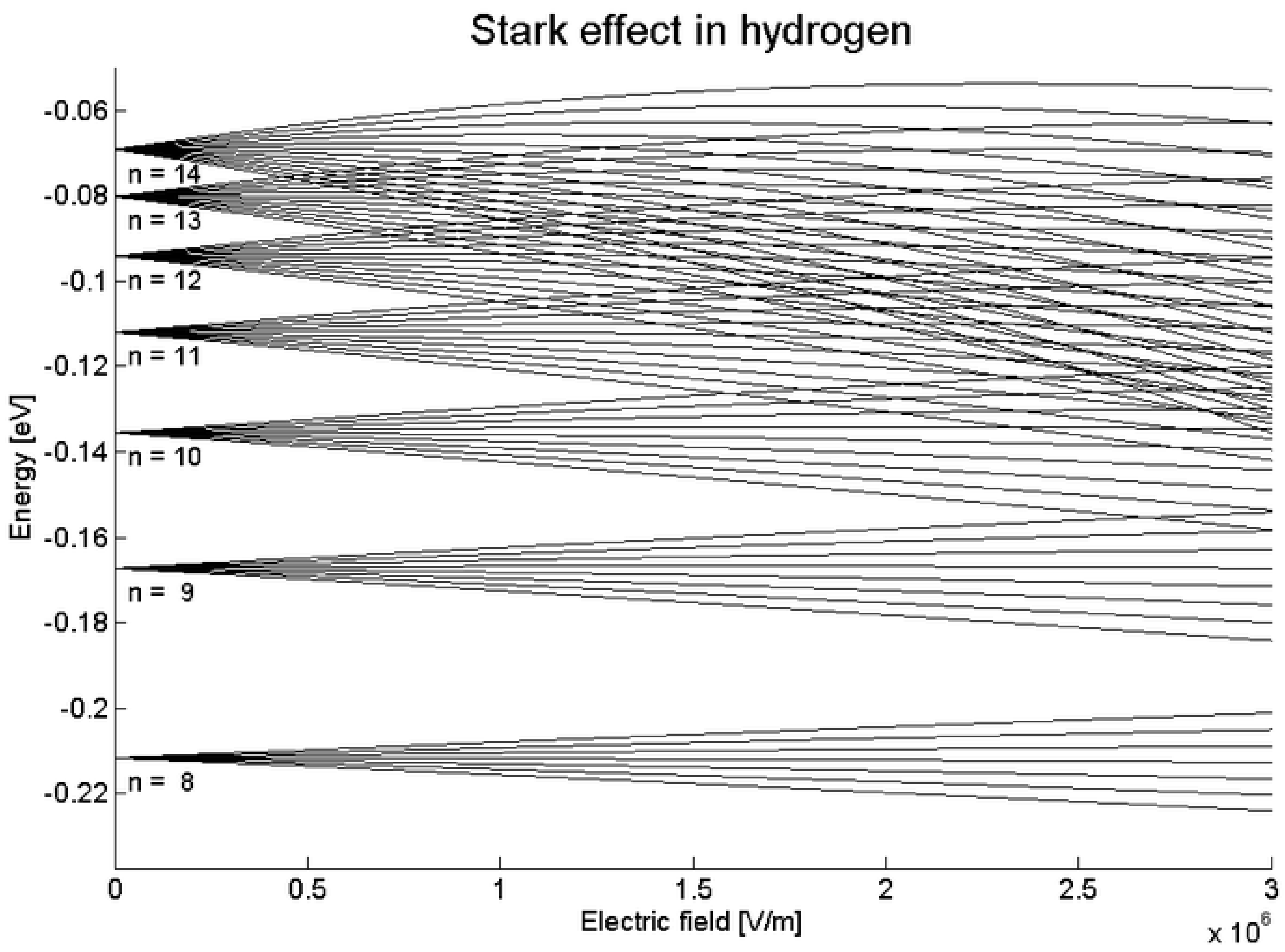
$$\lambda_D = \left(\frac{k_B T}{4\pi (n_e + n_p) e^2}\right)^{1/2}$$

If protons are included in the calculation of λ_D (as they *should be*), then λ_D decreases by a factor of $\sqrt{2}$

The Physics of Occupation Probability (OP)

H. Rausch von Traubenberg (1929—1931)





- Also called “continuum lowering” or “ionization potential depression”
- Due to the plasma environment, an atom can experience electric fields large enough that a bound electron may escape to the continuum
- This is not treated as a collisional or inelastic process
- An electron escaping by tunneling is an example that can decrease the occupation probability below 1.0
- There is a critical electric field (or distance of closest approach of the nearest ion) beyond which the state is assumed not to exist
- This process should modify the *strengths* and *shapes* of spectral lines

The Physics of Occupation Probability (OP)

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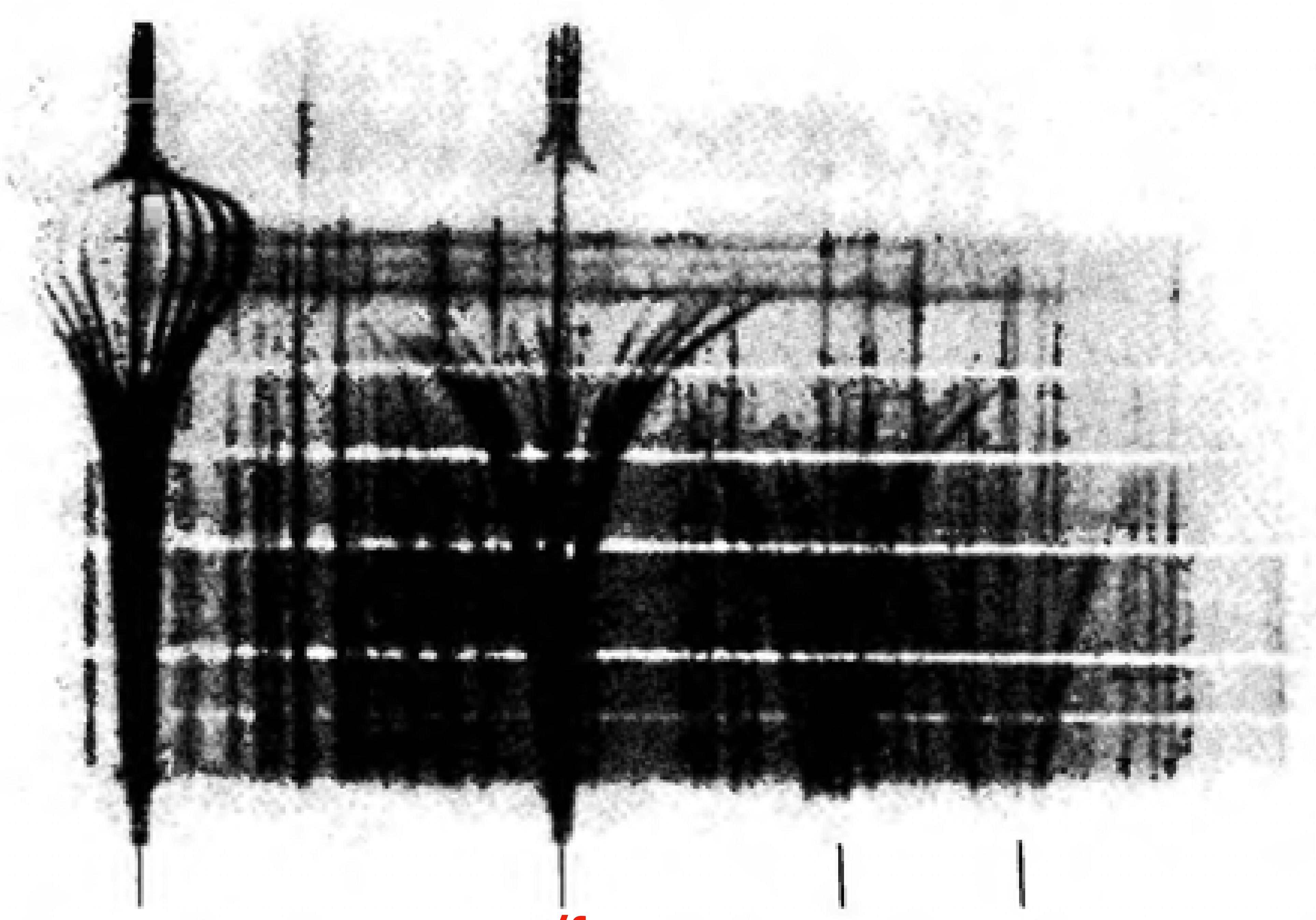
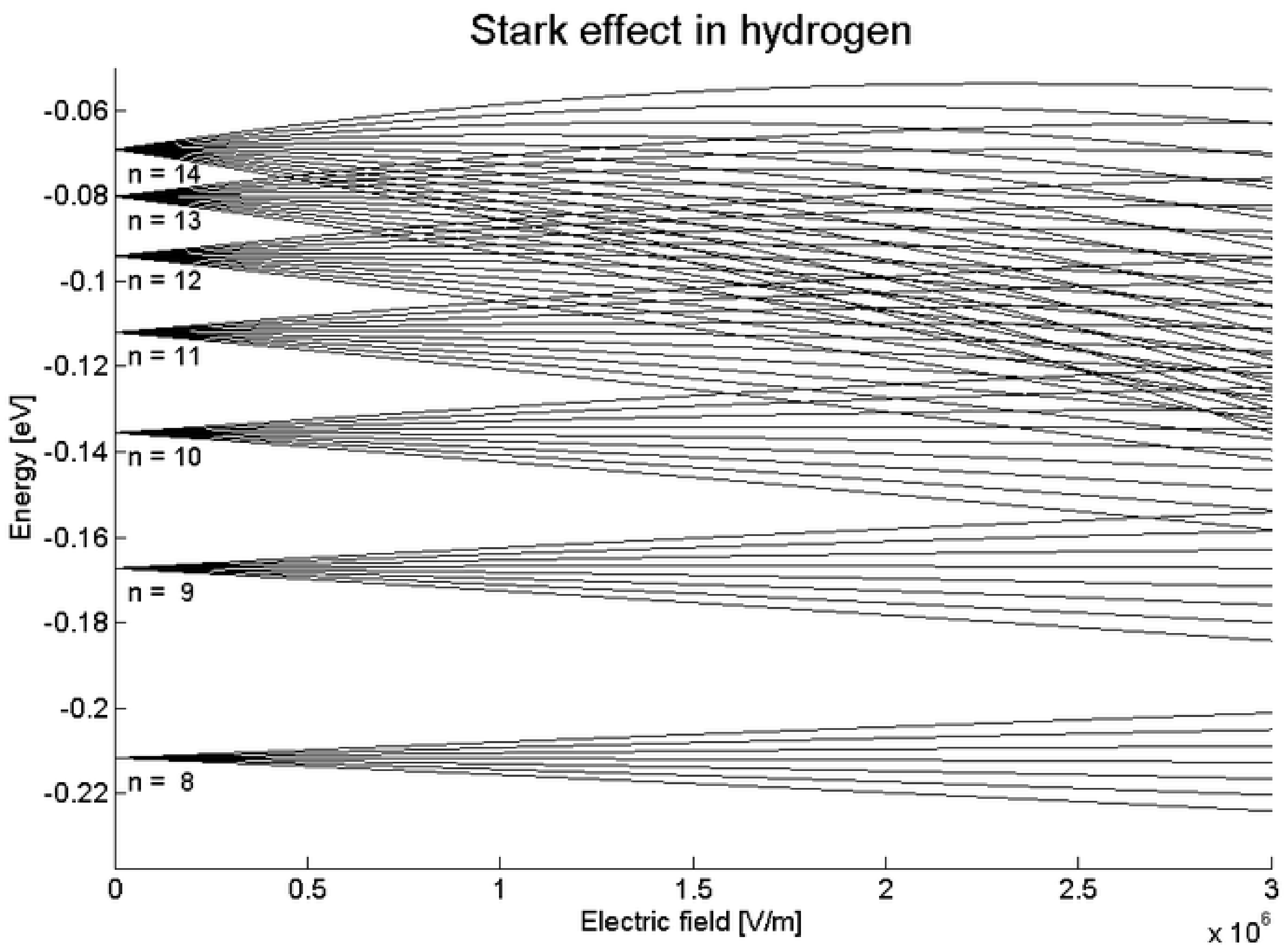
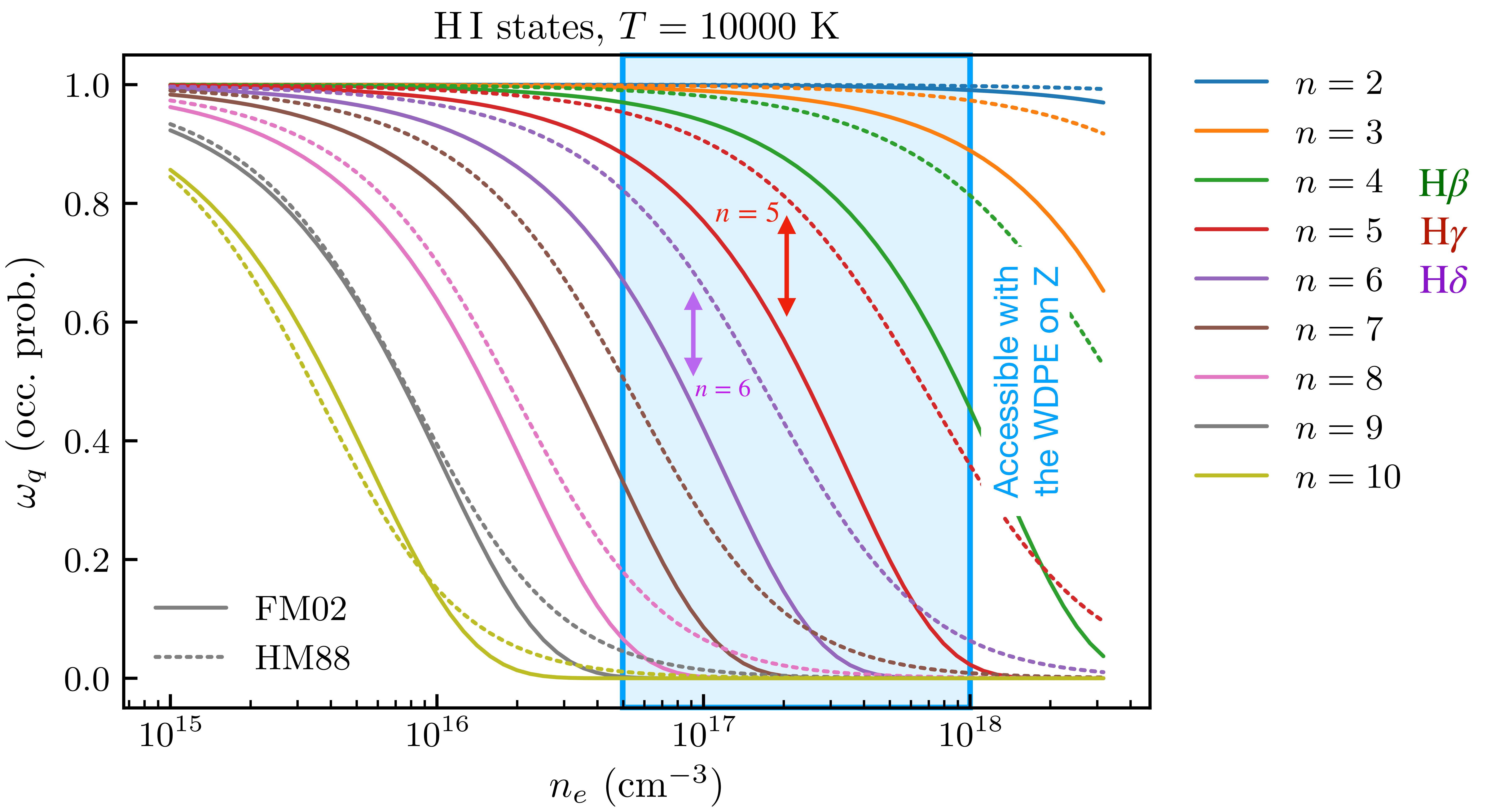




- Many different proposed criteria/treatments, often yielding somewhat similar answers:
  - Inglis-Teller (levels crossing, ApJ, 1939)
  - Hummer & Mihalas (ApJ, 1988, "HM88")
  - Däppen et al. (ApJ, 1987, "DAM")
  - Seaton (1990)
  - Bergeron (1991, "$2 \times \beta_{\rm crit}$")
  - Fisher & Maron (2002, "FM02")
- Invoking an OP formalism leads to partition functions that are convergent

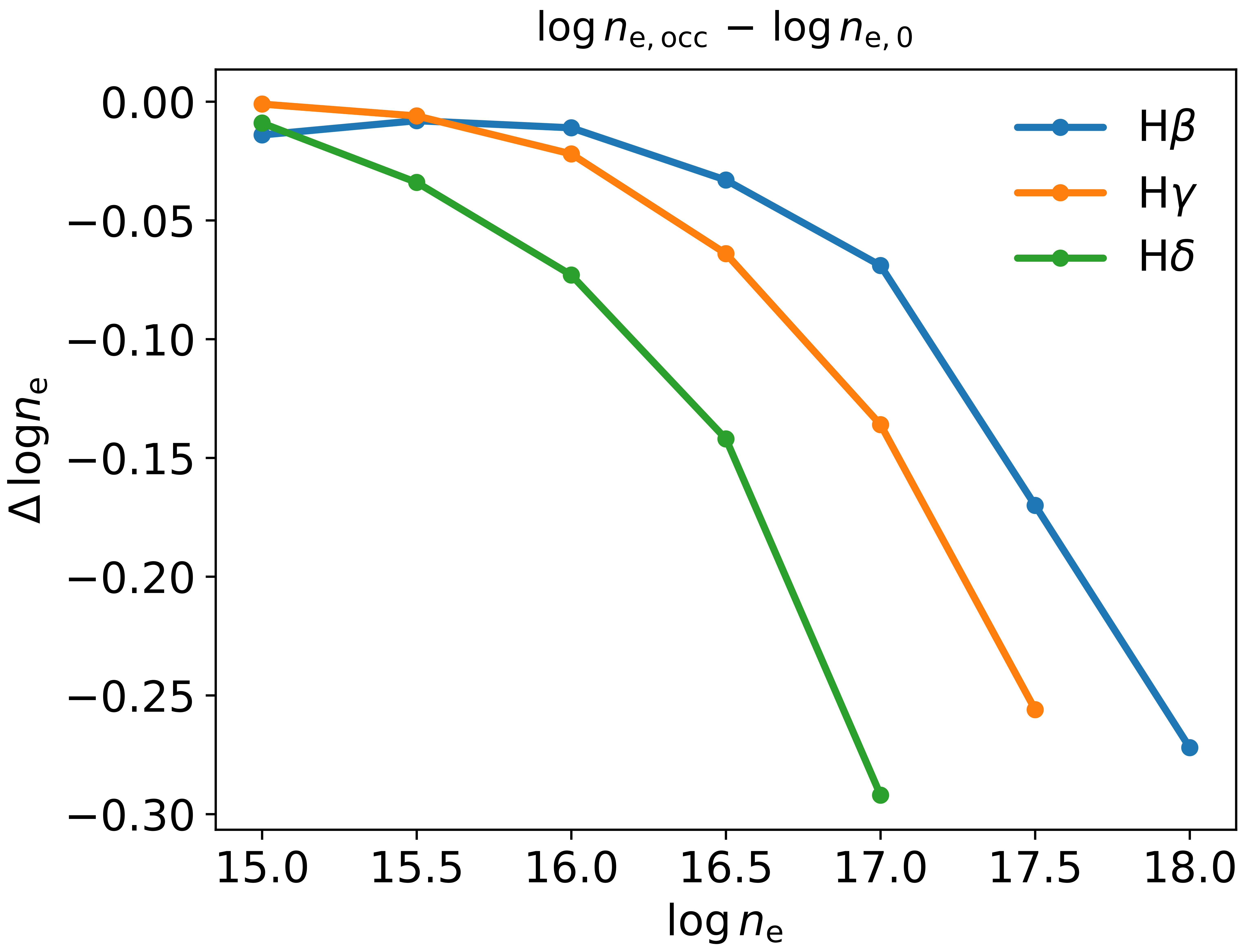
$$n_i/N_{\rm tot} = w_i\, g_i\, \exp\left(-E_i/kT\right)/Z$$

Comparison of HM88 and FM02 OP Prescriptions

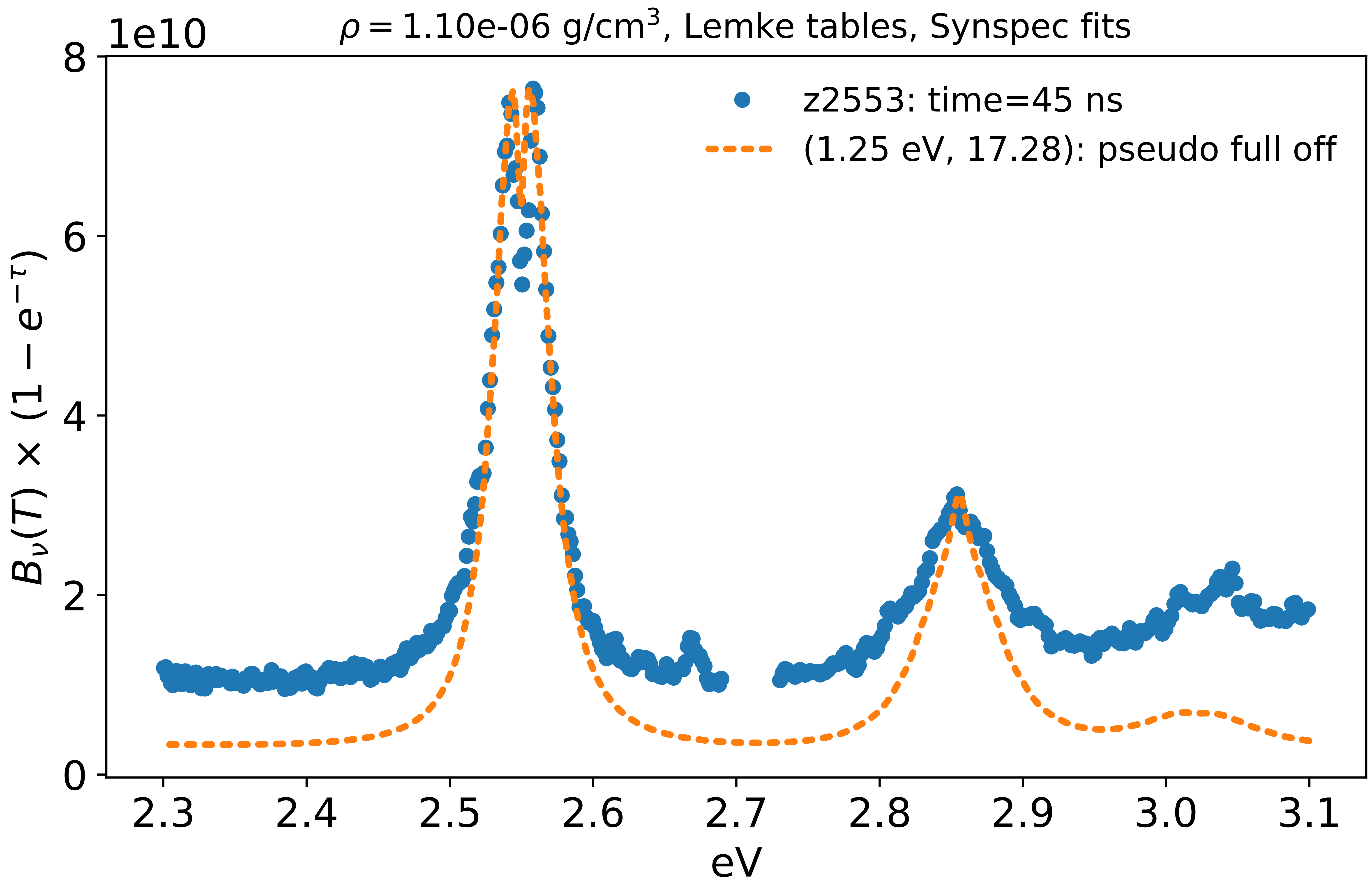


For $n \leq 8$, the Fisher & Maron OP (FM02) is lower than that of Hummer & Mihalas (HM88)

Density Offset with and without OP (using FM02)

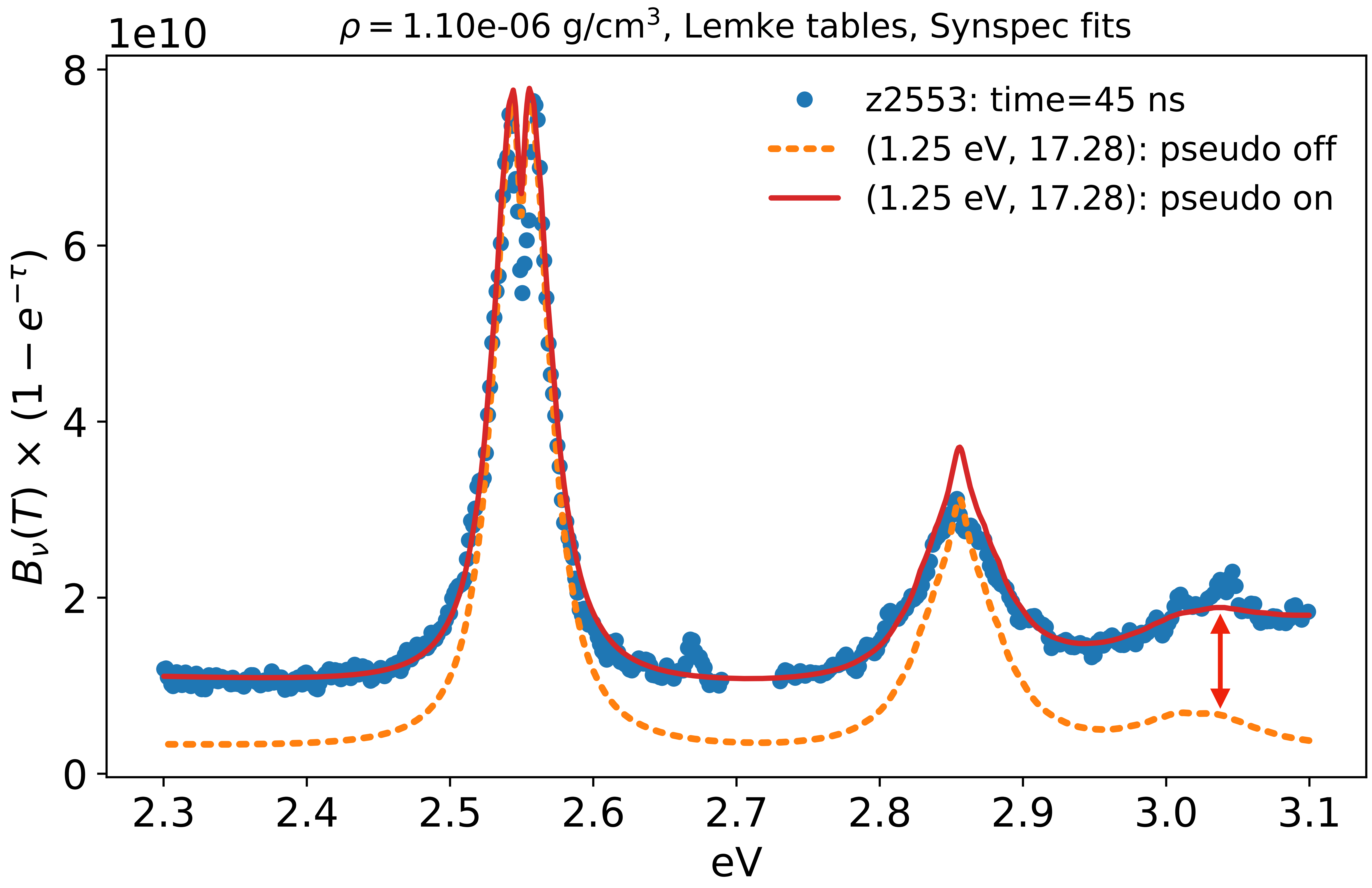


Effect of the Pseudo-continuum



These calculations use the code *Synspec*, part of the *Tlusty* suite (Ivan Hubeny), which is used to fit the observed spectra of white dwarf stars.

Effect of the Pseudo-continuum



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The Electric Field Calculation

- A line profile calculation is an “ensemble average” over electric field configurations of the electrons + protons
- We need thousands of time series of the electric field, and each time series contains thousands of time steps
    - much too expensive to compute with straightforward N-body codes
- The standard approach is to use non-interacting electrons and protons on straight-line trajectories, which is much less expensive computationally
- The particle interactions are “taken into account” by using screened potentials for the electrons and protons

The was examined by Stambulchik et al. for one density and one line, $H\alpha$

TMD = "Trivial Molecular Dynamics"

- singly-shielded electrons
- doubly-shielded protons

FMD = "Full Molecular Dynamics"

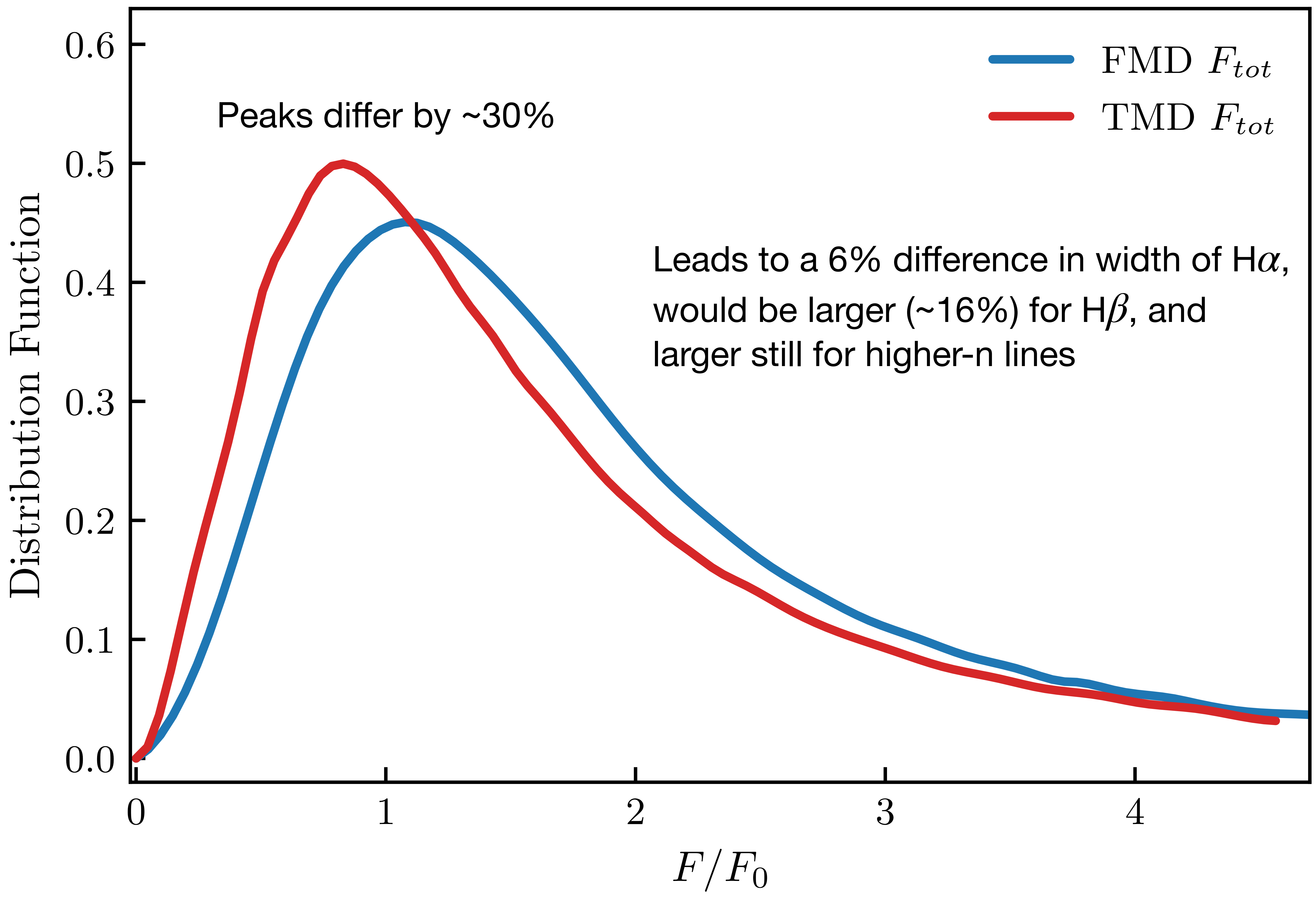
- fully interacting plasma
- Coulomb forces $(1/r^2)$

$$n_e = n_i = 10^{18}\,\mathrm{cm}^{-3}$$

$$T_e = T_i = 1\,\mathrm{eV}$$

$$\Gamma_e = \Gamma_i = 0.23$$

Stambulchik et al., 2007, HEDP, 3, 272

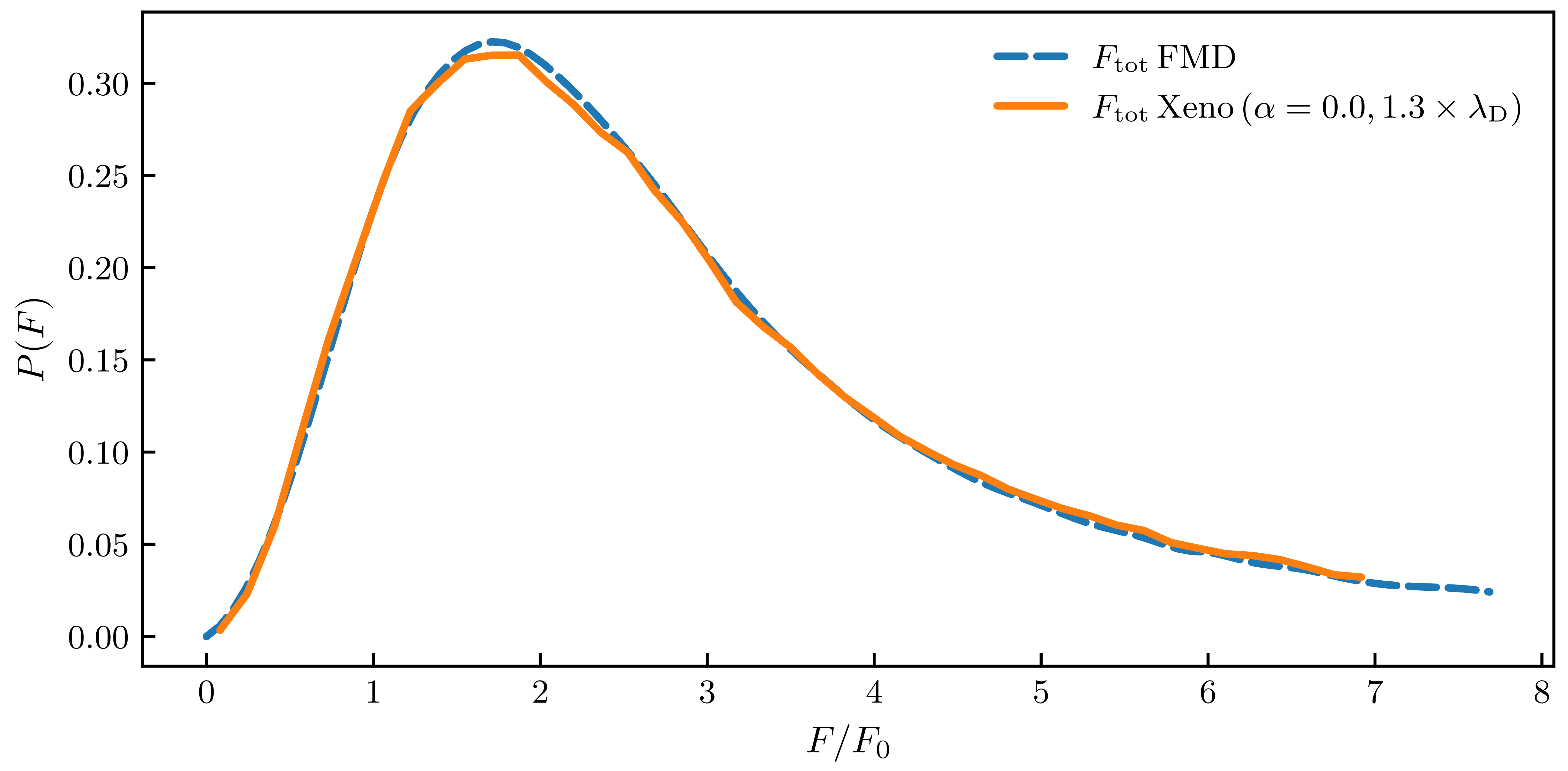


It turns out that it is possible to reproduce the electric microfield distribution with a different choice of screening…

FMD = “Full Molecular Dynamics”
- fully interacting plasma
- Coulomb forces $(1/r^2)$

Can reproduce E-field distribution of FMD by choosing

$$\lambda' = 1.3 \times \lambda_D$$



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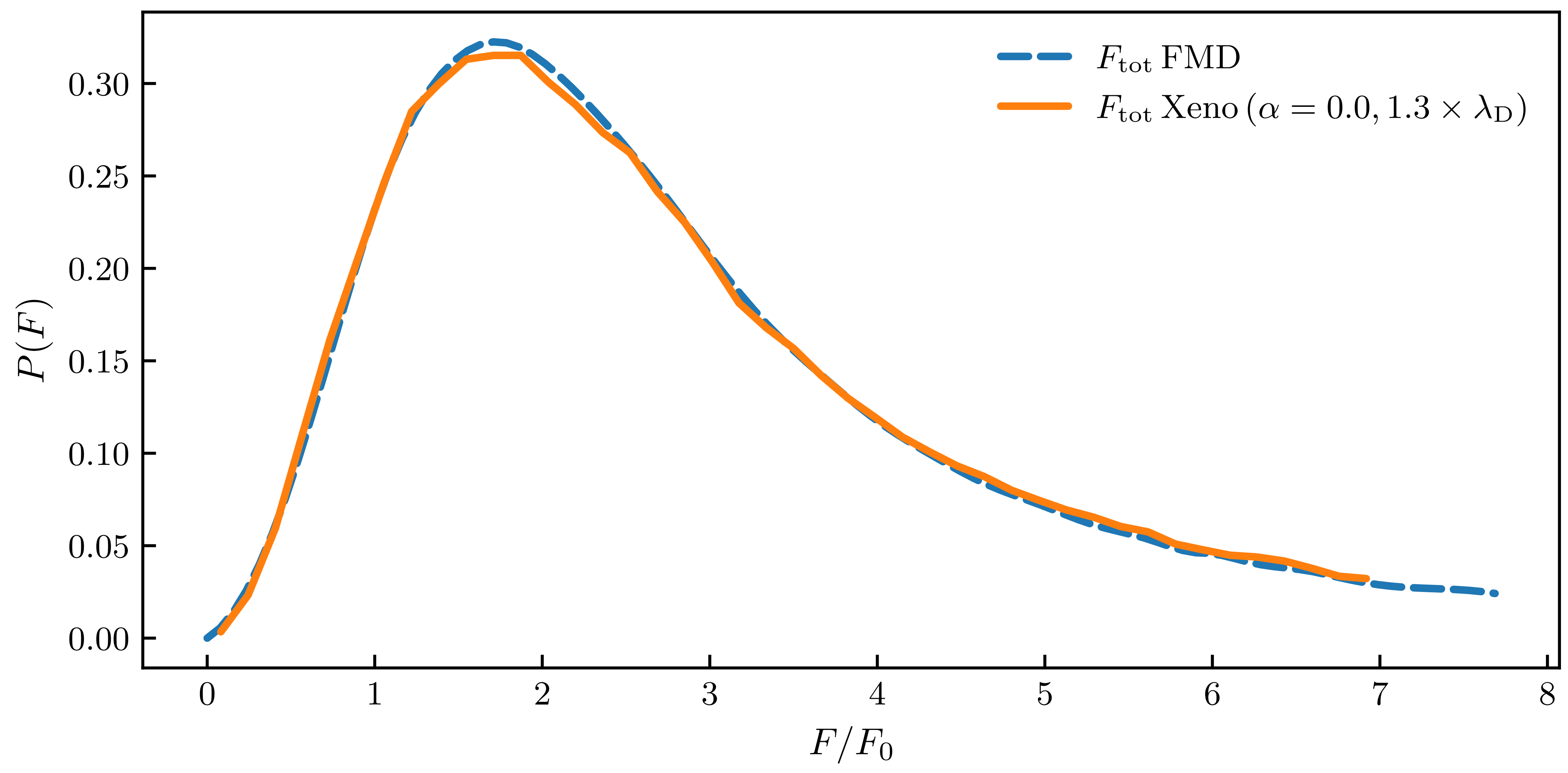
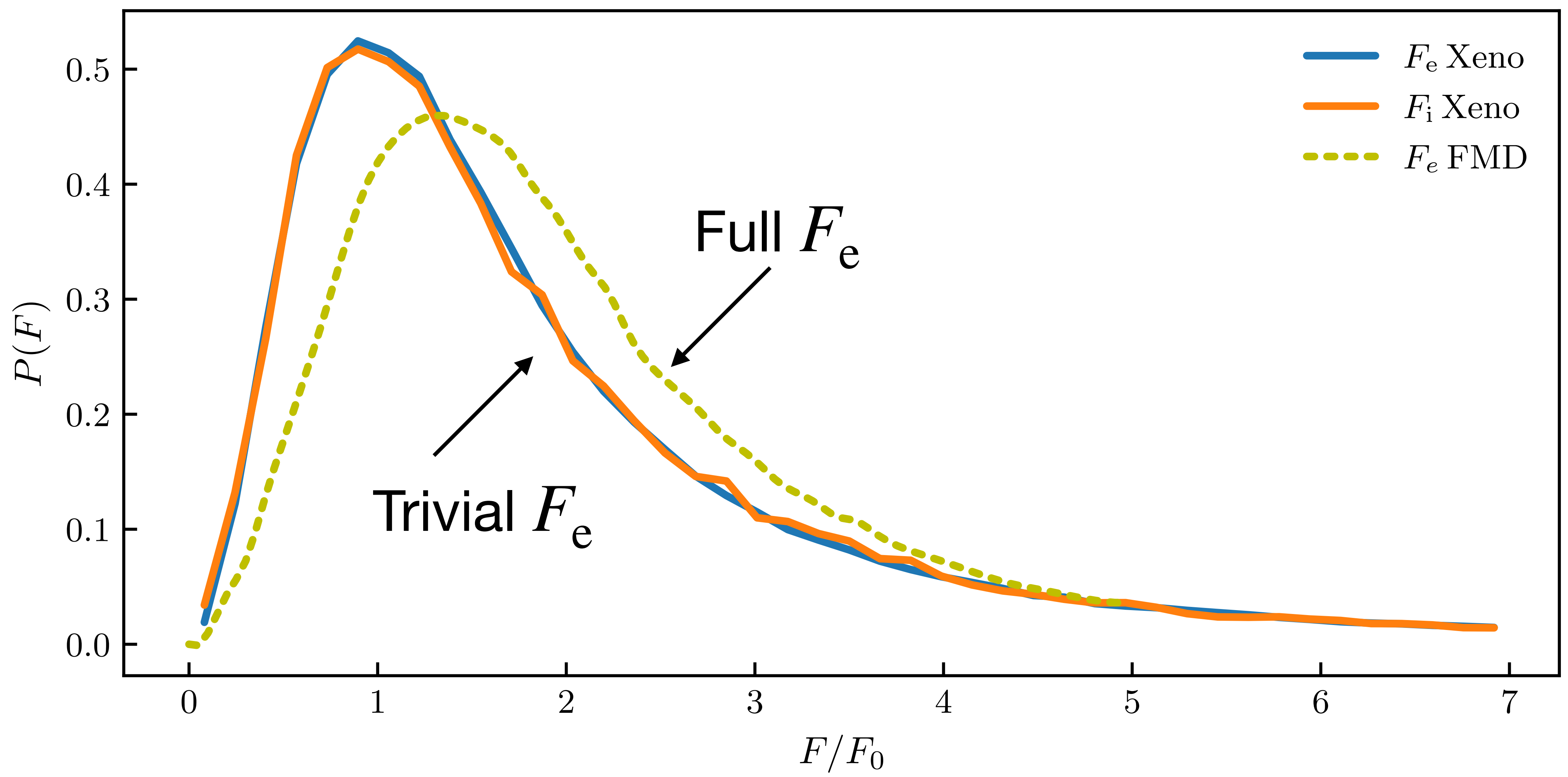
Can reproduce E-field distribution of FMD by choosing

$\lambda' = 1.3 \times \lambda_D$

But the individual electron and ion fields do not match those of the FMD





If we introduce a “correlation parameter” we can fit both using the trivial simulations...

FMD = “Full Molecular Dynamics”

- fully interacting plasma
- Coulomb forces $(1/r^2)$

Can reproduce E-field distribution of FMD by choosing

$$\vec{F}_{\mathrm{e}} = \vec{F}_{\bar{\mathrm{e}}} + \alpha \vec{F}_{\mathrm{i}}$$

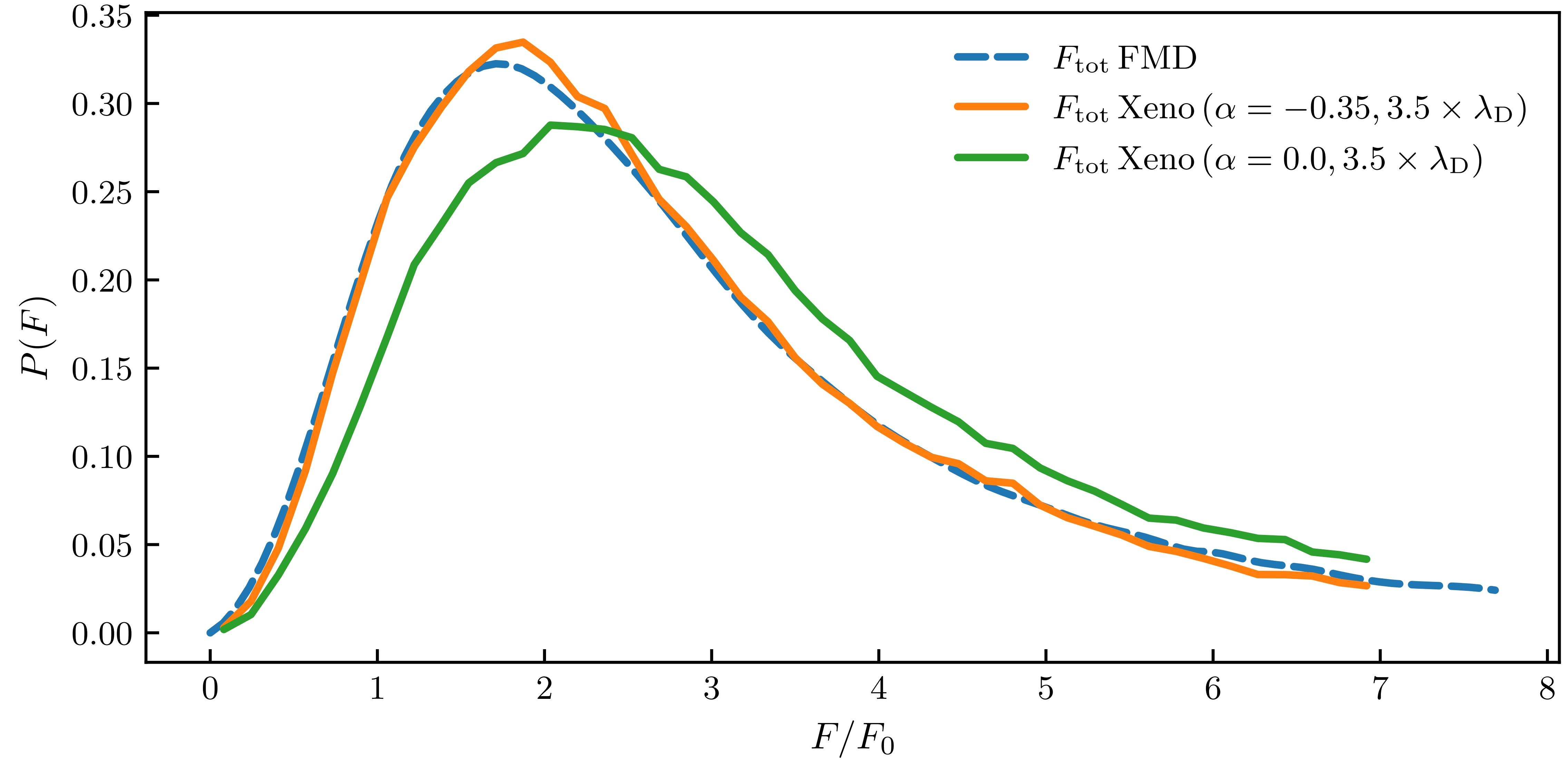
so that

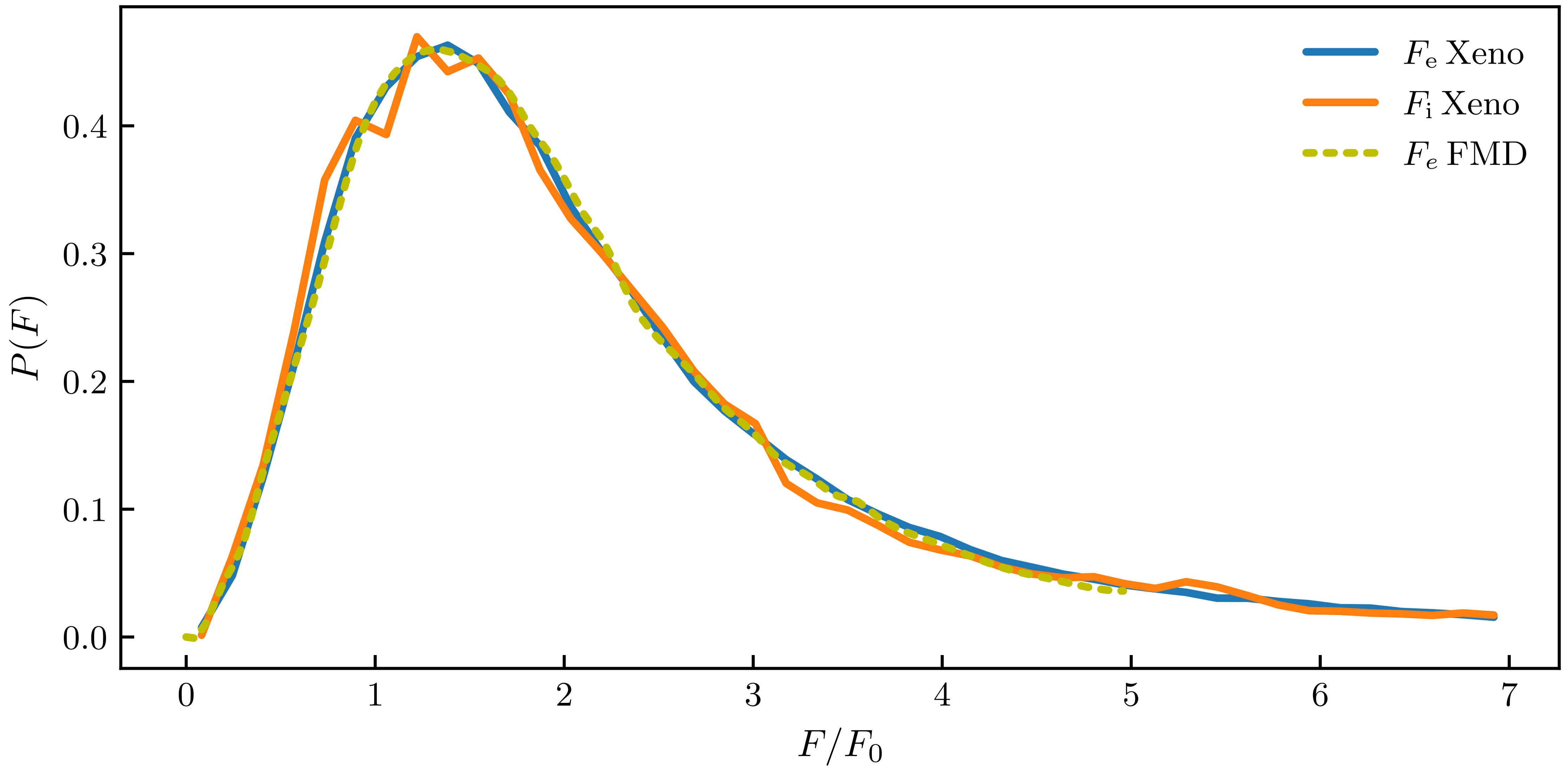
$$\vec{F}_{\mathrm{tot}} = \vec{F}_{\bar{\mathrm{e}}} + (1+\alpha) \vec{F}_{\mathrm{i}}$$

with $\alpha \approx -0.35$ and $\lambda' = 3.5 \times \lambda_D$

We need to see if $\alpha = -1.5\,\Gamma_{\mathrm{i}}$ is valid over a larger range of T and n_{e}

Stambulchik et al., 2007, HEDP, 3, 272





Summary

- While a theoretically solved problem, a practical way of generating 1000s of E-field time series is still a non-trivial problem
- The physics related to Occupation Probability (or Continuum Lowering or Ionization Potential Depression) is important in our regimes of interest $(16 \leq \log\, n_e \leq 18,\ \ 10{,}000\,\mathrm{K} \leq T \leq 40{,}000\,\mathrm{K})$
  - Laboratory plasmas
  - White Dwarf photospheres
- Occupation Probability affects both the shapes and strengths of the lines
- Using multiple lines may allow us to constrain different parameterizations of this effect
- Laboratory data will be crucial for making progress