

COSMOLOGICAL HYDROGEN RECOMBINATION: The effect of extremely high- n states and forbidden transitions

arXiv:0911.1359, submitted to Phys. Rev. D.

Daniel Grin

in collaboration with Christopher M. Hirata

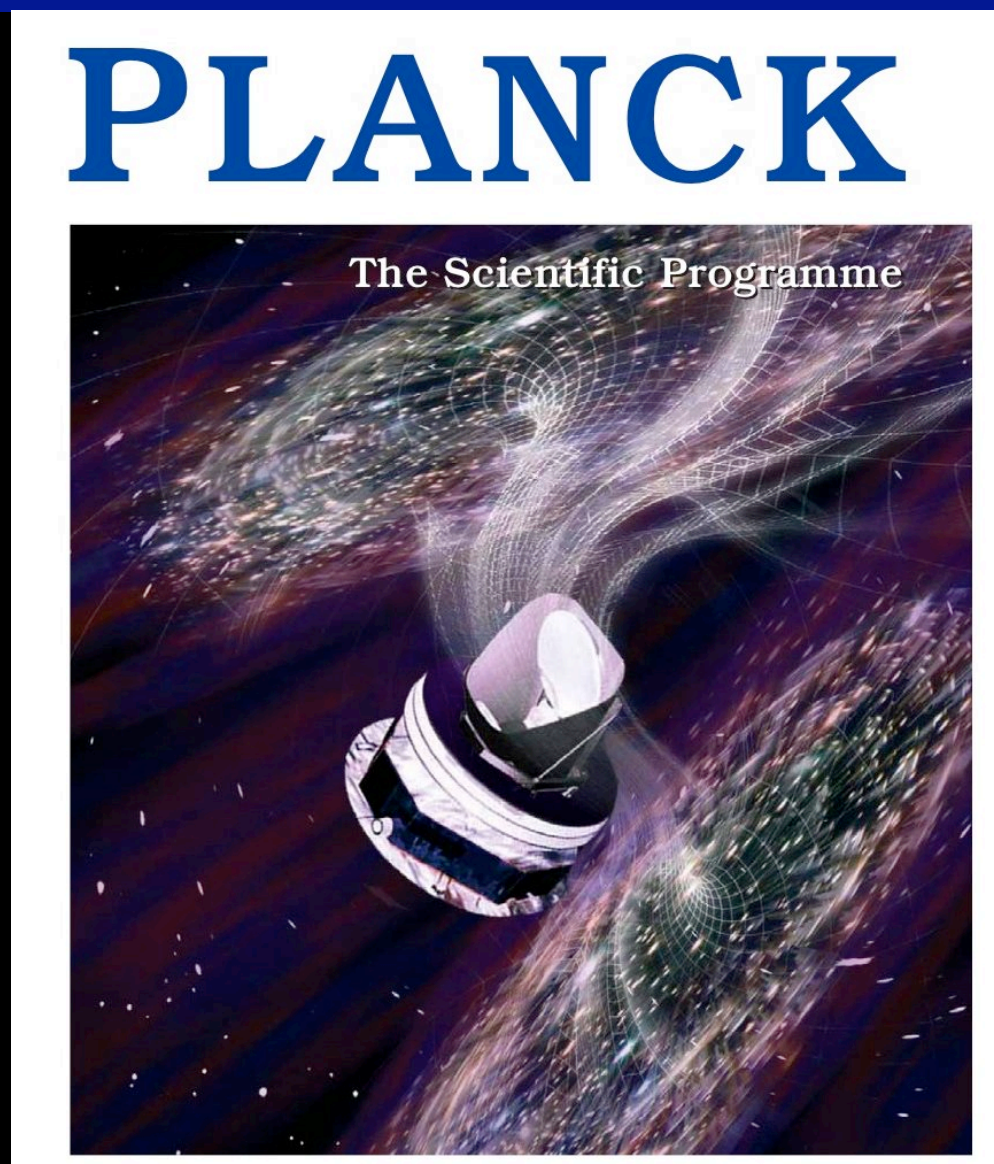
University of Pennsylvania Seminar

12/1/09

OUTLINE

- * Motivation: CMB anisotropies and recombination spectra
- * Recombination in a nutshell
- * Breaking the Peebles/RecFAST mold
- * **RecSparse**: a new tool for high-n states
- * Forbidden transitions
- * Results
- * Ongoing/future work

WALK THE PLANCK

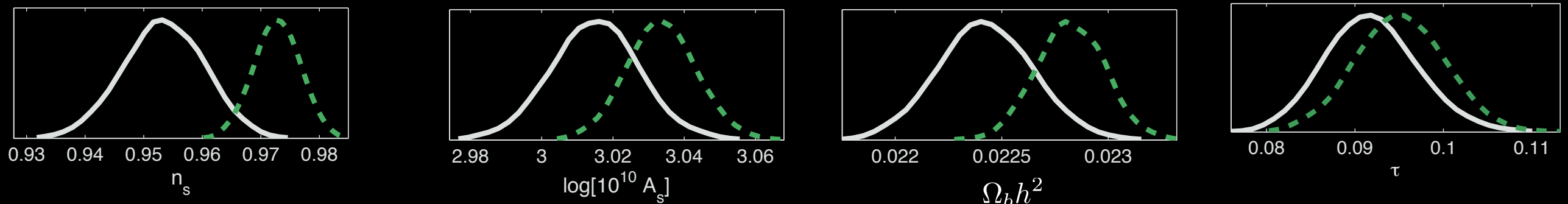


- * Planck (launched May 2009) will make cosmic-variance limited CMB anisotropy measurements up to $l \sim 2500$ (T), and $l \sim 1500$ (E)
- * Wong 2007 and Lewis 2006 show that $x_e(z)$ needs to be predicted to several parts in 10^4 accuracy for Planck data analysis

RECOMBINATION, INFLATION, AND REIONIZATION

$$P(k) = A_s (k\eta_0)^{n_s}$$

* Planck uncertainty forecasts using MCMC



- * Cosmological parameter inferences will be off if recombination is improperly modeled (Wong/Moss/Scott 2007)
- * Leverage on new physics comes from high l . Here the details of recombination matter!
- * Inferences about inflation will be wrong if recombination is improperly modeled

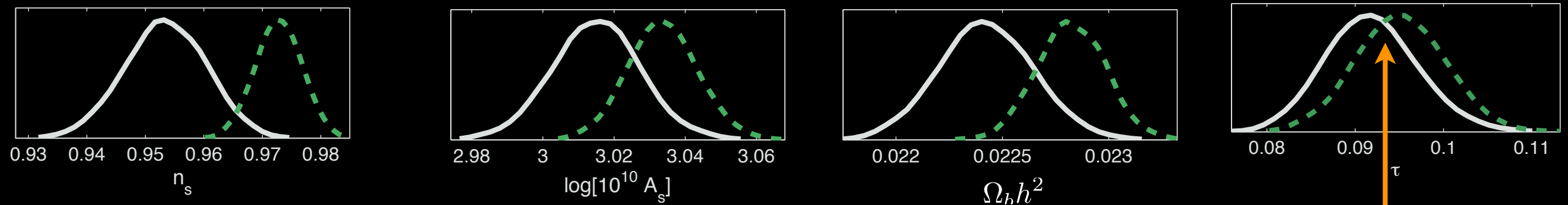
$$n_s = 1 - 4\epsilon + 2\eta \quad \epsilon = \frac{m_{\text{pl}}^2}{16\pi} \left[\frac{V'(\phi)}{V(\phi)} \right]^2 \quad A_s^2 = \frac{32}{75} \frac{V}{m_{\text{pl}}^4 \epsilon} \Big|_{k_{\text{pivot}}=aH}$$

CAVEAT EMPTOR: $3 \lesssim ? \lesssim 16$

Need to do eV physics right to infer anything about 10^7 GeV physics! 4

RECOMBINATION, INFLATION, AND REIONIZATION

* Planck uncertainty forecasts using MCMC



Bad recombination history yields biased inferences about reionization

PHYSICAL RELEVANCE FOR CMB: SMEARING AND MOVING THE SURFACE OF LAST SCATTERING (SLS)

- * Photons kin. decouple when Thompson scattering freezes out

$$\gamma + e^- \Leftrightarrow \gamma + e^-$$

- * Acoustic mode evolution influenced by visibility function

$$g = \dot{\tau} e^{-\tau} \qquad \tau(z) = \int_0^{\eta(z)} n_e \sigma_T a(\eta') d\eta'$$

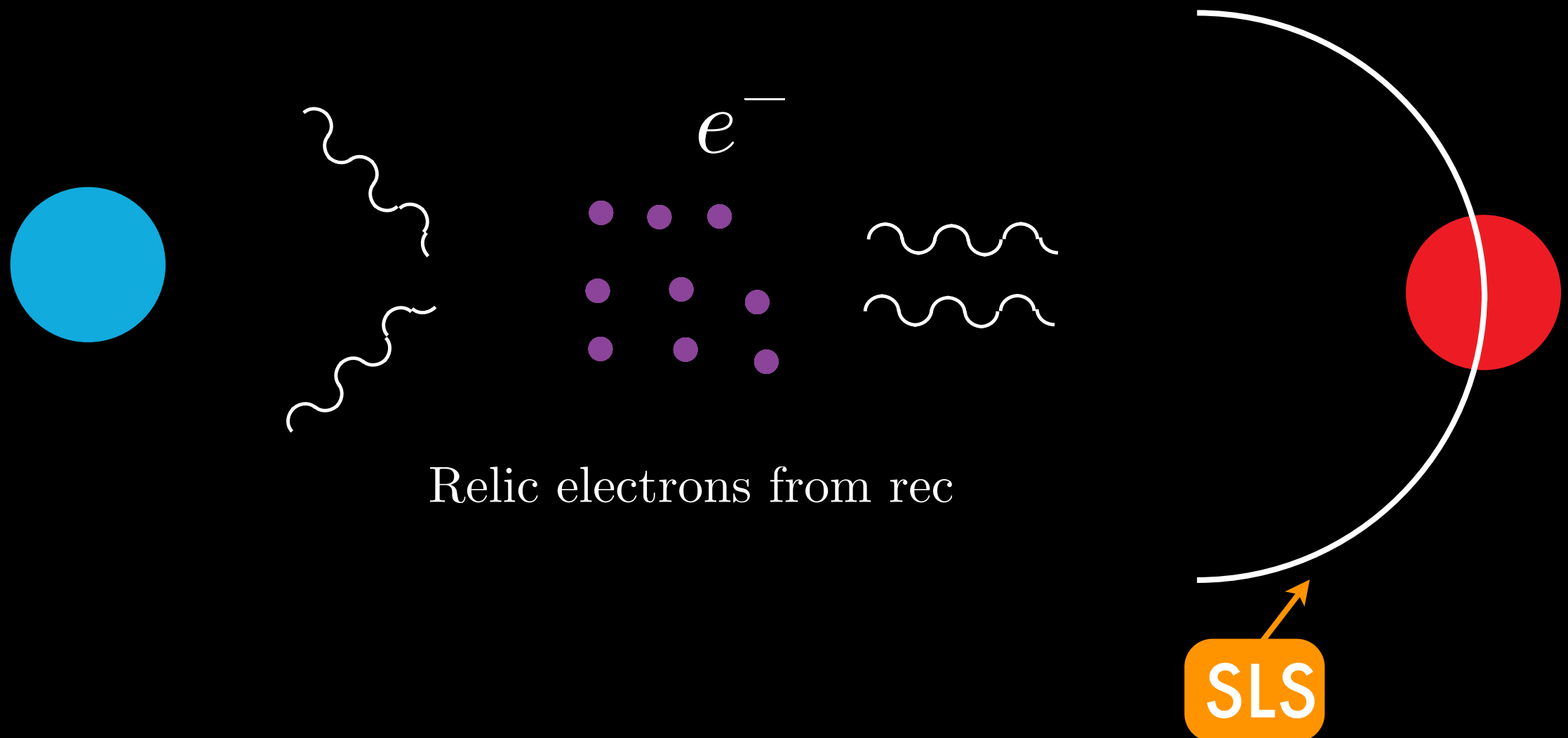
- * $z_{\text{dec}} \simeq 1100$: Decoupling occurs during recombination

$$C_l \rightarrow C_l e^{-2\tau(z)} \text{ if } l > \eta_{\text{dec}}/\eta(z)$$

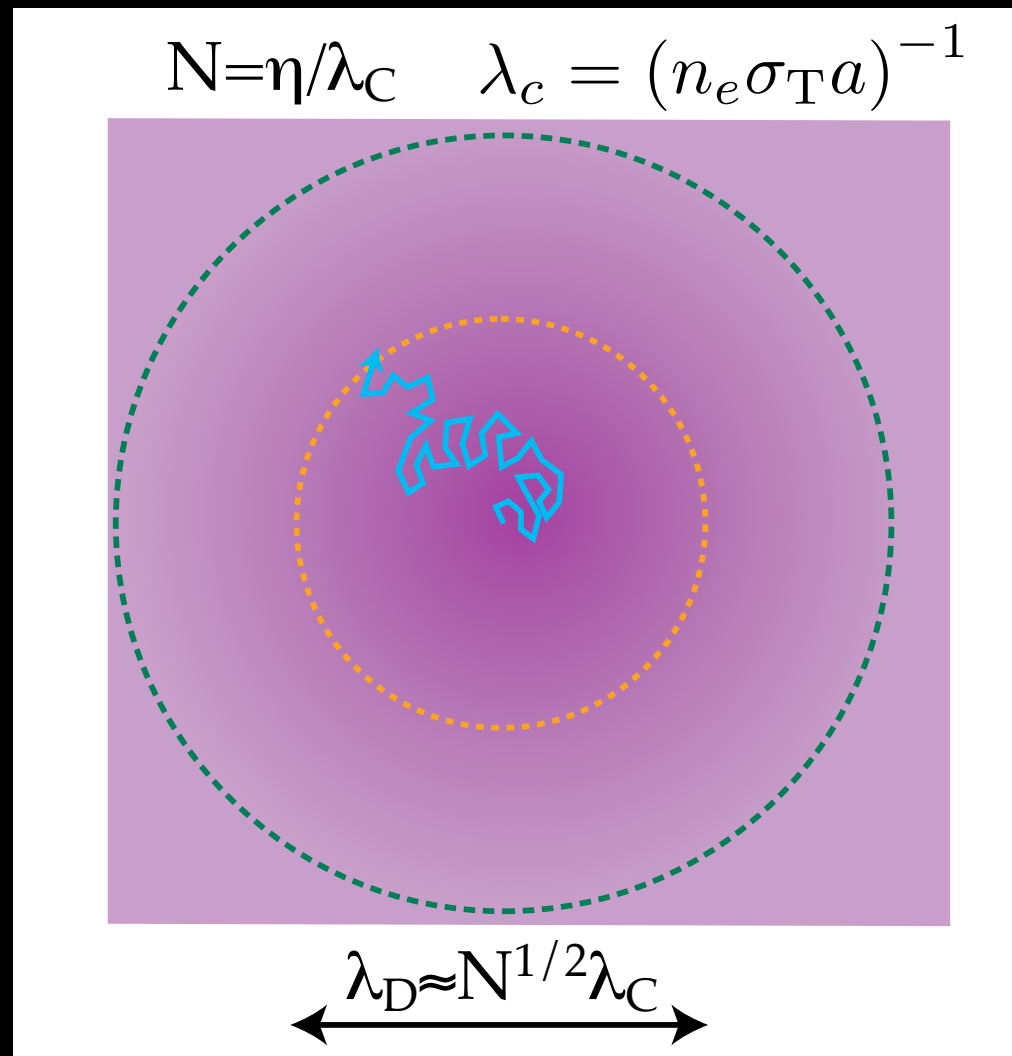
PHYSICAL RELEVANCE FOR CMB: SMEARING AND MOVING THE SURFACE OF LAST SCATTERING (SLS)

* Photons kin. decouple when Thompson scattering freezes out

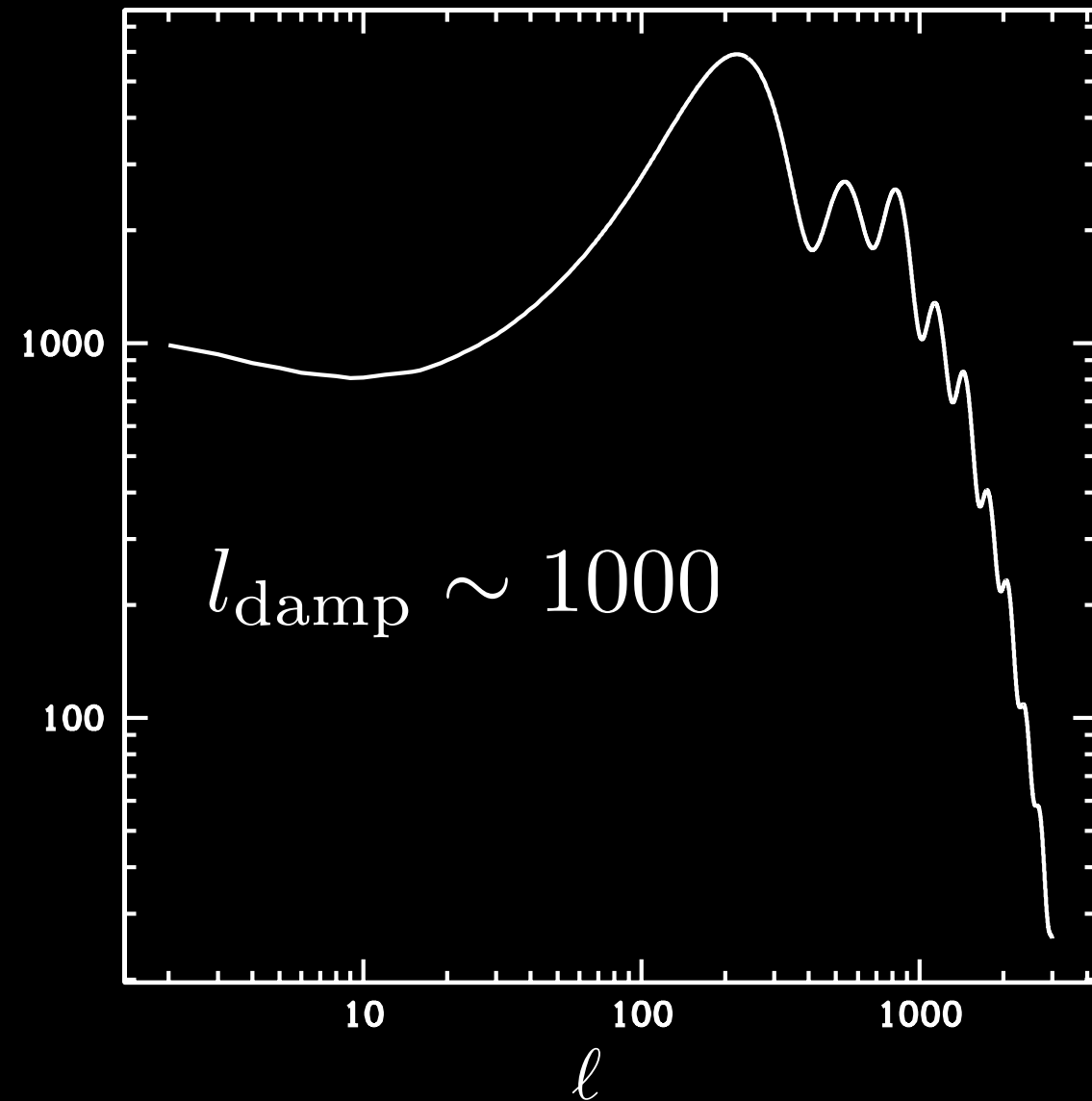
$$\gamma + e^{-} \Leftrightarrow \gamma + e^{-}$$



PHYSICAL RELEVANCE FOR CMB: THE SILK DAMPING TAIL



$$C_\ell^{\text{TT}} (\mu K^2)$$



✳ Inhomogeneities are damped for $\lambda < \lambda_D$

PHYSICAL RELEVANCE FOR CMB: POLARIZATION

Isotropic radiation

Quadrupole moment

No polarization

Polarization

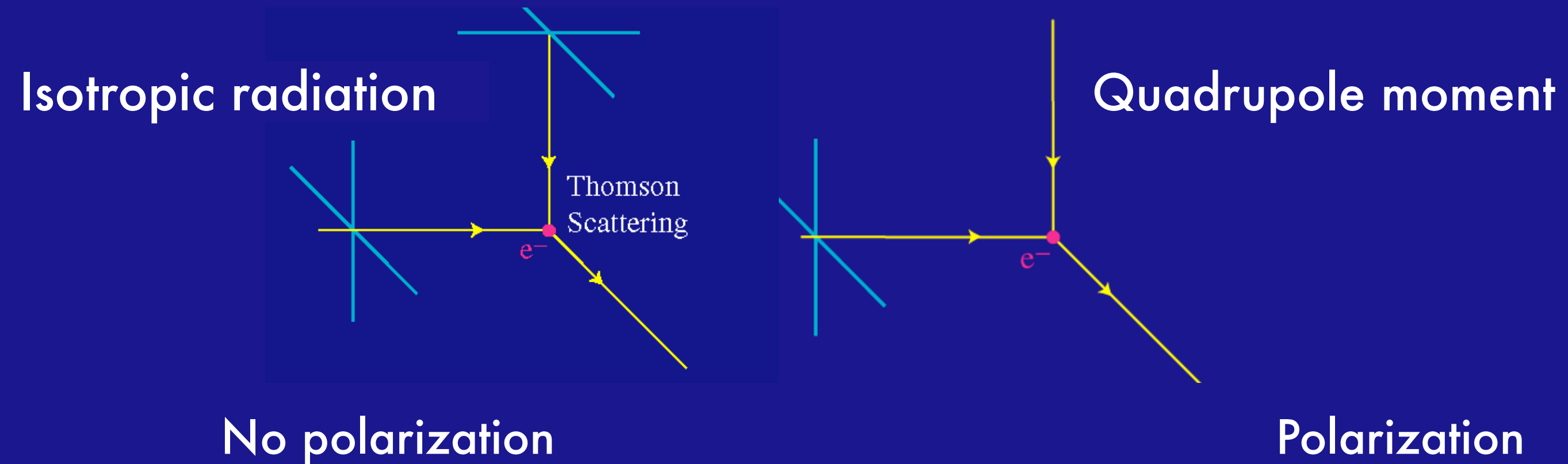
From Wayne Hu's website

* Need time to develop a quadrupole

$$\Theta_l(k\eta) \sim \frac{k\eta}{2\tau} \Theta_{l+1}(k\eta) \ll \Theta_{l+1}(k\eta) \text{ if } l \geq 2, \text{ in tight coupling regime}$$

* Need to scatter quadrupole to polarize CMB

PHYSICAL RELEVANCE FOR CMB: POLARIZATION



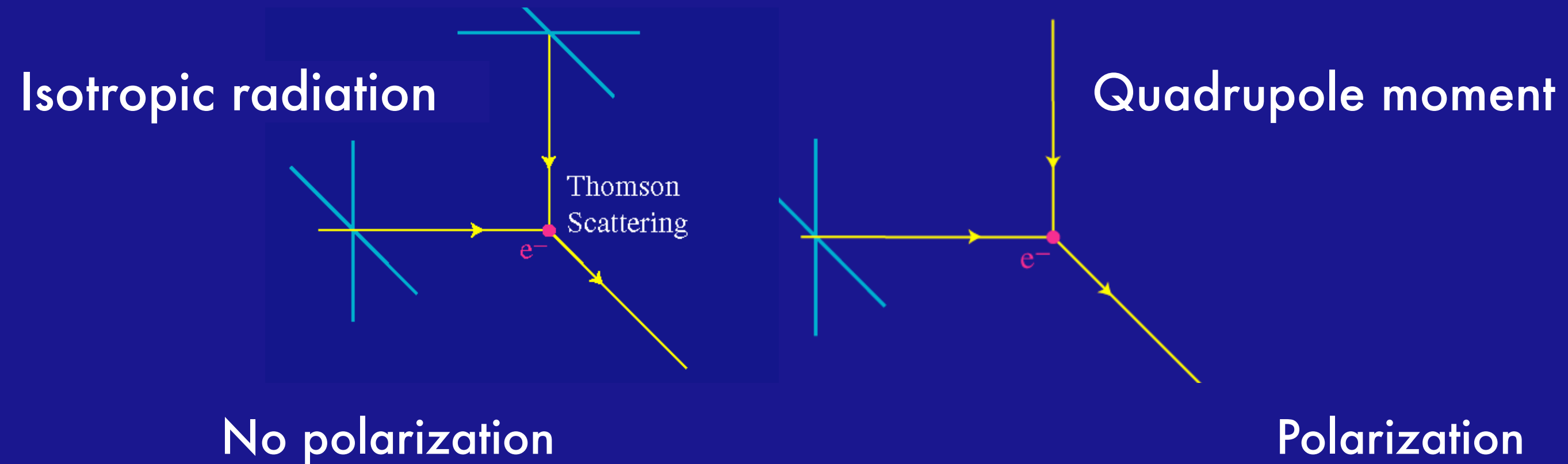
From Wayne Hu's website

* Need time to develop a quadrupole

$$\Theta_l(k\eta) \sim \frac{k\eta}{2\tau} \Theta_{l+1}(k\eta) \ll \Theta_{l+1}(k\eta) \text{ if } l \geq 2, \text{ in tight coupling regime}$$

* Need to scatter quadrupole to polarize CMB

PHYSICAL RELEVANCE FOR CMB: POLARIZATION



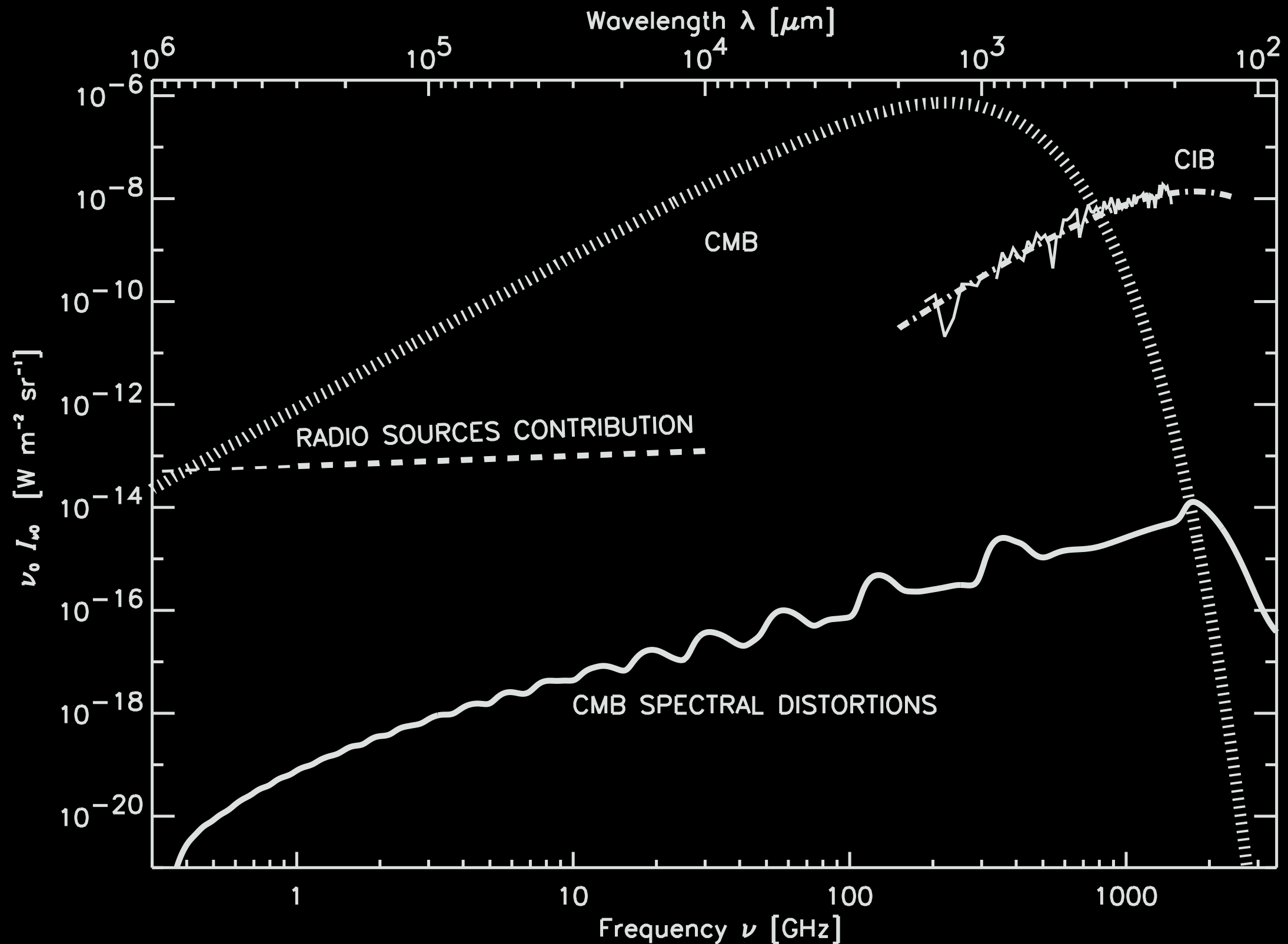
From Wayne Hu's website

* Need time to develop a quadrupole

$$\Theta_l(k\eta) \sim \frac{k\eta}{2\tau} \Theta_{l+1}(k\eta) \ll \Theta_{l+1}(k\eta) \text{ if } l \geq 2, \text{ in tight coupling regime}$$

* Need to scatter quadrupole to polarize CMB

PHYSICAL RELEVANCE FOR CMB: SPECTRAL DISTORTIONS FROM RECOMBINATION



SAHA EQUILIBRIUM IS INADEQUATE



- * Chemical equilibrium does reasonably well predicting “moment of recombination”

$$\frac{x_e^2}{1 - x_e} = \left(\frac{13.6}{T_{\text{eV}}} \right)^{3/2} e^{35.9 - 13.6/T_{\text{eV}}}$$

$$x_e = 0.5 \text{ when } T = T_{\text{rec}} \simeq 0.3 \text{ eV} \qquad z_{\text{rec}} \simeq 1300$$

- * Further evolution falls prey to reaction freeze-out

$$\Gamma < H \text{ when } T < T_{\text{F}} \simeq 0.25 \text{ eV}$$

BOTTLENECKS/ESCAPE ROUTES

BOTTLENECKS

- * Ground state recombinations are ineffective

$$\Gamma_{c \rightarrow 1s} = 10^{-1} \text{ s}^{-1} \gg H \simeq 10^{-12} \text{ s}^{-1}$$

- * Resonance photons are re-captured, e.g. Lyman α

$$\Gamma_{2p \rightarrow 1s} = 10^{-2} \text{ s}^{-1} \gg H \simeq 10^{-12} \text{ s}^{-1}$$

ESCAPE ROUTES (e.g. n=2)

- * Two-photon processes

$$H^{2s} \rightarrow H^{1s} + \gamma + \gamma \quad \Lambda_{2s \rightarrow 1s} = 8.22 \text{ s}^{-1}$$

- * Redshifting off resonance

$$R \sim (n_H \lambda_\alpha^3)^{-1} H$$

THE PEEBLES PUNCHLINE

- * Only n=2 bottlenecks are treated
- * Net Rate is suppressed by bottleneck vs. escape factor

$$-\frac{dx_e}{dt} = \mathcal{S} \sum_{n,l>1s} \alpha_{nl}(T) \{nx_e^2 - x_{1s}f(T)\}$$

THE PEEBLES PUNCHLINE

- * Only $n=2$ bottlenecks are treated
- * Net Rate is suppressed by bottleneck vs. escape factor

$$-\frac{dx_e}{dt} = \mathcal{S} \sum_{n,l>1s} \alpha_{nl}(T) \{ nx_e^2 - x_{1s} f(T) \}$$

Recombination rate



THE PEEBLES PUNCHLINE

- * Only n=2 bottlenecks are treated
- * Net Rate is suppressed by bottleneck vs. escape factor

$$-\frac{dx_e}{dt} = \mathcal{S} \sum_{n,l>1s} \alpha_{nl}(T) \{ nx_e^2 - x_{1s} f(T) \}$$

Ionization rate



THE PEEBLES PUNCHLINE

* Only $n=2$ bottlenecks are treated

* Net Rate is suppressed by bottleneck vs. escape factor

$$-\frac{dx_e}{dt} = S \sum_{n,l>1s} \alpha_{nl}(T) \{nx_e^2 - x_{1s}f(T)\}$$

THE PEEBLES MODEL

*Net Rate is suppressed by bottleneck vs. escape factor

$$\mathcal{S} = \frac{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + \Lambda_{2s \rightarrow 1s}}{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + (\Lambda_{2s \rightarrow 1s} + \beta_c)}$$

THE PEEBLES MODEL

*Net Rate is suppressed by bottleneck vs. escape factor

$$\mathcal{S} = \frac{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + \Lambda_{2s \rightarrow 1s}}{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + (\Lambda_{2s \rightarrow 1s} + \beta_c)}$$

Redshifting term

THE PEEBLES MODEL

*Net Rate is suppressed by bottleneck vs. escape factor

$$\mathcal{S} = \frac{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + \Lambda_{2s \rightarrow 1s}}{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + (\Lambda_{2s \rightarrow 1s} + \beta_c)}$$

→ 2γ term

THE PEEBLES MODEL

*Net Rate is suppressed by bottleneck vs. escape factor

$$\mathcal{S} = \frac{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + \Lambda_{2s \rightarrow 1s}}{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + (\Lambda_{2s \rightarrow 1s} + \beta_c)} \rightarrow \text{Ionization Term}$$

THE PEEBLES MODEL

*Net Rate is suppressed by bottleneck vs. escape factor

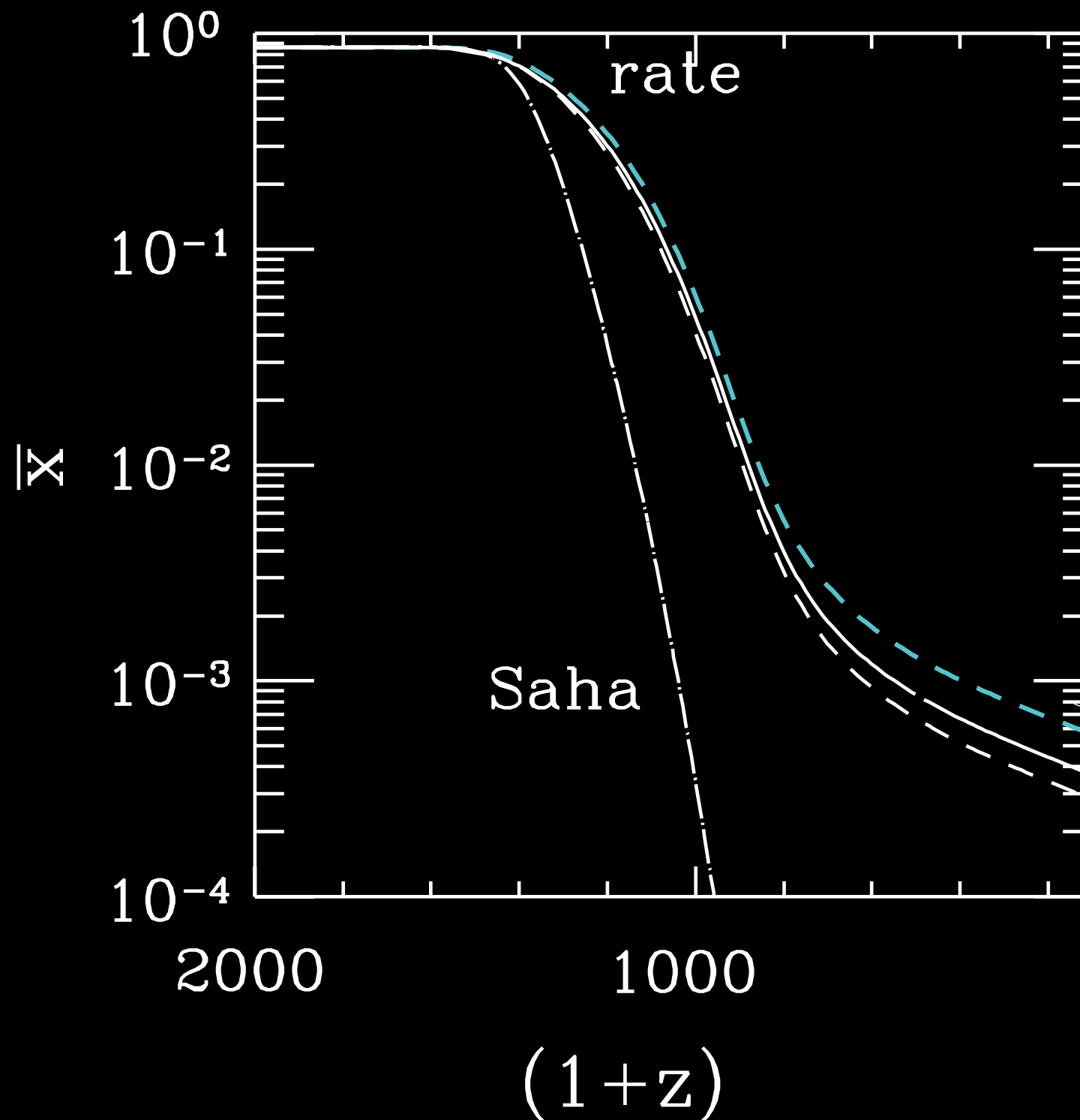
$$\mathcal{S} = \frac{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + \Lambda_{2s \rightarrow 1s}}{\frac{8\pi}{\lambda_{\alpha}^3 n_{1s}} H + (\Lambda_{2s \rightarrow 1s} + \beta_c)} \rightarrow \text{Ionization Term}$$

$$\frac{\text{redshift term}}{2\gamma \text{ term}} \simeq 0.02 \frac{\Omega_m^{1/2}}{(1 - x_e[z]) \left(\frac{1+z}{1100}\right)^{3/2}}$$

2γ process dominates until late times ($z \lesssim 850$)

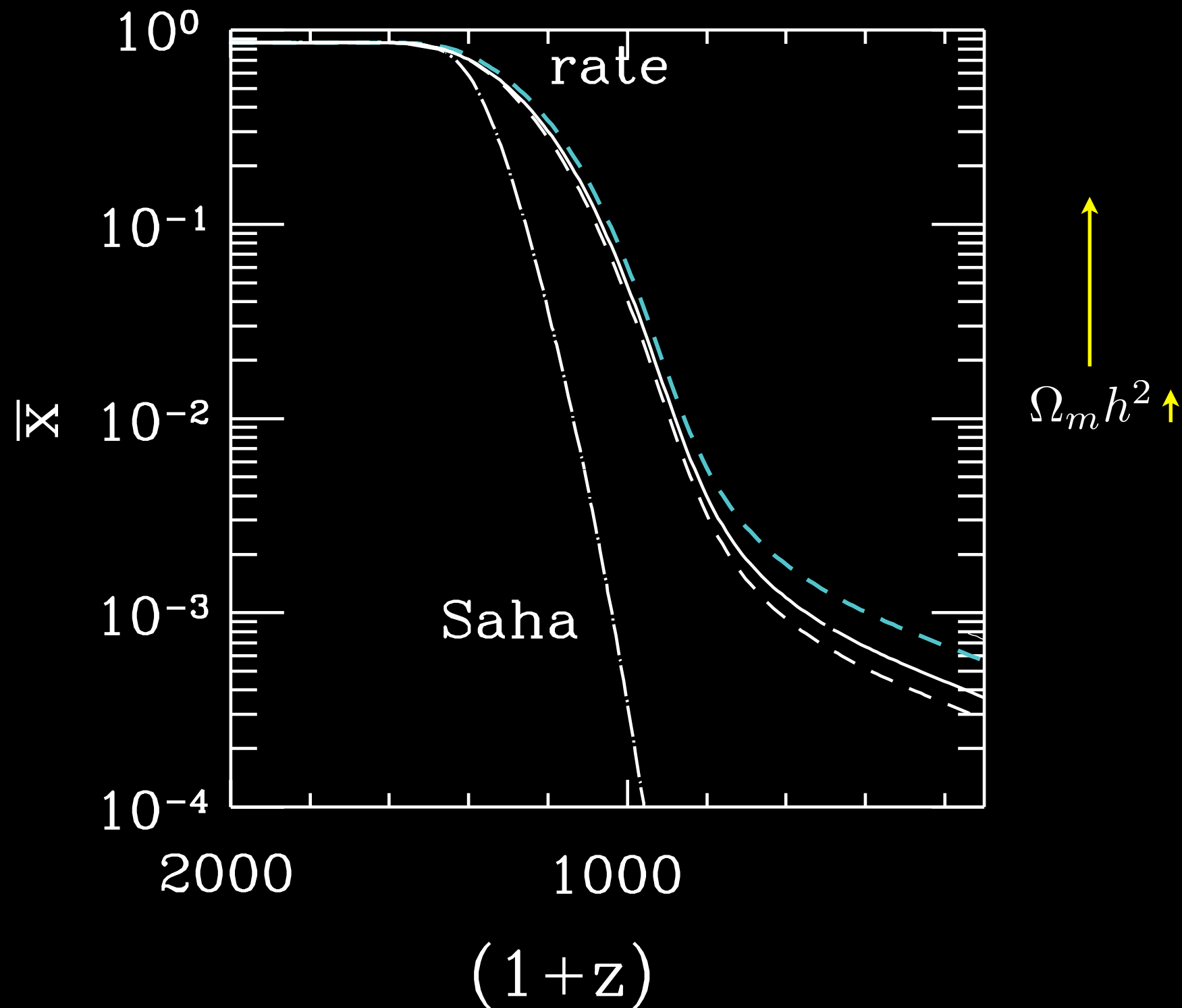
THE PEEBLES MODEL

✦ Peebles 1967: State of the Art for 30 years!



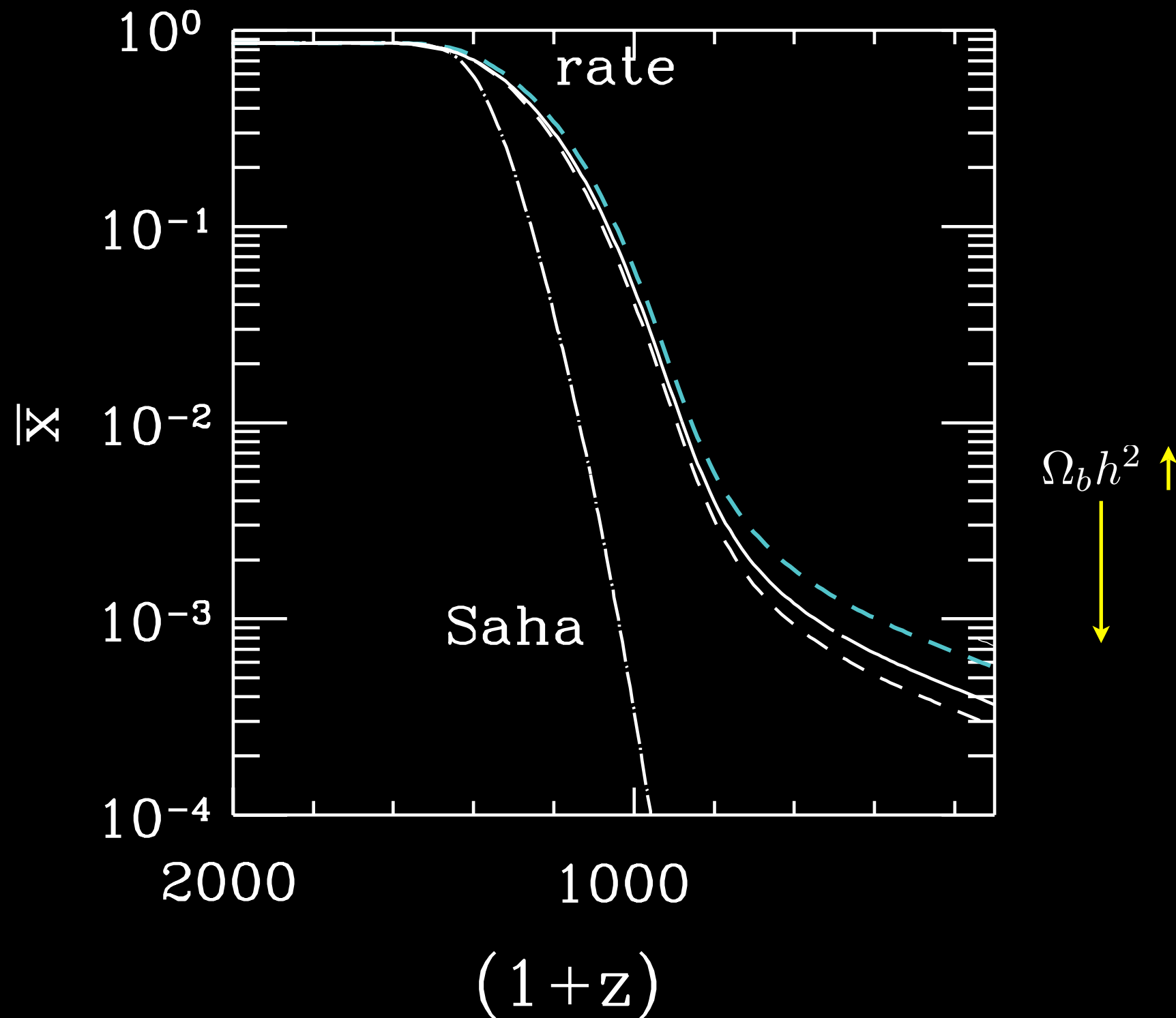
THE PEEBLES MODEL

✦ Peebles 1967: State of the Art for 30 years!



THE PEEBLES MODEL

✦ Peebles 1967: State of the Art for 30 years!



EQUILIBRIUM ASSUMPTIONS

*Radiative/collisional eq. between different l

$$\mathcal{N}_{nl} = \mathcal{N}_n \frac{(2l+1)}{n^2}$$

* Radiative eq. between different n -states

$$\mathcal{N}_n = \sum_l \mathcal{N}_{nl} = \mathcal{N}_2 e^{-(E_n - E_2)/T}$$

Non-eq rate equations

*Matter in eq. with radiation due to Thompson scattering

$$T_m = T_\gamma \text{ since } \frac{\sigma_T a T_\gamma^4 c}{m_e c^2} < H(T)$$

EQUILIBRIUM ASSUMPTIONS

*Radiative/collisional eq. between different l

$$\mathcal{N}_{nl} = \mathcal{N}_n \frac{(2l+1)}{n^2}$$

Seager/Scott/Sasselov 2000/RECFAST!

* Radiative eq. between different n-states

$$\mathcal{N}_n = \sum_l \mathcal{N}_{nl} = \mathcal{N}_2 e^{-(E_n - E_2)/T}$$

Non-eq rate equations

*Matter in eq. with radiation due to Thompson scattering

$$T_m = T_\gamma \text{ since } \frac{\sigma_T a T_\gamma^4 c}{m_e c^2} < H(T)$$

BREAKING EQUILIBRIUM

- * Chluba et al. (2005,6) follow l , n separately, get to $n_{\max} = 100$
- * 0.1 %-level corrections to CMB anisotropies at $n_{\max} = 100$
- * Equilibrium between l states: $\Delta l = \pm 1$ bottleneck
- * Beyond this, testing convergence with n_{\max} is hard!

$$t_{\text{compute}} \sim \mathcal{O}(\text{years}) \text{ for } n_{\max} = 300$$

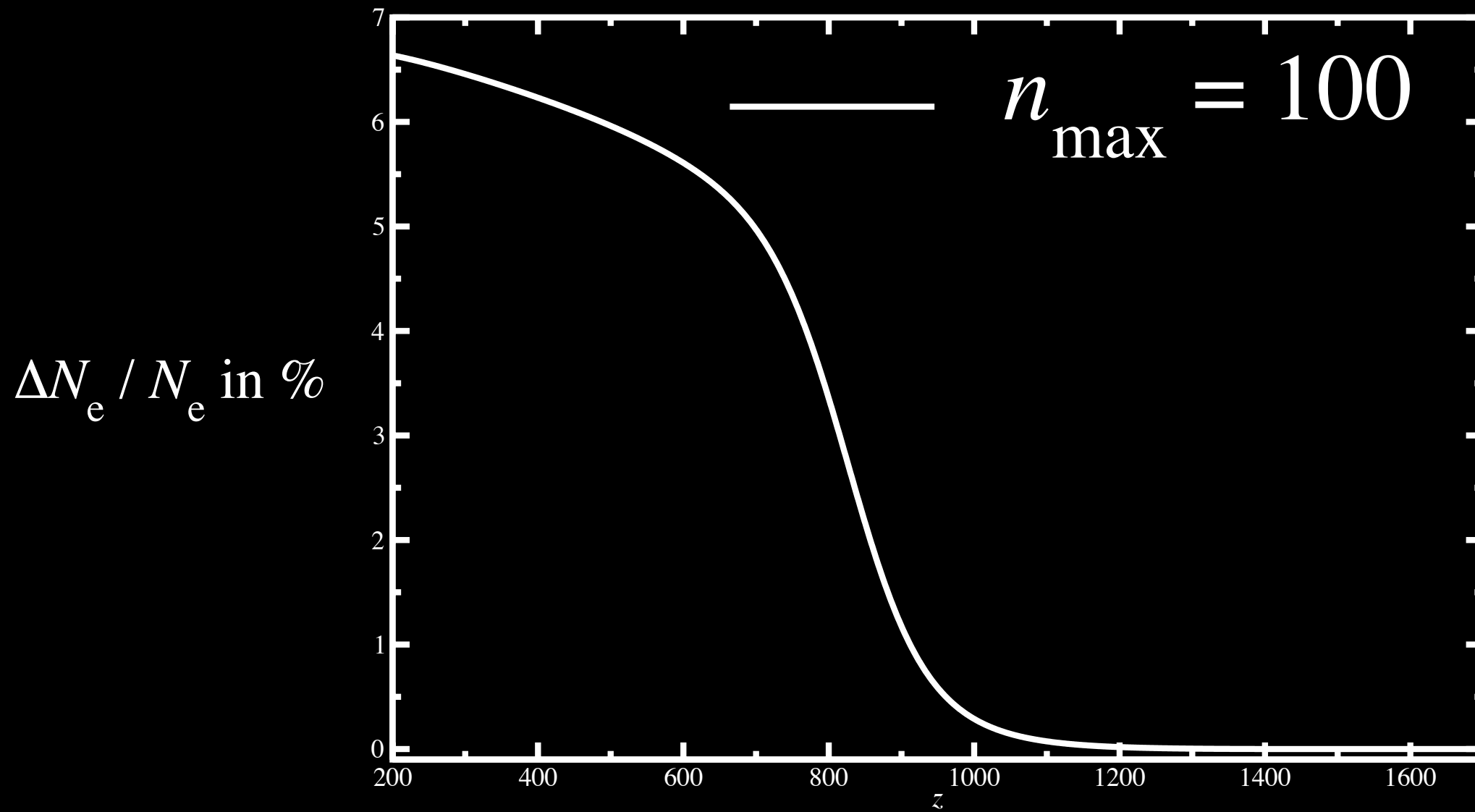
How to proceed if we want $\mathcal{O}(1) \times 10^{-4}$ accuracy in C_ℓ ?

THESE ARE REAL STATES

- * Still inside plasma shielding length for $n < 100000$
- * $r \sim a_0 n^2$ is as large as $2\mu\text{m}$ for $n_{\text{max}} = 200$
- * $\frac{\Delta E|_{\text{thermal}}}{E} < \frac{2}{n^3}$
- * Similarly high n are seen in emission line nebulae

THE EFFECT OF RESOLVING l - SUBSTATES

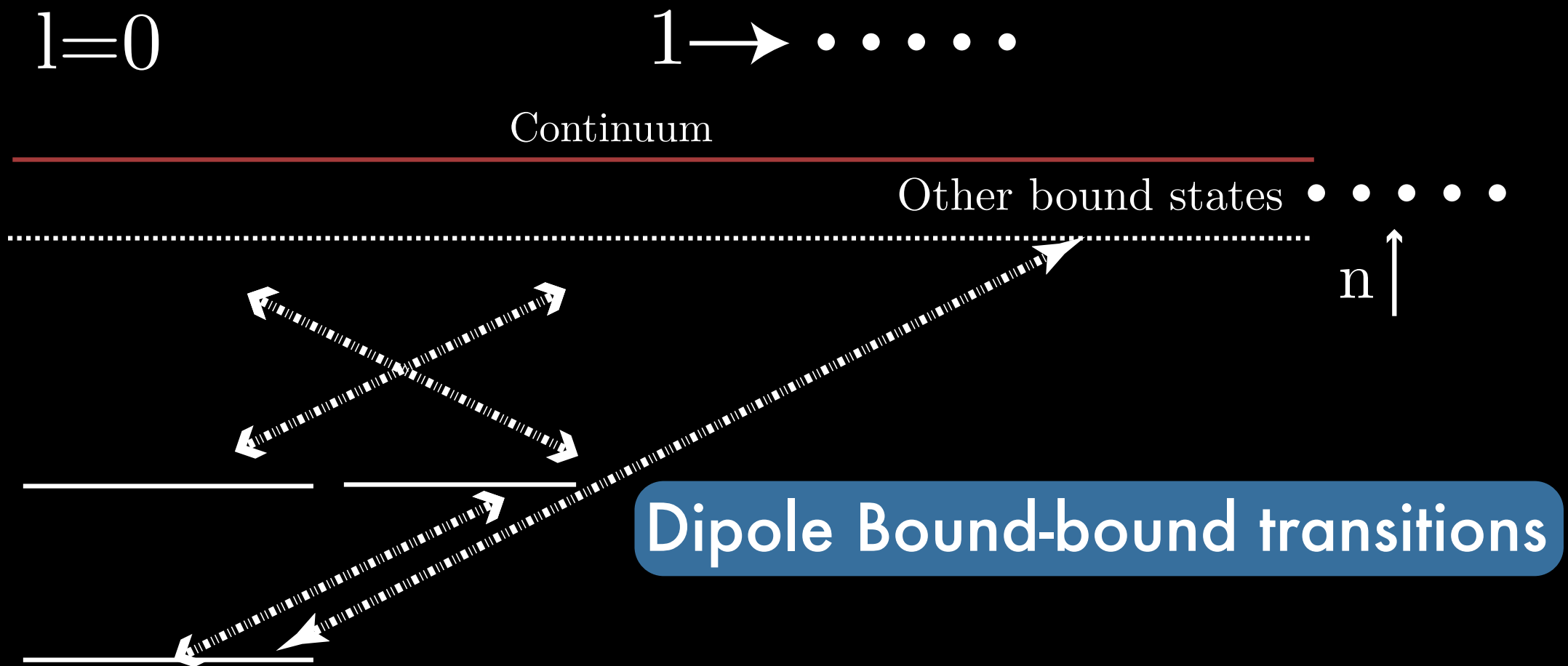
Resolved l vs unresolved l



From Chluba et al. 2006

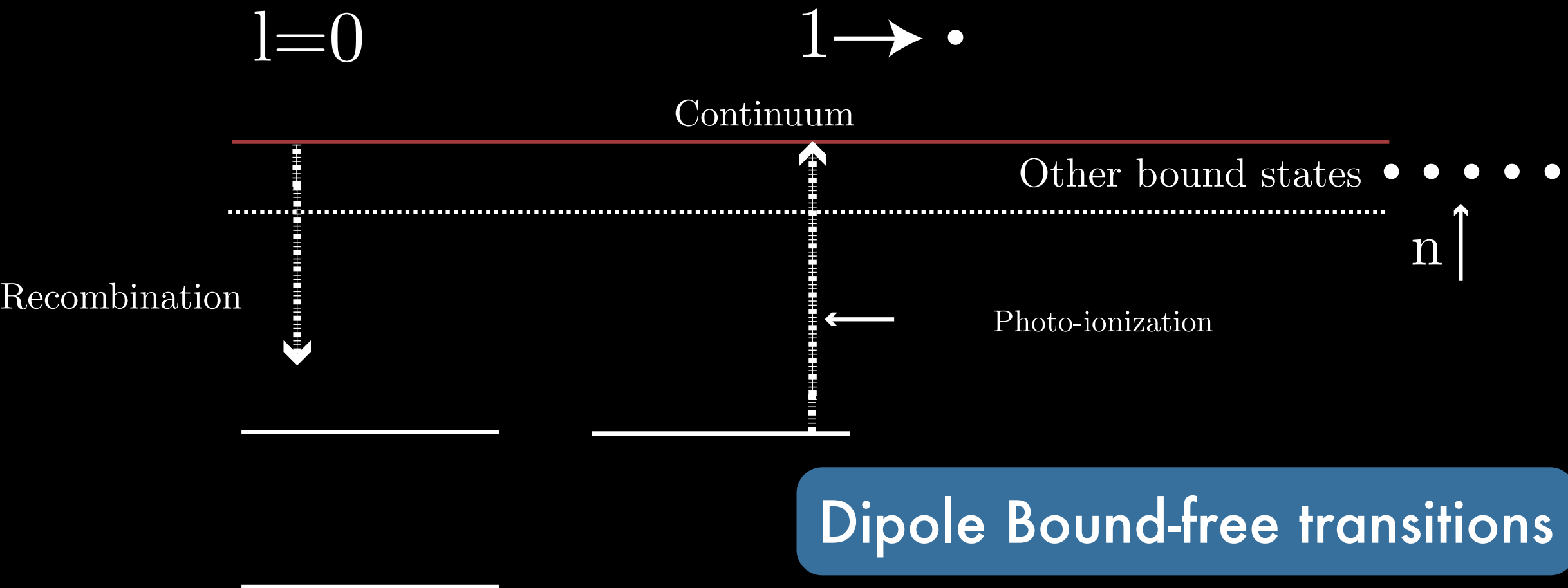
✳ 'Bottlenecked' l -substates decay slowly to 1s: Recombination is slower; Chluba et al. 2006

RECSPARSE AND THE MULTI-LEVEL ATOM



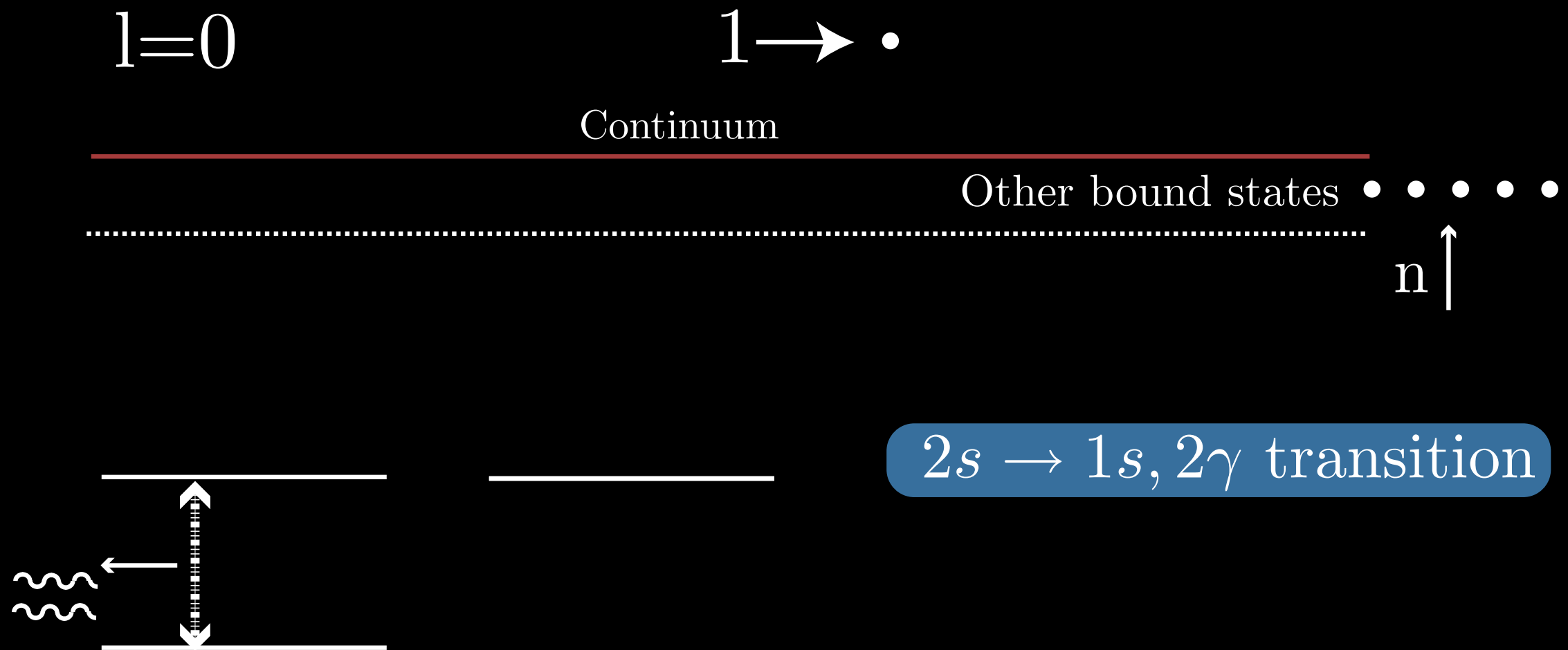
- * We implement a multi-level atom computation in a new code, **RecSparse!**
- * Boltzmann eq. solved for $T_m (T_\gamma)$
- * Spontaneous/stimulated emission/absorption included

RECSPARSE AND THE MULTI-LEVEL ATOM



- * We implement a multi-level atom computation in a new code, **RecSparse!**
- * Boltzmann eq. solved for $T_m (T_\gamma)$
- * Spontaneous/stimulated emission/absorption included

RECSPARSE AND THE MULTI-LEVEL ATOM



- * We implement a multi-level atom computation in a new code, **RecSparse!**
- * Boltzmann eq. solved for $T_m (T_\gamma)$
- * Spontaneous/stimulated emission/absorption included

RECSPARSE AND THE MULTI-LEVEL ATOM

✱ Free electron fraction evolved according to

$$\begin{aligned}\dot{x}_e &= -\dot{x}_{1s} \\ &= -\Lambda_{2s \rightarrow 1s} \left(x_{2s} - x_{1s} e^{-E_{2s \rightarrow 1s}/T_\gamma} \right) + \sum_{n,l > 1s} A_{n1}^{l0} P_{n1}^{l0} \{g(T, n, l)\}\end{aligned}$$

2s-1s decay rate

RECSPARSE AND THE MULTI-LEVEL ATOM

✱ Free electron fraction evolved according to

$$\begin{aligned}\dot{x}_e &= -\dot{x}_{1s} \\ &= -\Lambda_{2s \rightarrow 1s} \left(x_{2s} - x_{1s} e^{-E_{2s \rightarrow 1s}/T_\gamma} \right) + \sum_{n,l > 1s} A_{n1}^{l0} P_{n1}^{l0} \{g(T, n, l)\}\end{aligned}$$

Lyman series current to ground state

RECSPARSE AND THE MULTI-LEVEL ATOM

✳ Free electron fraction evolved according to

$$\begin{aligned}\dot{x}_e &= -\dot{x}_{1s} \\ &= -\Lambda_{2s \rightarrow 1s} \left(x_{2s} - x_{1s} e^{-E_{2s \rightarrow 1s}/T_\gamma} \right) + \sum_{n,l > 1s} A_{n1}^{l0} P_{n1}^{l0} \{g(T, n, l)\}\end{aligned}$$

Einstein coeff.

RECSPARSE AND THE MULTI-LEVEL ATOM

✱ Free electron fraction evolved according to

$$\begin{aligned}\dot{x}_e &= -\dot{x}_{1s} \\ &= -\Lambda_{2s \rightarrow 1s} \left(x_{2s} - x_{1s} e^{-E_{2s \rightarrow 1s}/T_\gamma} \right) + \sum_{n,l > 1s} A_{n1}^{l0} P_{n1}^{l0} \{g(T, n, l)\}\end{aligned}$$

Escape probability



RADIATION FIELD: BLACK BODY +

- * Escape probability treated in Sobolev approx: depends on steady-state and incoherent scattering approximations

$$P_{n,n'}^{l,l'} = \frac{1 - e^{-\tau_s}}{\tau_s}$$

$$\tau_s \propto \frac{n_H x_n^l A_{nn'}^{ll'}}{H(z)} \quad n' > n$$

- * RecSparse includes radiative feedback
- * Ongoing work in field focuses on corrections to simple radiative transfer picture
- * Ultimate goal is to combine all new atomic physics effect in one fast recombination code

RADIATION FIELD: BLACK BODY +

- * Escape probability treated in Sobolev approx: depends on steady-state and incoherent scattering approximations

Resonant absorber density

$$\tau_s \propto \frac{n_H x_n^l A_{nn'}^{ll'}}{H(z)} \quad n' > n$$

- * RecSparse includes radiative feedback
- * Ongoing work in field focuses on corrections to simple radiative transfer picture
- * Ultimate goal is to combine all new atomic physics effect in one fast recombination code

RADIATION FIELD: BLACK BODY +

- * Escape probability treated in Sobolev approx: depends on steady-state and incoherent scattering approximations

Einstein coefficient

$$\tau_s \propto \frac{n_{\text{H}} x_n^l A_{nn'}^{ll'}}{H(z)} \quad n' > n$$

- * RecSparse includes radiative feedback
- * Ongoing work in field focuses on corrections to simple radiative transfer picture
- * Ultimate goal is to combine all new atomic physics effect in one fast recombination code

RADIATION FIELD: BLACK BODY +

- * Escape probability treated in Sobolev approx: depends on steady-state and incoherent scattering approximations

Cosmological expansion

$$\tau_s \propto \frac{n_{\text{H}} x_n^l A_{nn'}^{ll'}}{H(z)} \quad n' > n$$

- * RecSparse includes radiative feedback
- * Ongoing work in field focuses on corrections to simple radiative transfer picture
- * Ultimate goal is to combine all new atomic physics effect in one fast recombination code

OTHER CORRECTIONS TO RECOMBINATION

- * Deviations from steady-state approx (Chluba/Sunyaev 2008)
- * Coherent scattering (Forbes and Hirata 2009, Switzer/Hirata 2007)
- * Atomic recoil (Forbes and Hirata 2009, Dubrovich and Grachev 2008)
- * Diffusion near resonance lines
- * Line overlap (Ali-Haimoud, Grin, Hirata in progress)
- * Feedback from hydrogen/helium (Chluba/Sunyaev 2007)
- * Higher-n two-photon processes (Chluba/Sunyaev 2007, Hirata 2008) in hydrogen and Helium (Switzer/Hirata 2007)
- * Deuterium
- * Additional effects in Helium (Switzer/Hirata 2007)

STEADY-STATE FOR EXCITED LEVELS

✱ Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$

STEADY-STATE FOR EXCITED LEVELS

* Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$

$\vec{x} =$

$$\begin{pmatrix} \vec{x}_0 \\ \vec{x}_1 \\ \dots \\ \vec{x}_l \\ \dots \\ \vec{x}_{l_{\max}} \end{pmatrix}$$

STEADY-STATE FOR EXCITED LEVELS

- * Evolution equations may be re-written in matrix form

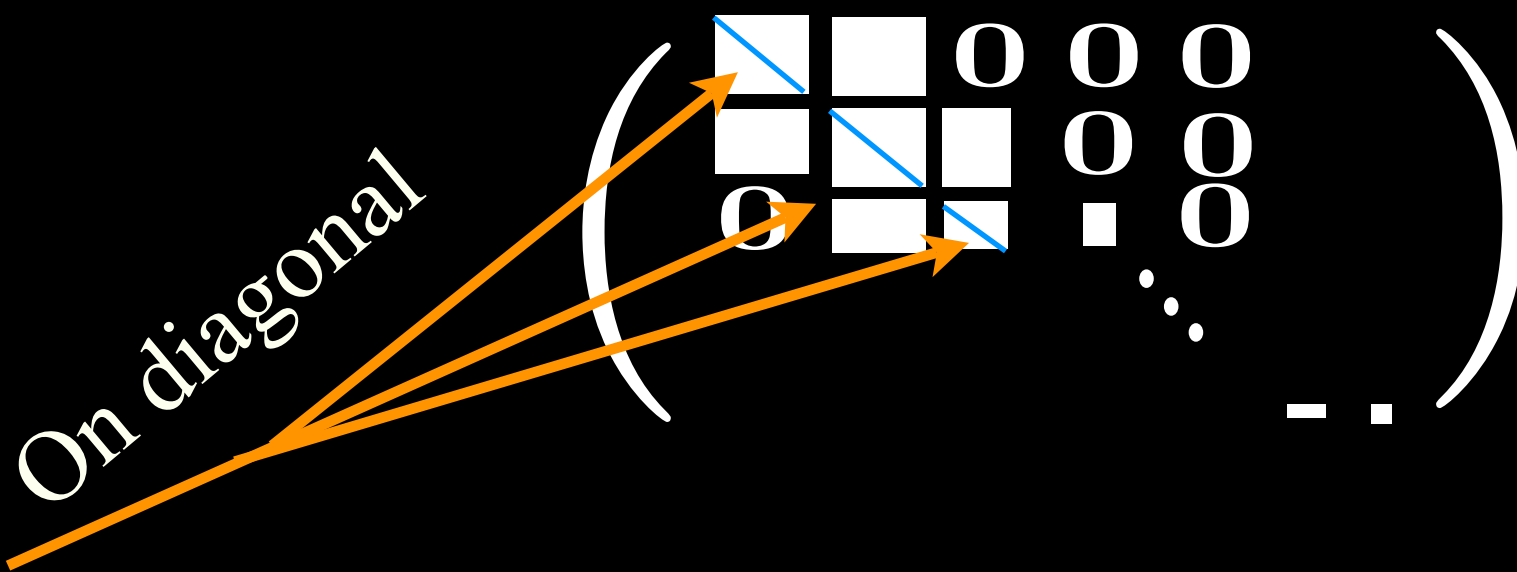
$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$

The diagram illustrates the relationship between a sub-vector \vec{x}_l and a full vector \vec{x} . On the left, a blue rounded rectangle contains the equation $\vec{x}_l = \begin{pmatrix} x_{l,l+1} \\ \dots \\ x_{l,n_{\max}} \end{pmatrix}$. On the right, a large white vector $\vec{x} = \begin{pmatrix} \vec{x}_0 \\ \vec{x}_1 \\ \dots \\ \vec{x}_l \\ \dots \\ \vec{x}_{l_{\max}} \end{pmatrix}$ is shown. An orange arrow points from the \vec{x}_l element within the large vector to the blue box on the left, indicating that \vec{x}_l is a sub-vector of \vec{x} .

STEADY-STATE FOR EXCITED LEVELS

* Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$



For state 1, includes BB transitions out of 1 to all other 1'',
photo-ionization, 2γ transitions to ground state

STEADY-STATE FOR EXCITED LEVELS

- * Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$




Off diagonal

For state 1, includes BB transitions into 1 from all other l'

STEADY-STATE FOR EXCITED LEVELS

- * Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$


Includes recombination to 1,
1 and 2γ transitions from ground state

STEADY-STATE FOR EXCITED LEVELS

- * Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$

For $n > 1$, $\mathbf{R}, \vec{s} \geq 1 \text{ s}^{-1}$ e.g. Lyman- α

STEADY-STATE FOR EXCITED LEVELS

* Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$

$$t_{\text{rec}}^{-1} \sim 10^{-12} \text{ s}^{-1}$$

For $n > 1$, $\mathbf{R}, \vec{s} \geq 1 \text{ s}^{-1}$ e.g. Lyman- α

STEADY-STATE FOR EXCITED LEVELS

* Evolution equations may be re-written in matrix form

$$\frac{d\vec{x}}{dt}$$

$$= \mathbf{R}\vec{x} + \vec{s}$$

LHS \ll RHS

$$\vec{x} \simeq -\mathbf{R}^{-1}\vec{s}$$

$$t_{\text{rec}}^{-1} \sim 10^{-12} \text{ s}^{-1}$$

For $n > 1$, $\mathbf{R}, \vec{s} \geq 1 \text{ s}^{-1}$ e.g. Lyman- α

RAPID MATRIX INVERSION: SPARSITY TO THE RESCUE

* Matrix is $\sim n_{max}^2 \times n_{max}^2$

* Brute force would require $An_{max}^6 \sim 10^5$ s for $n_{max} = 200$ for a single time step

* Dipole selection rules: $\Delta l = \pm 1$

$$M_{l,l-1}\vec{x}_{l-1} + M_{l,l}\vec{x}_l + M_{l,l+1}\vec{x}_{l+1} = \vec{s}_l \quad \left(\begin{array}{ccccc} \blacksquare & \blacksquare & 0 & 0 & 0 \\ \blacksquare & \blacksquare & \blacksquare & 0 & 0 \\ 0 & \blacksquare & \blacksquare & \blacksquare & 0 \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{array} \right) \begin{pmatrix} \vec{x}_0 \\ \vec{x}_1 \\ \dots \\ \vec{x}_{n_{max}-1} \end{pmatrix} = \vec{s}_l$$

* Physics imposes sparseness on the problem. Solved in closed form to yield algebraic $\vec{x}_{l_{max}}$, then \vec{x}_l in terms of \vec{x}_{l+1}

RAPID MATRIX INVERSION: SPARSITY TO THE RESCUE

- * Einstein coefficients to states with $n > n_{\max}$ are set $A = 0$: more later!
- * **RecSparse** generates rec. history with computation time $\sim n_{\max}^{2.5}$: Huge improvement!
- * Case of $n_{\max} = 100$ runs in less than a day, $n_{\max} = 200$ takes ~ 4 days.

FORBIDDEN TRANSITIONS AND RECOMBINATION

- * Higher- n 2γ transitions in H important at $7\text{-}\sigma$ for Planck (TT/EE) data analysis (Hirata 2008, Kholupenko 2006)
- * Some forbidden transitions are important in Helium recombination (Dubrovich 2005, Lewis 2006) and would bias cosmological parameter estimation.
- * *Are other forbidden transitions in hydrogen important, particularly for Planck data analysis? How about electric quadrupole (E2) transitions?*

QUADRUPOLE TRANSITIONS AND RECOMBINATION

- * Ground-state electric quadrupole (E2) lines are optically thick!

$$P_{n,n'}^{l,l'} = \frac{1 - e^{-\tau_s}}{\tau_s}$$

$$R \propto AP \propto A/\tau \text{ if } \tau \gg 1$$

$$\tau \propto A \rightarrow R \rightarrow A/A \rightarrow \text{const}$$

- * Coupling to ground state will overwhelmingly dominate:

$$\frac{A_{n,2 \rightarrow 1,0}^{\text{quad}}}{A_{n,2 \rightarrow m,0}^{\text{quad}}} \propto \frac{\omega_{n1}^5}{\omega_{nm}^5} \geq 10^3 \text{ if } m \geq 2$$

QUADRUPOLE TRANSITIONS AND RECOMBINATION

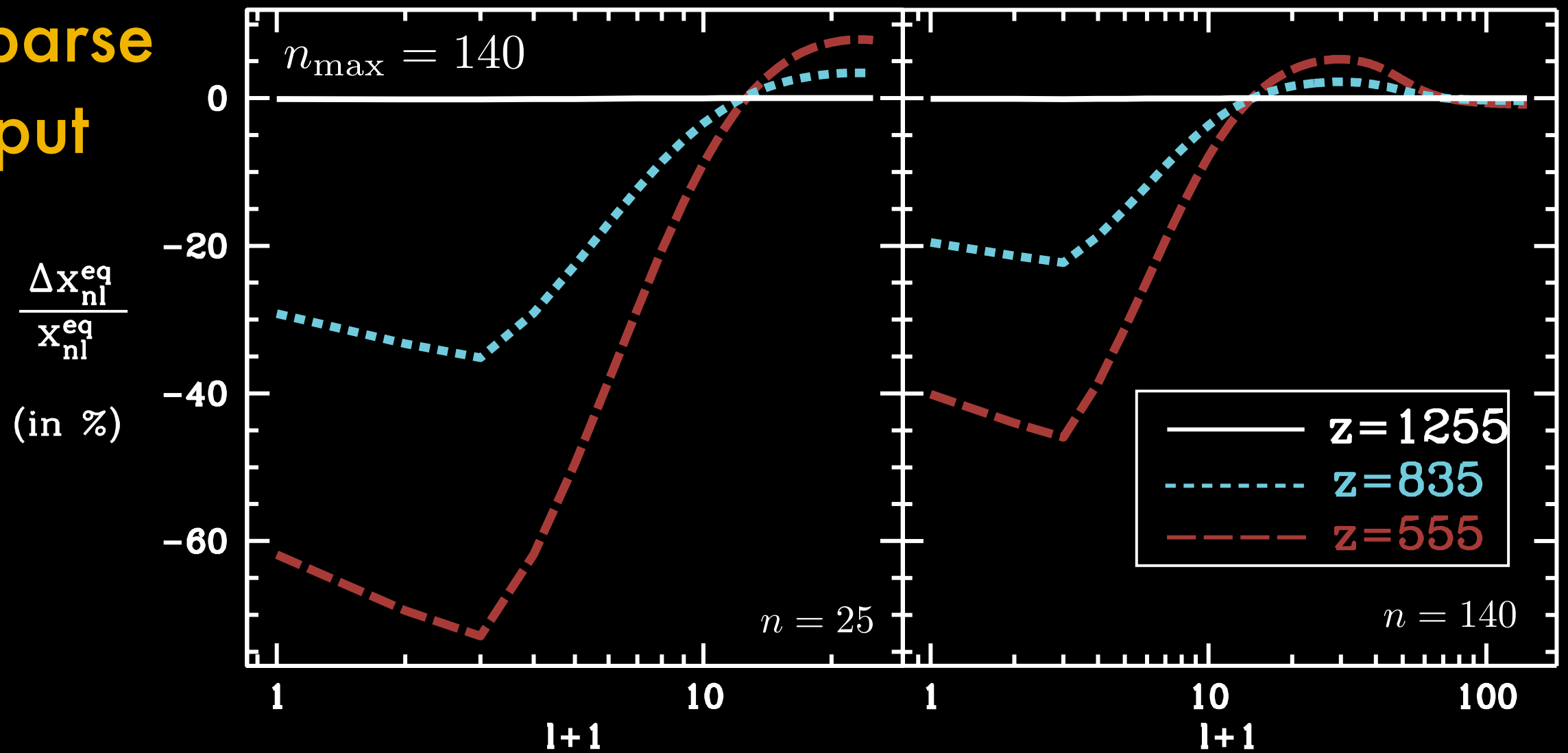
- * Lyman lines are optically thick, so $nd \rightarrow 1s$ immediately followed by $1s \rightarrow np$, so this can be treated as an effective $d \rightarrow p$ process with rate $A_{nd \rightarrow 1s} x_{nd}$.
- * Same sparsity pattern of rate matrix, similar to l-changing collisions
- * Detailed balance yields net rate

$$R_{nd \rightarrow np}^{\text{quad}} = A_{nd \rightarrow 1s} \left(x_{nd} - \frac{5}{3} x_{np} \right)$$

RESULTS: STATE OF THE GAS

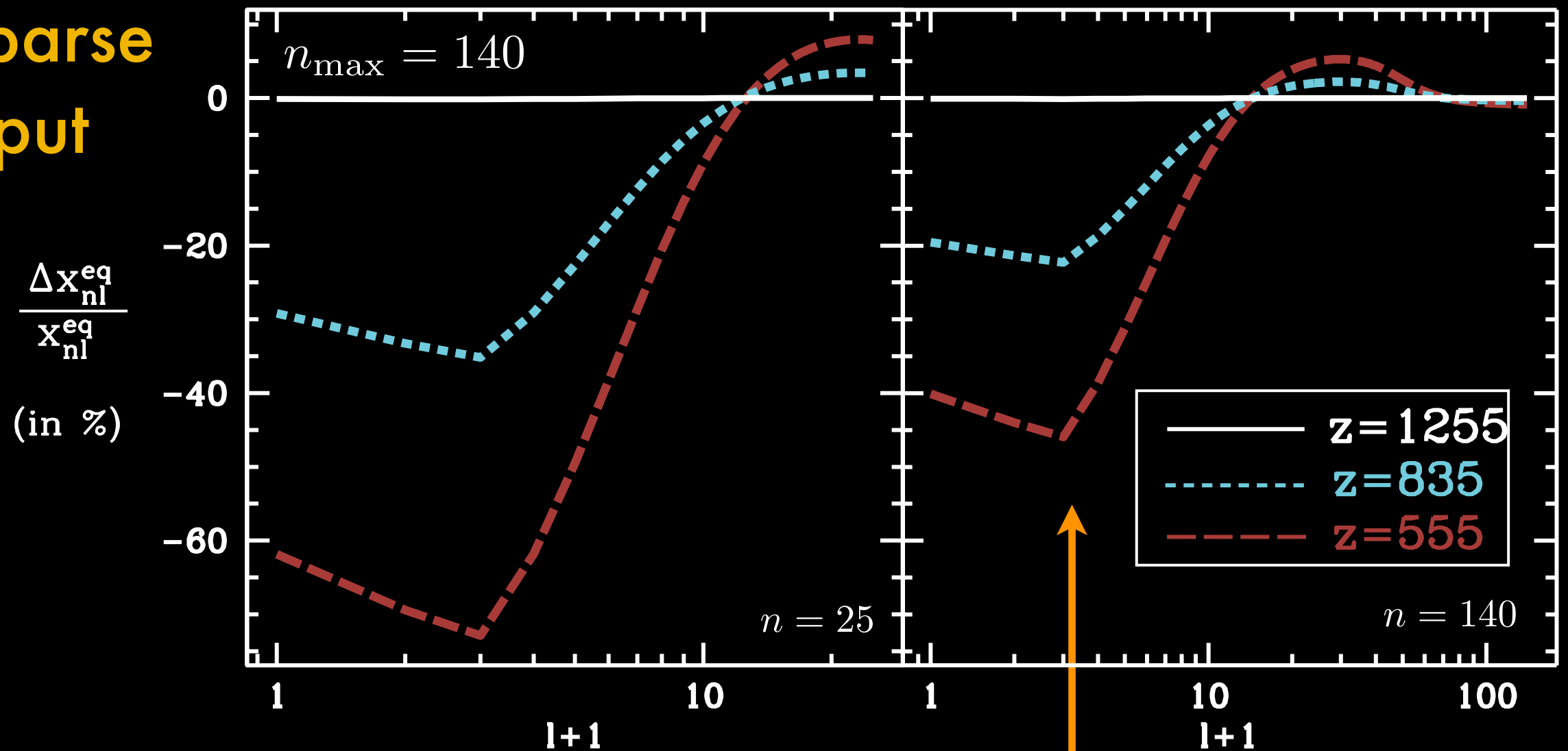
DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

RecSparse
output



DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

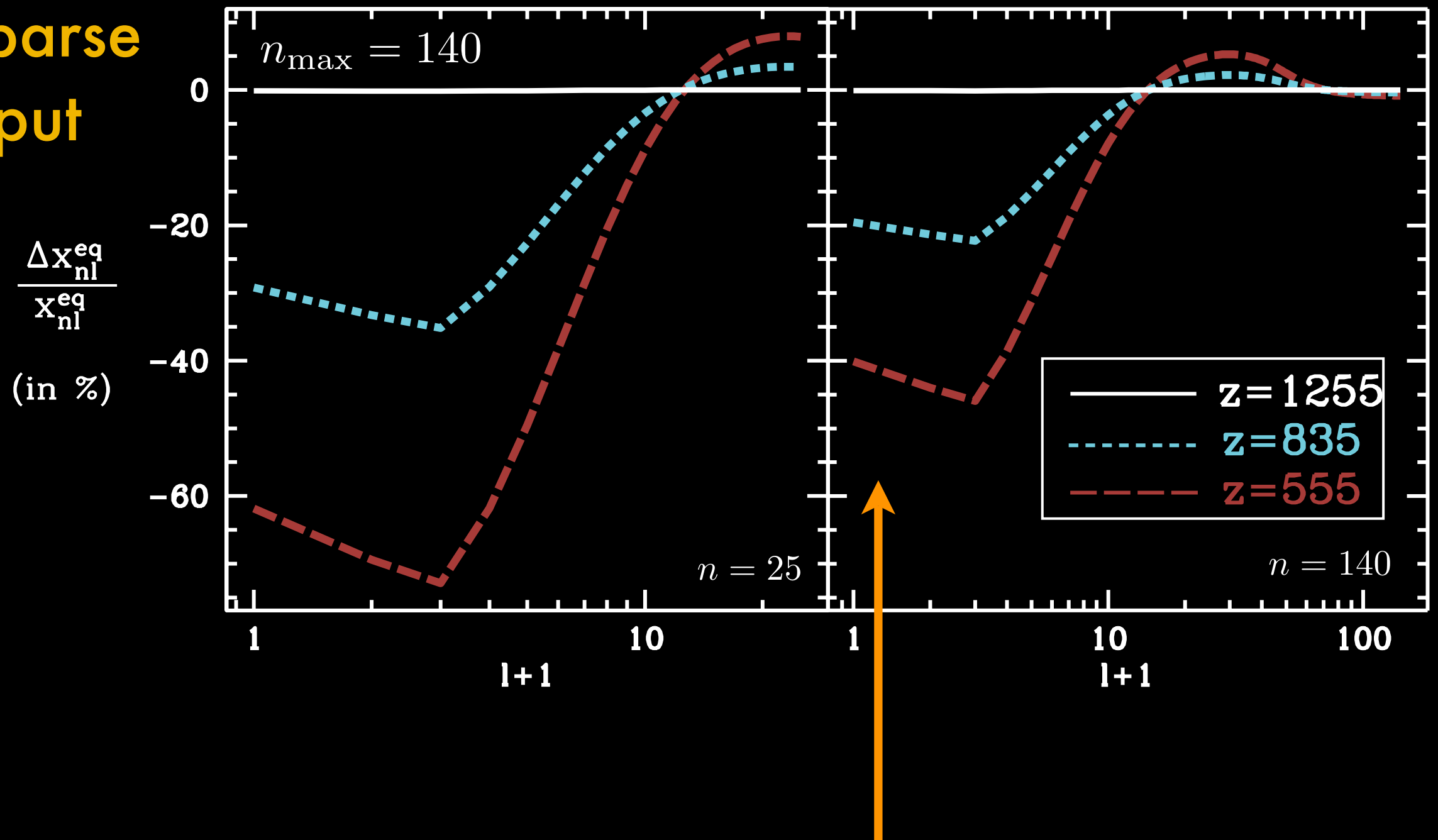
RecSparse
output



Lower l states can easily cascade down,
and are relatively under-populated

DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

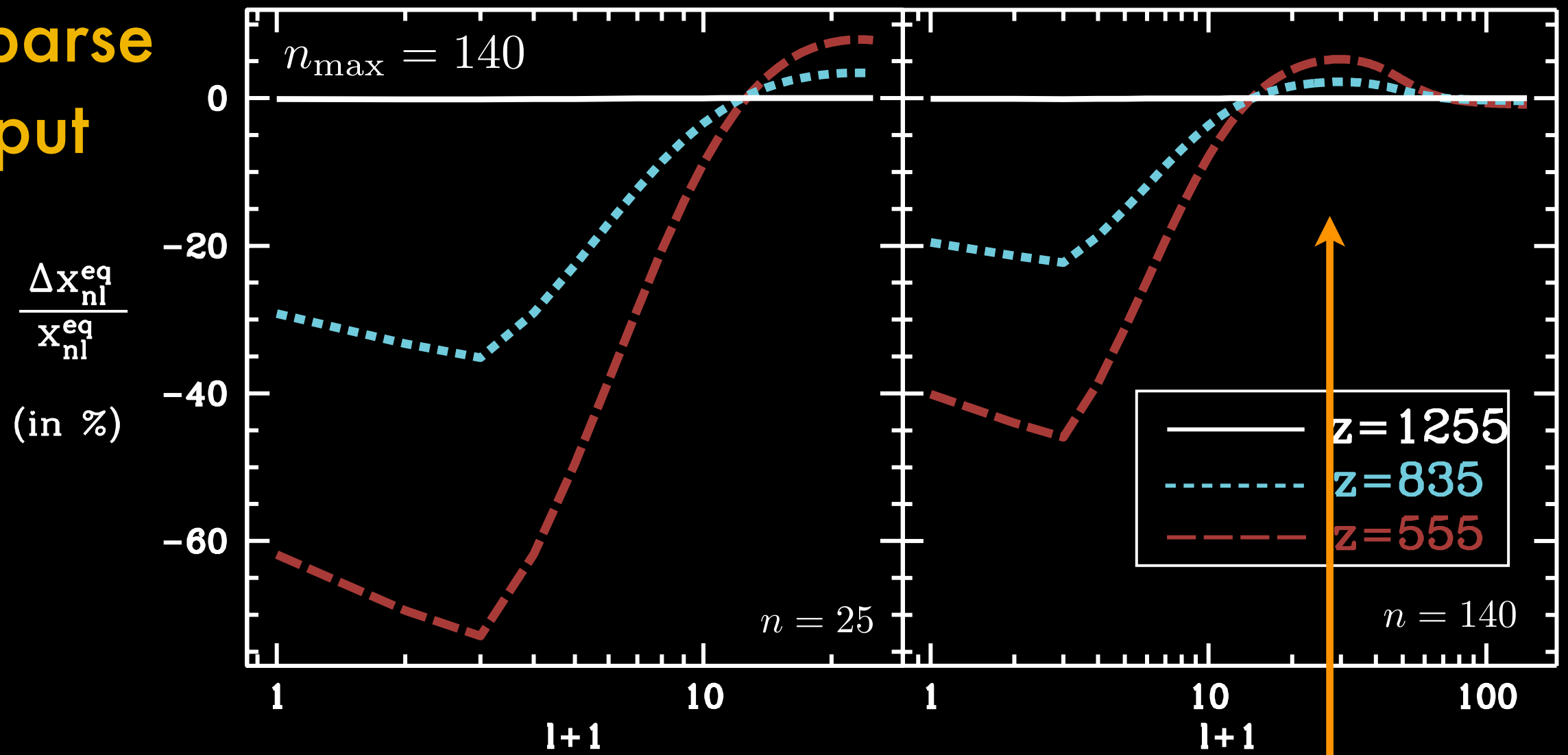
RecSparse
output



$l=0$ can't cascade down, so s states are not as under-populated

DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

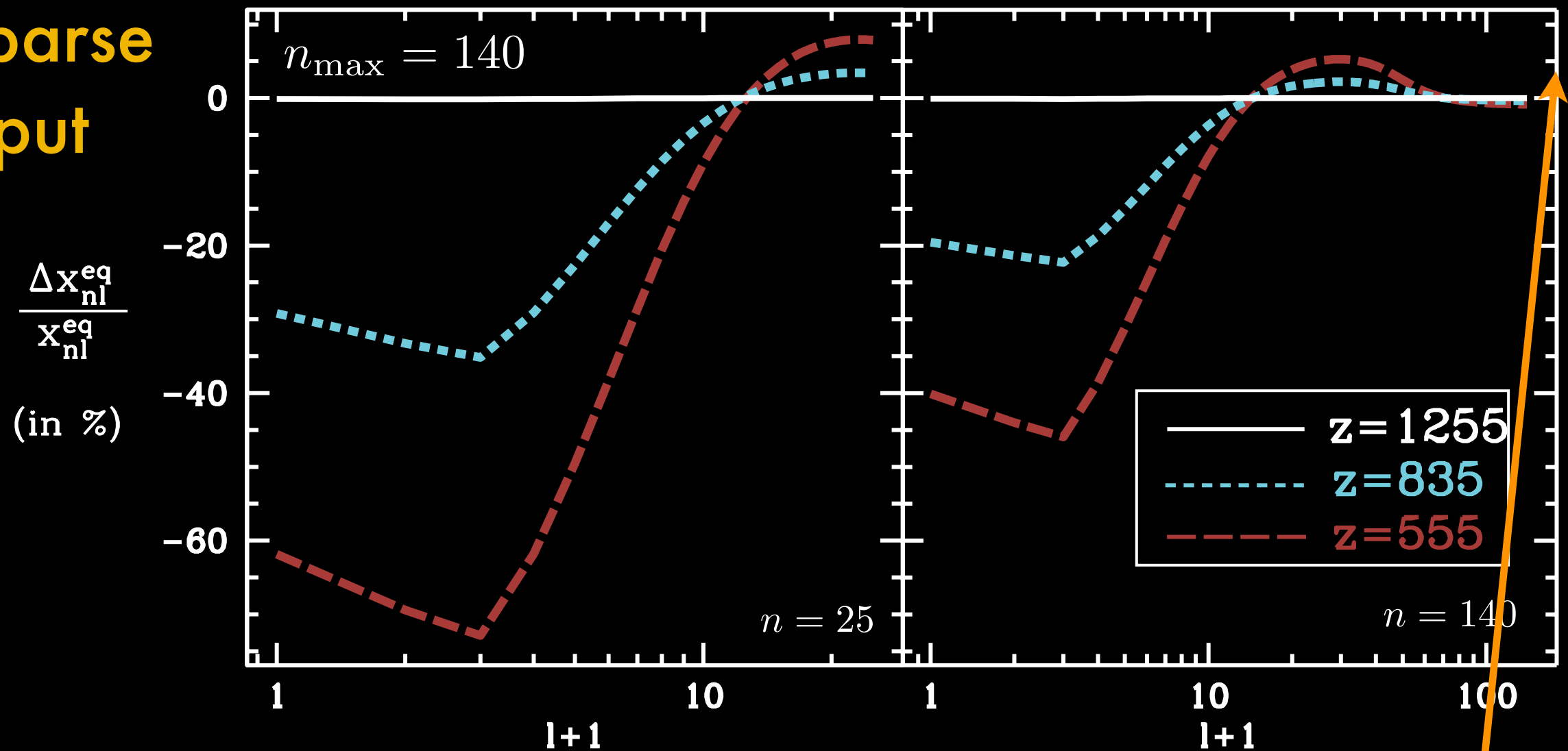
RecSparse
output



Higher l are bottlenecked by $\Delta l = \pm 1$ (over-pop)

DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

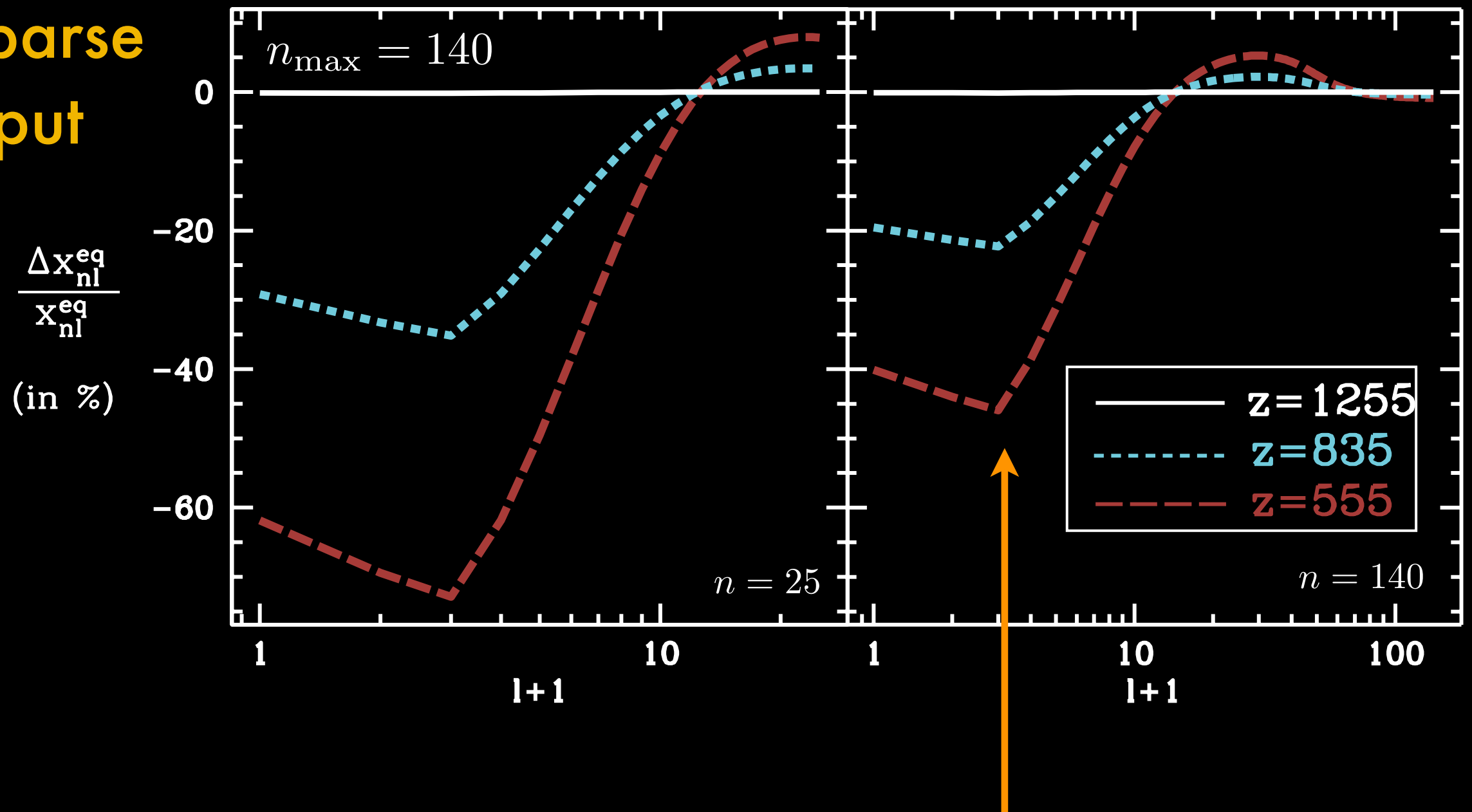
RecSparse
output



Highest l states recombine inefficiently, and are under-populated

DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

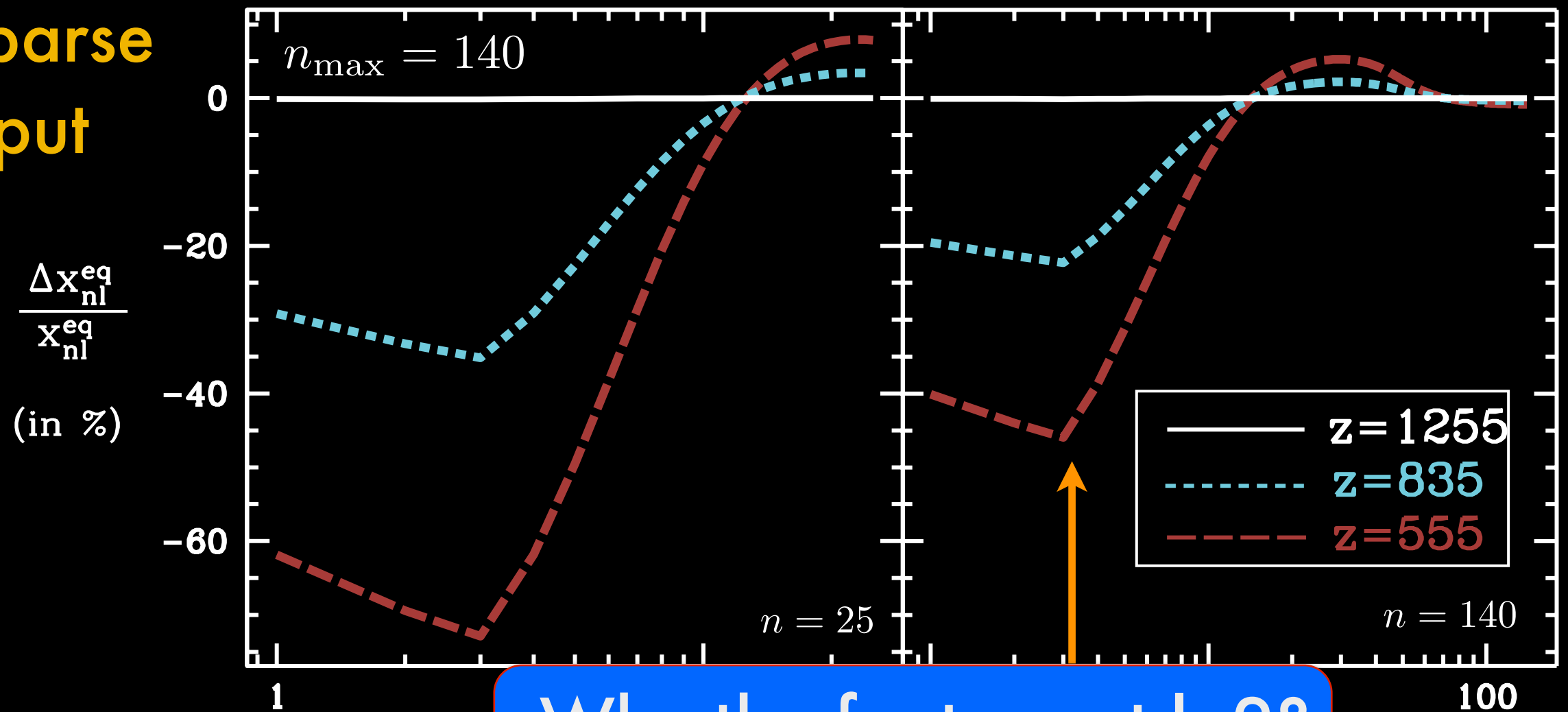
RecSparse
output



l -substates are highly out of Boltzmann eqb'm at late times

DEVIATIONS FROM BOLTZMANN EQ: l -SUBSTATES

RecSparse
output



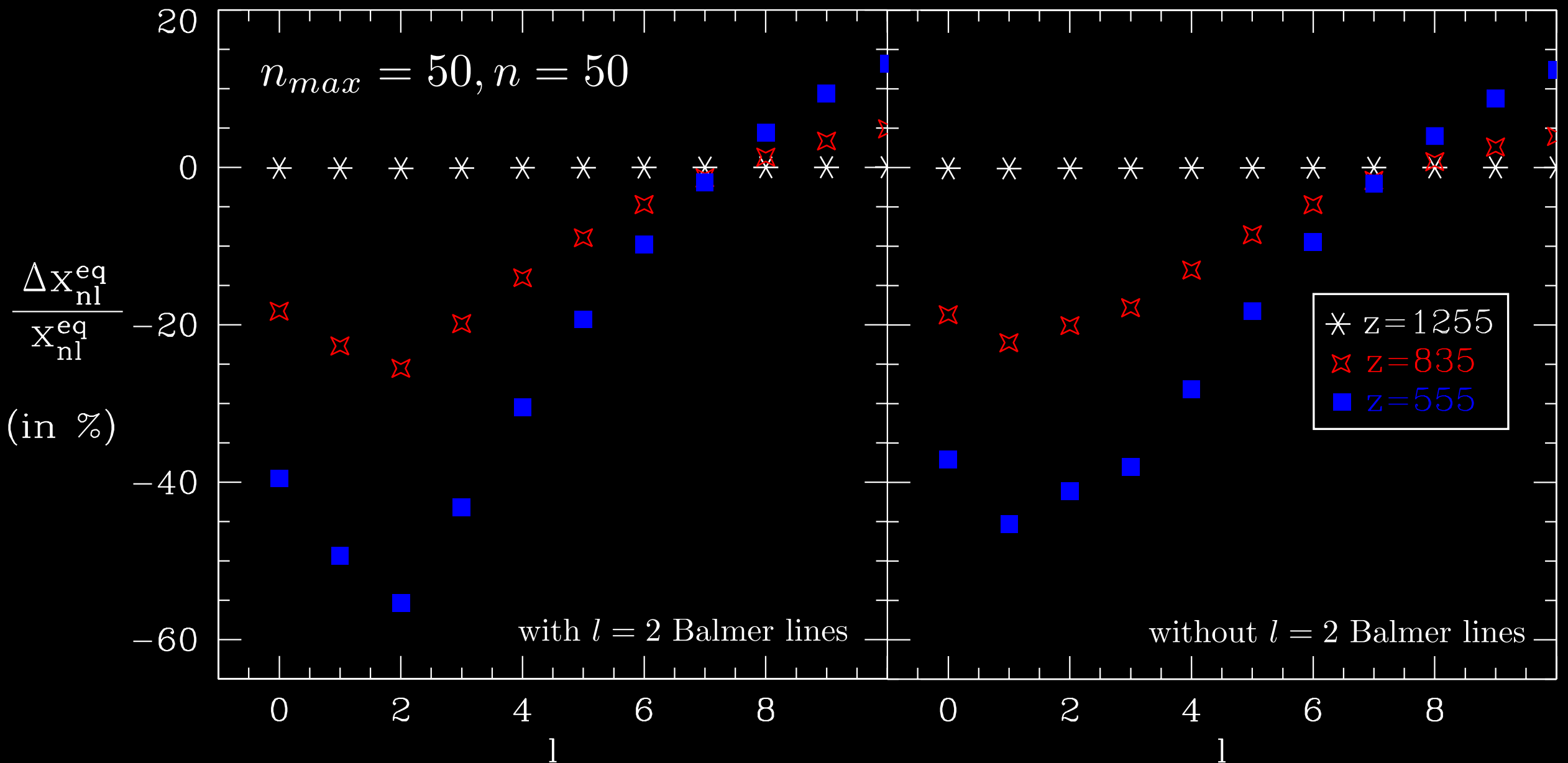
Why the feature at $l=2$?

WHAT IS THE ORIGIN OF THE $l=2$ DIP?

$$A_{nd \rightarrow 2p} > A_{np \rightarrow 2s} > A_{ns \rightarrow 2p}$$

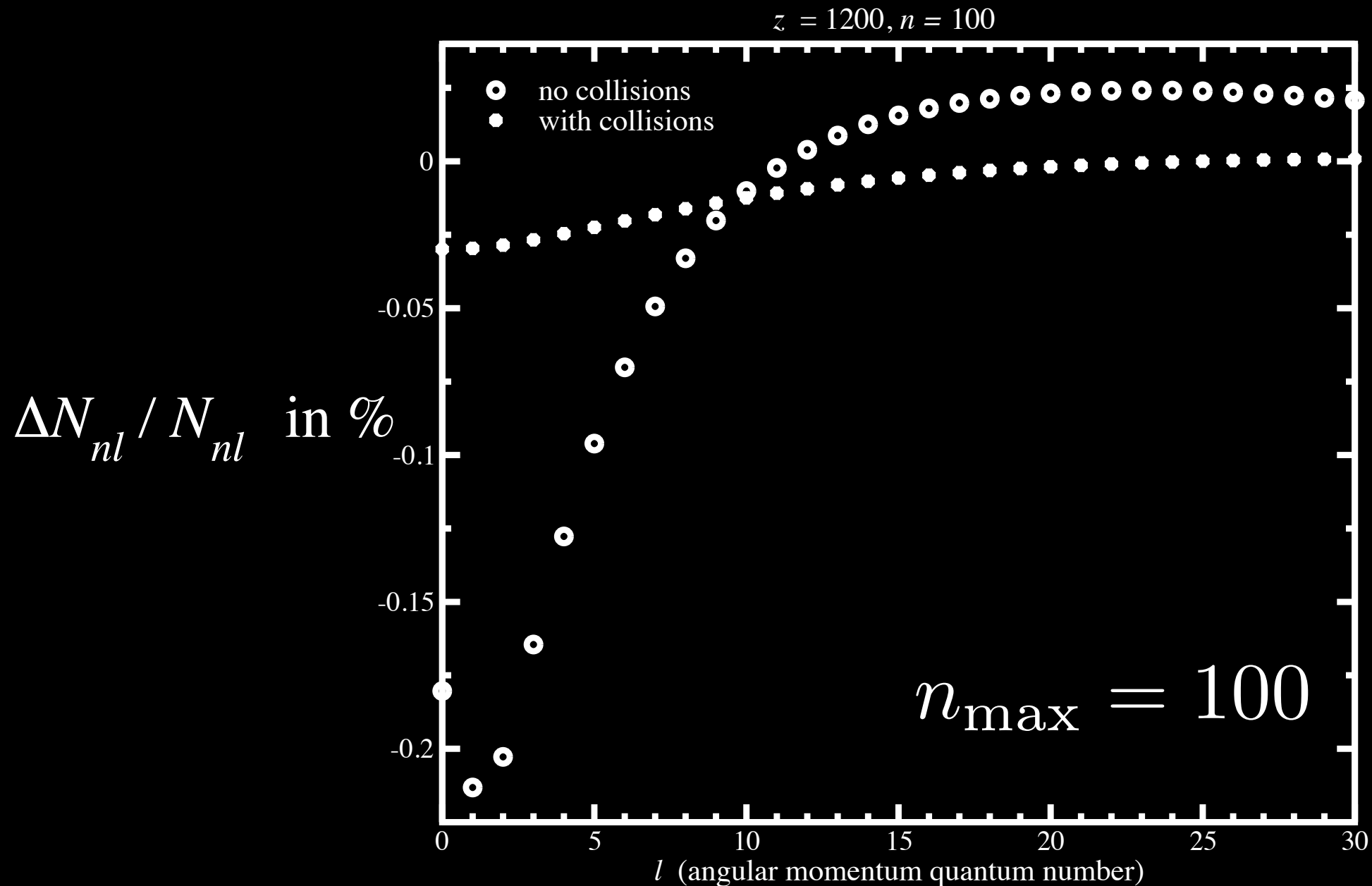
- * $l=2$ depopulates more rapidly than $l=1$ for higher ($n>2$) excited states
- * We can test if this explains the dip at $l=2$ by running the code with these Balmer transitions the blip should move to $l=1$

L-SUBSTATE POPULATIONS, BALMER LINES OFF



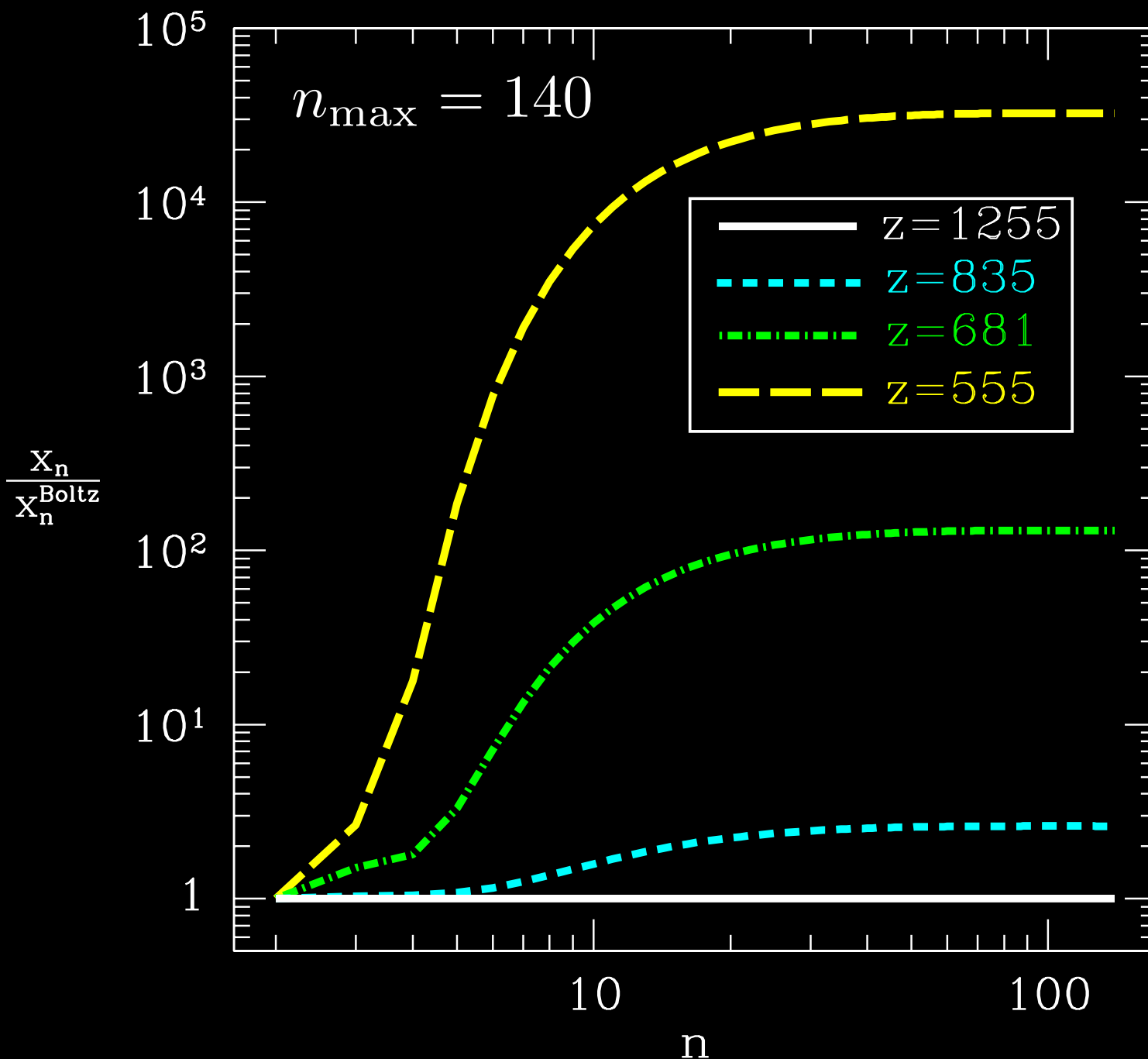
Dip moves as expected when Balmer lines are off!

ATOMIC COLLISIONS



- * l-changing collisions bring l-substates closer to statistical equilibrium (SE) (Chluba, Rubino Martin, Sunyaev 2006)
- * Theoretical collision rates unknown to factors of 2!

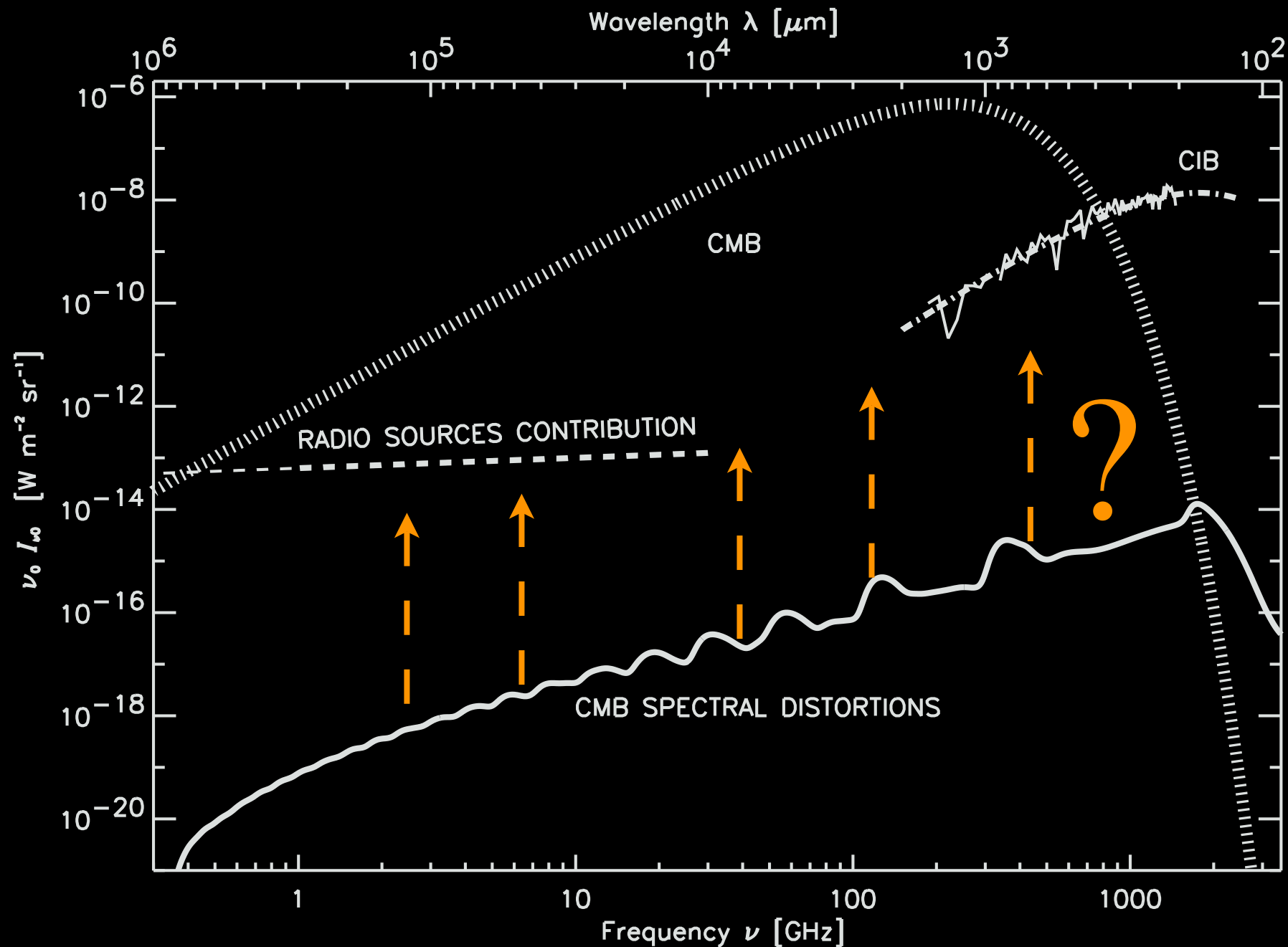
DEVIATIONS FROM BOLTZMANN EQUILIBRIUM: DIFFERENT n -SHELLS



$$\alpha_n n_e > \sum_{n'l}^{n' < n} A_{nn'}^{ll \pm 1}$$

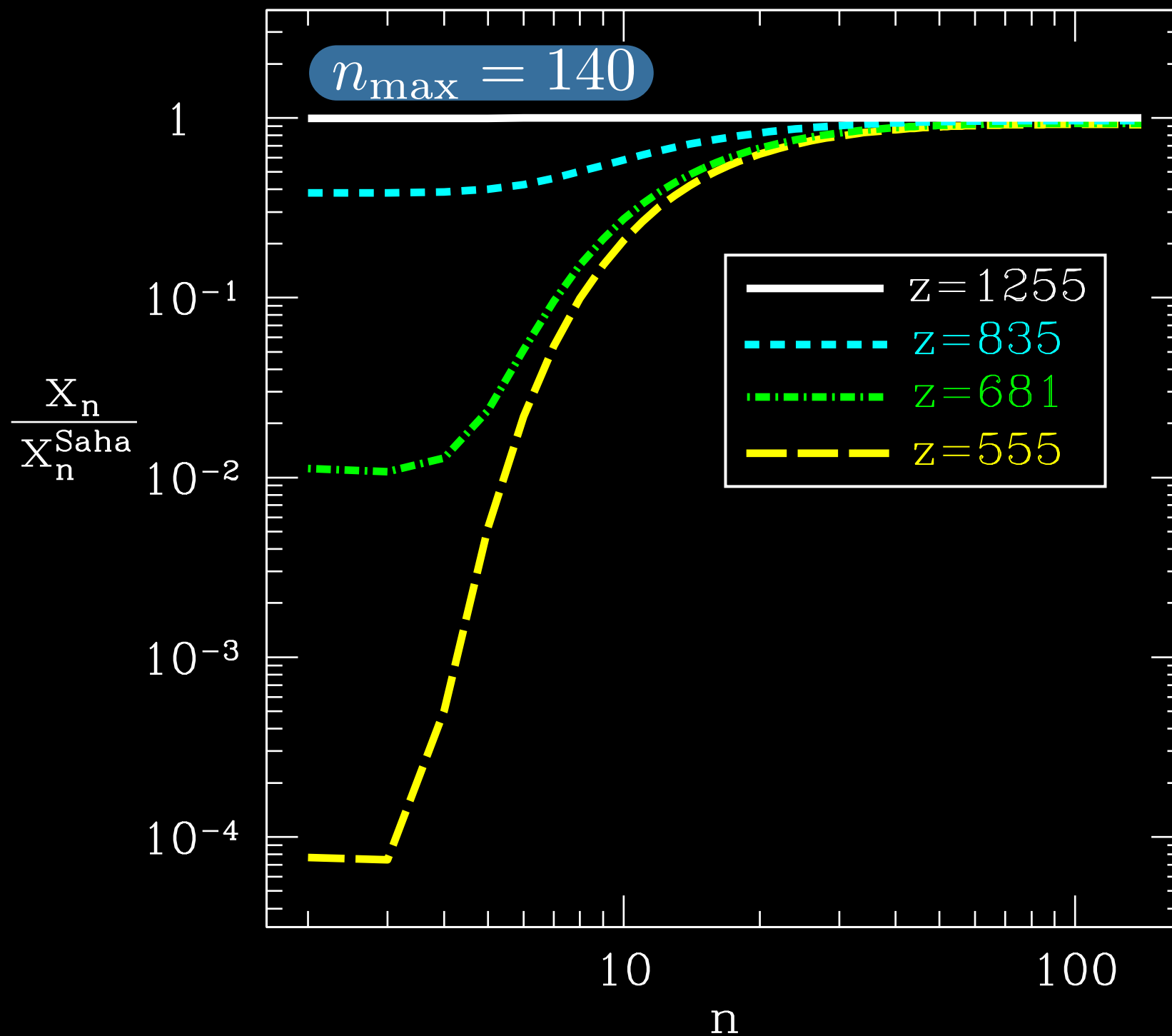
- * No inversion relative to $n=2$ (just over-population)
- * Population inversion seen between some excited states: Does radiation stay coherent? Does recombination make?

DEVIATIONS FROM BOLTZMANN EQUILIBRIUM: DIFFERENT n -SHELLS



**Masing could make spectral
distortions detectable!**

DEVIATIONS FROM SAHA EQUILIBRIUM

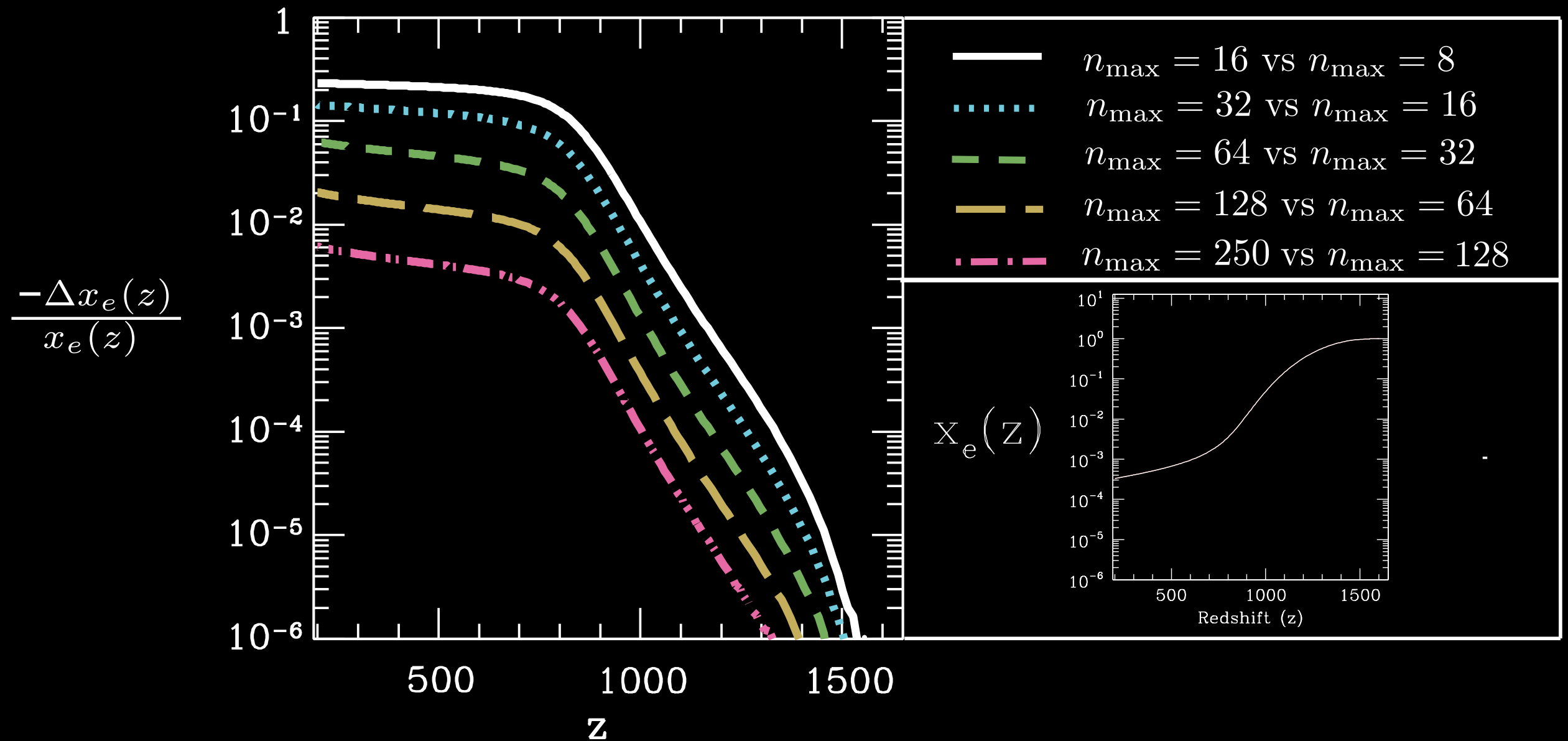


HUGE DEVIATIONS
FROM SAHA EQ!

- ✳ Effect of states with $n > n_{\max}$ could be approximated using asymptotic Einstein coeffs. and Saha eq, but Saha is elusive at high n /late times.
- ✳ At $z=200$, $n_{\max} \sim 1000$ needed, unless collisions included

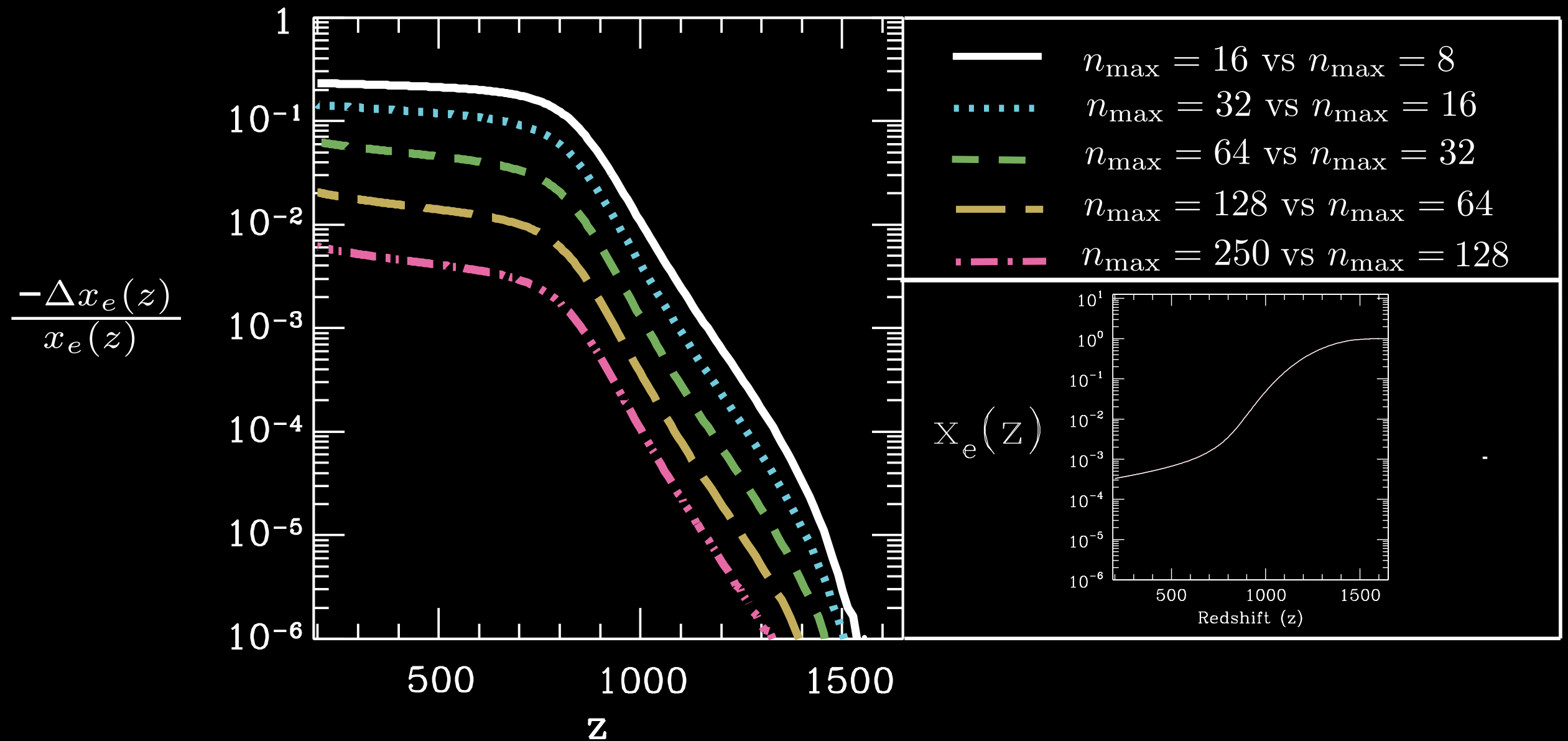
RESULTS: RECOMBINATION HISTORIES

RESULTS: RECOMBINATION HISTORIES INCLUDING HIGH- n



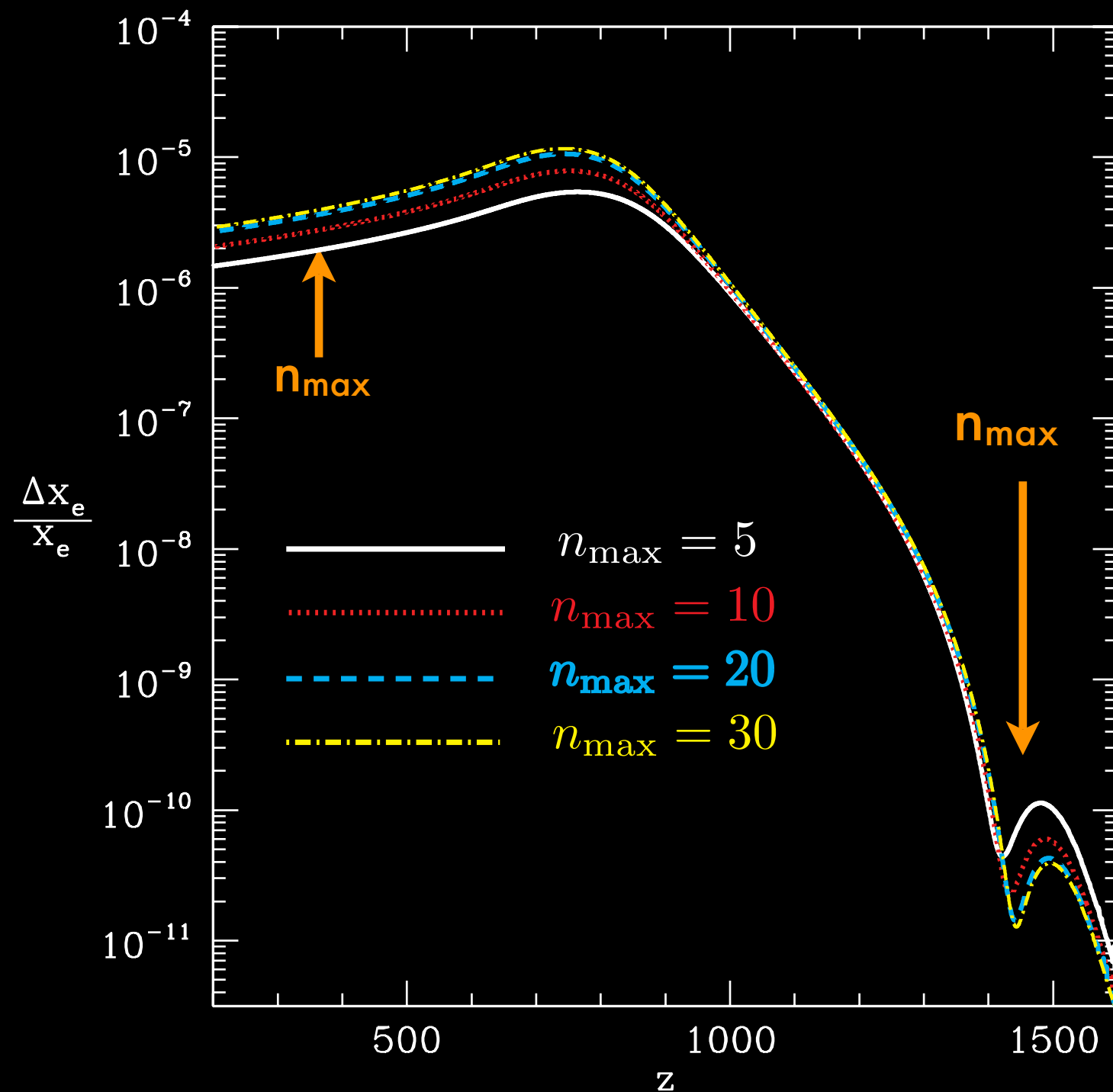
- * $x_e(z)$ falls with increasing $n_{\max} = 10 \rightarrow 250$, as expected.
- * Rec Rate > downward BB Rate > Ionization, upward BB rate
- * For $n_{\max} = 100$, code computes in only 2 hours

RESULTS: RECOMBINATION HISTORIES INCLUDING HIGH- n



- * Relative convergence is not the same thing as absolute convergence: Want to see Saha asymptote and impose well-motivated cutoff! Collisions could help
- * These are lower limits to the actual error
- * $n_{\max}=300$ just completed

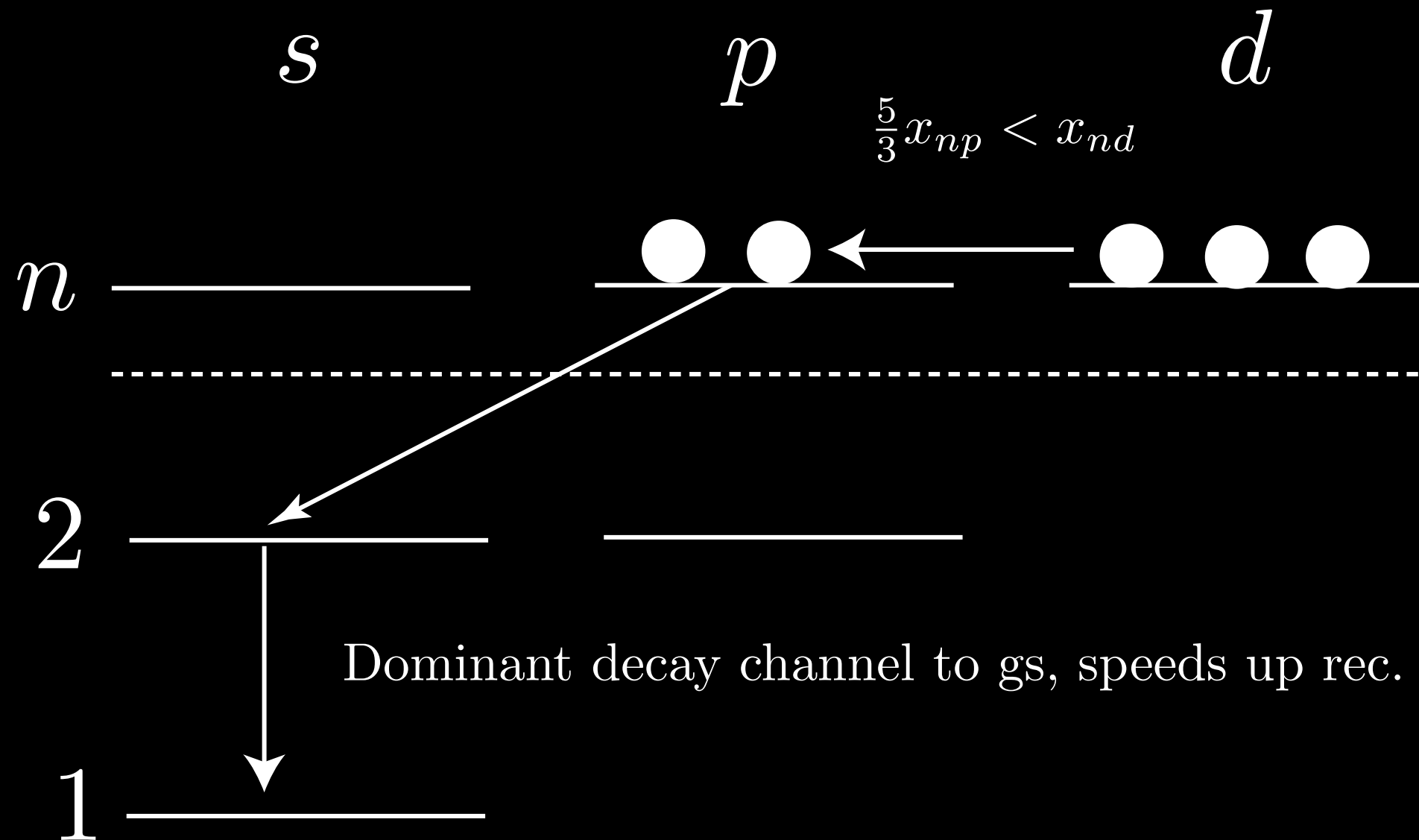
RESULTS: RECOMBINATION WITH HYDROGEN



$$\Delta x_e \equiv x_e|_{\text{no } E2 \text{ transitions}} - x_e|_{\text{with } E2 \text{ transitions}}$$

Negligible for Planck!

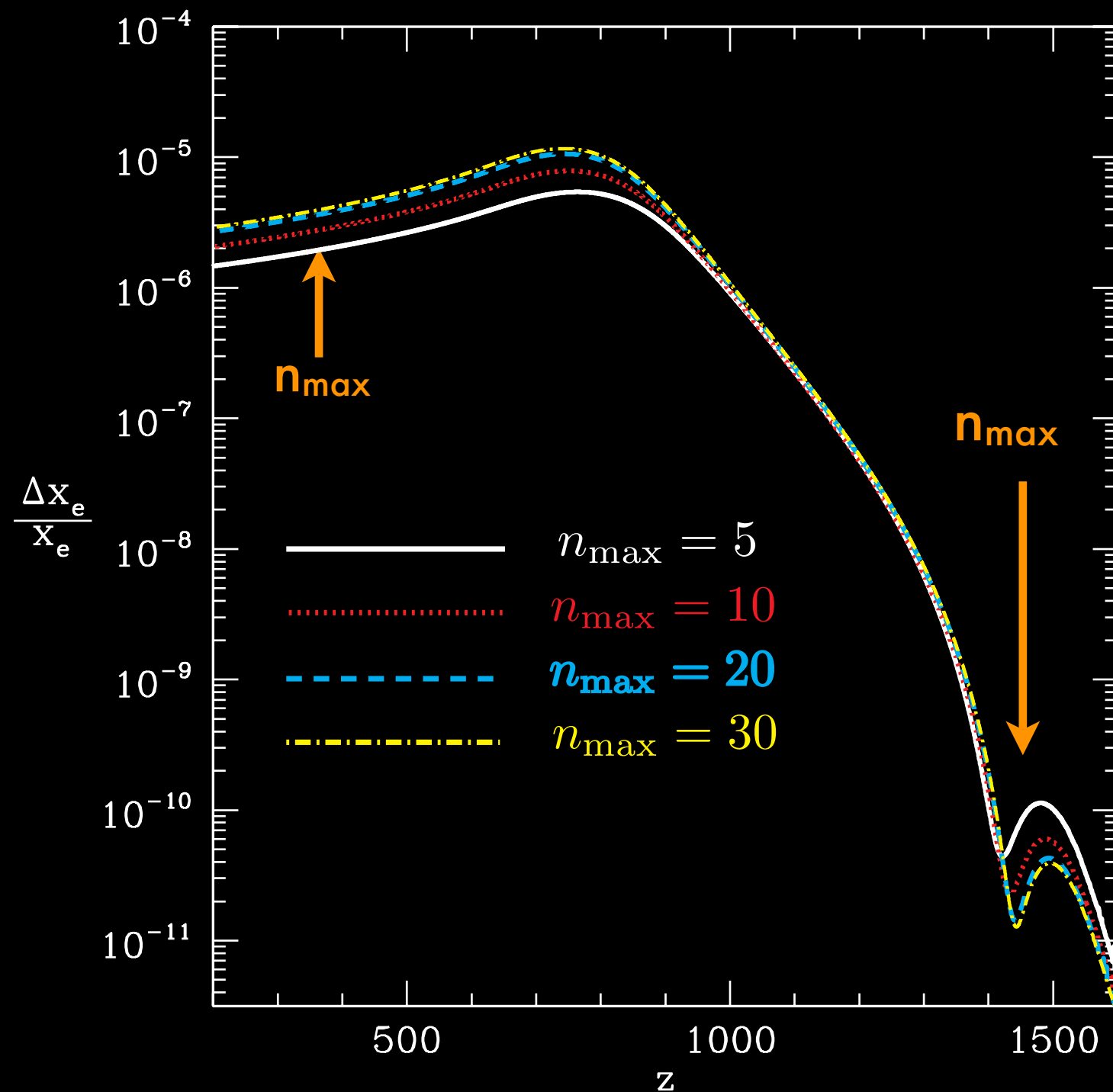
RESULTS: RECOMBINATION WITH HYDROGEN



$$R_{nd \rightarrow np}^{\text{quad}} = A_{nd \rightarrow 1s} \left(x_{nd} - \frac{5}{3}x_{np} \right)$$

$n < 5$, early times

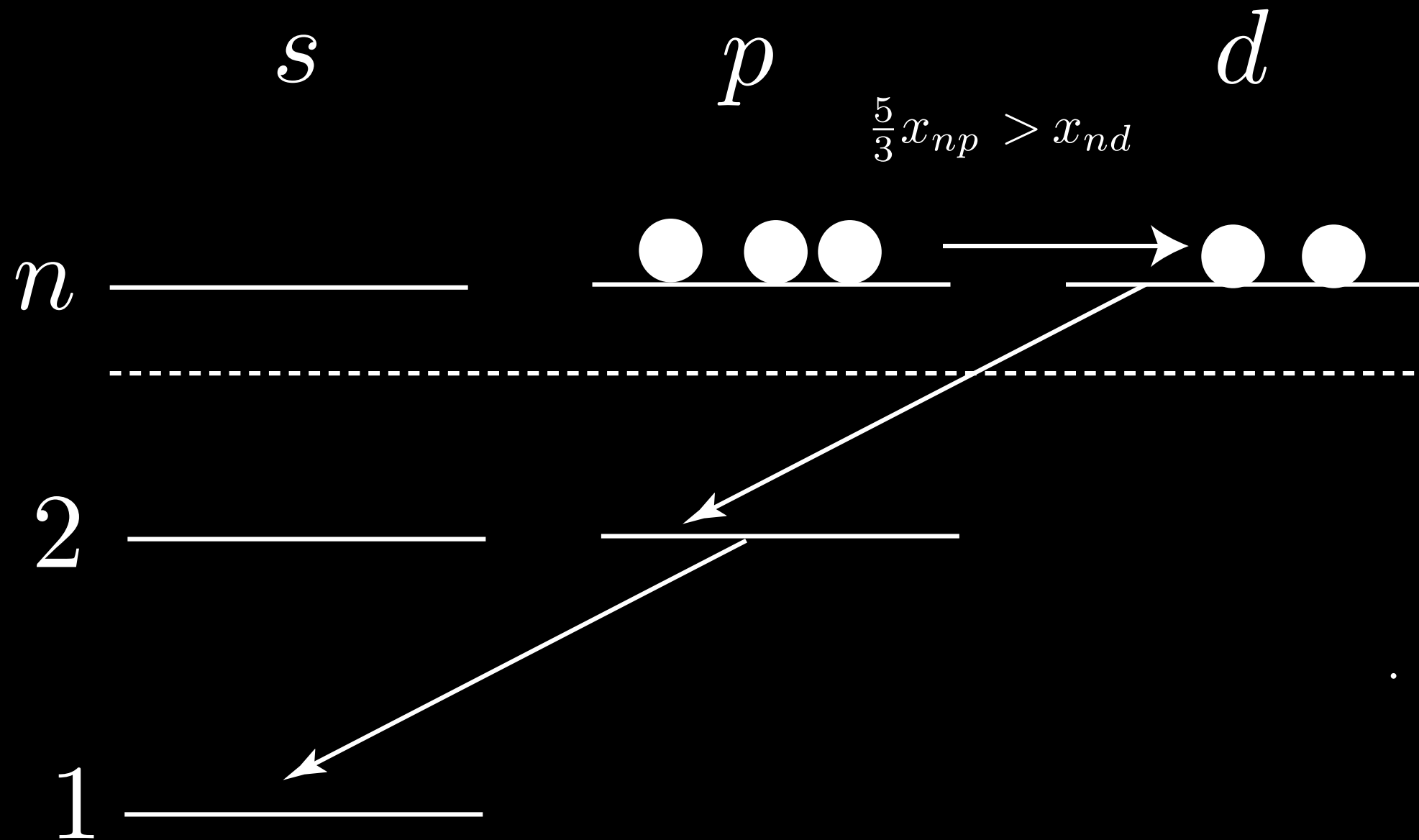
RESULTS: RECOMBINATION WITH HYDROGEN



$$\Delta x_e \equiv x_e|_{\text{no } E2 \text{ transitions}} - x_e|_{\text{with } E2 \text{ transitions}}$$

Negligible for Planck!

RESULTS: RECOMBINATION WITH HYDROGEN

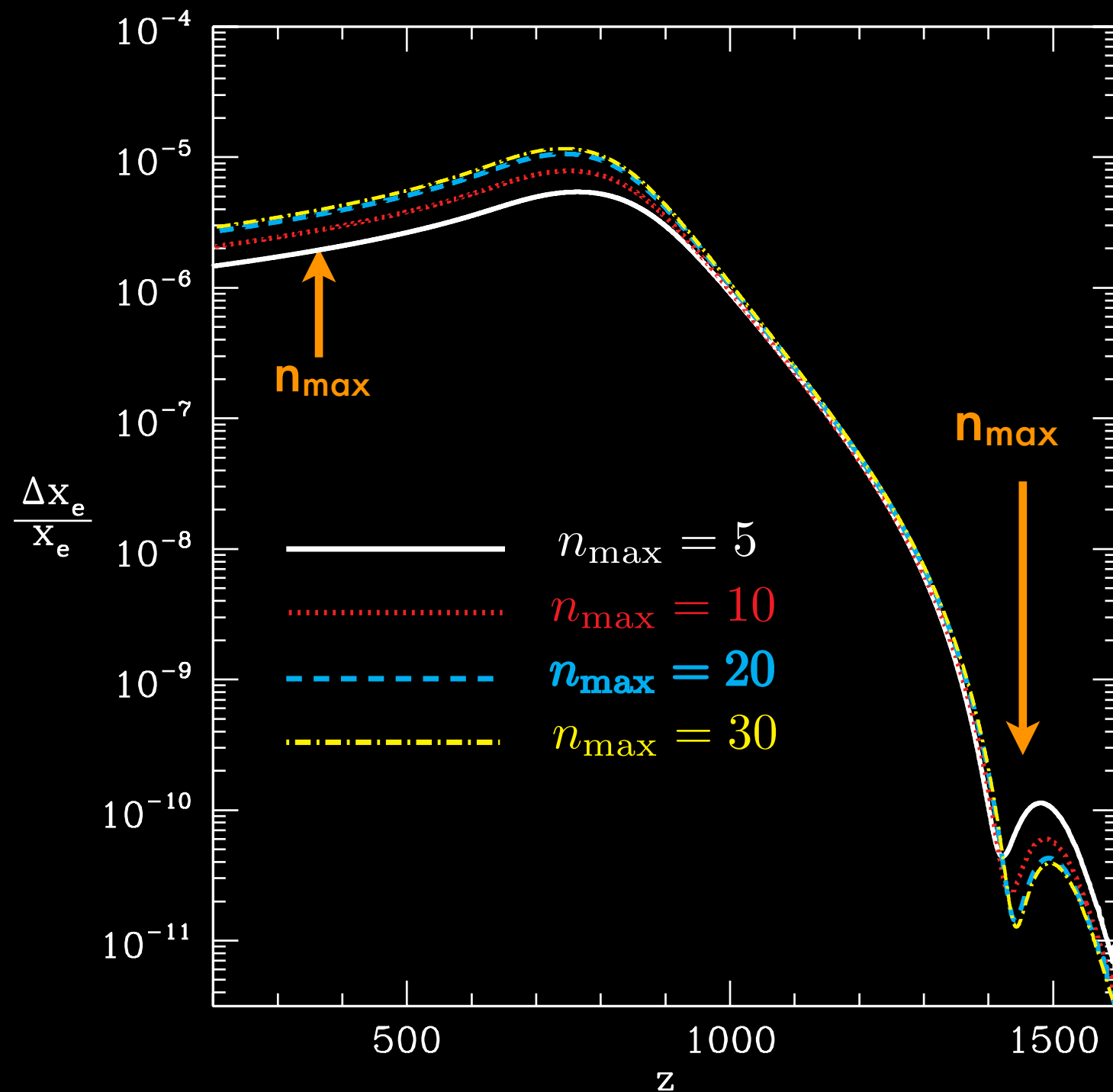


Sub-Dominant decay channel to gs, slows rec down rel. to $n < 5$

$$R_{nd \rightarrow np}^{\text{quad}} = A_{nd \rightarrow 1s} \left(x_{nd} - \frac{5}{3}x_{np} \right)$$

$n \geq 5$, early times

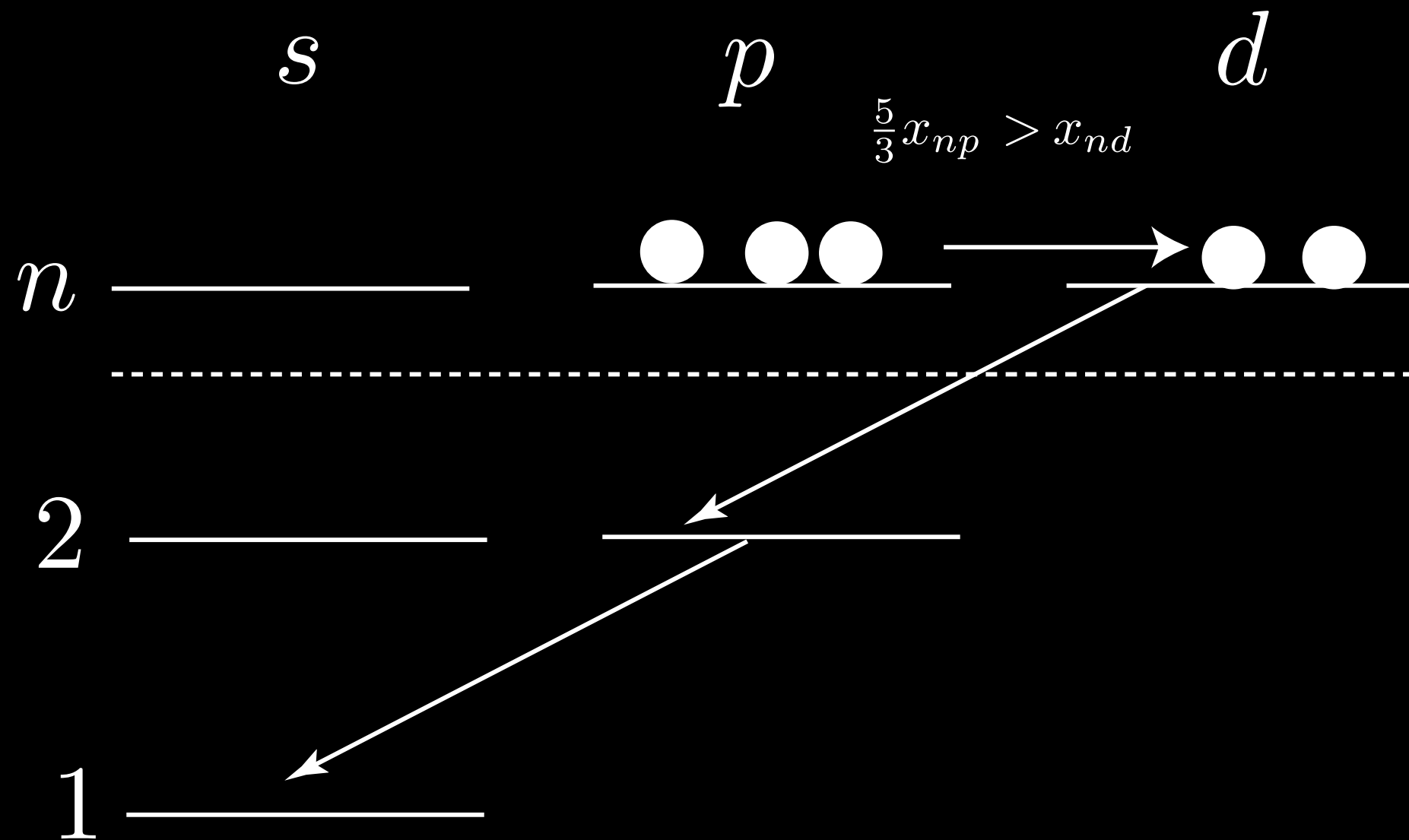
RESULTS: RECOMBINATION WITH HYDROGEN



$$\Delta x_e \equiv x_e|_{\text{no } E2 \text{ transitions}} - x_e|_{\text{with } E2 \text{ transitions}}$$

Negligible for Planck!

RESULTS: RECOMBINATION WITH HYDROGEN

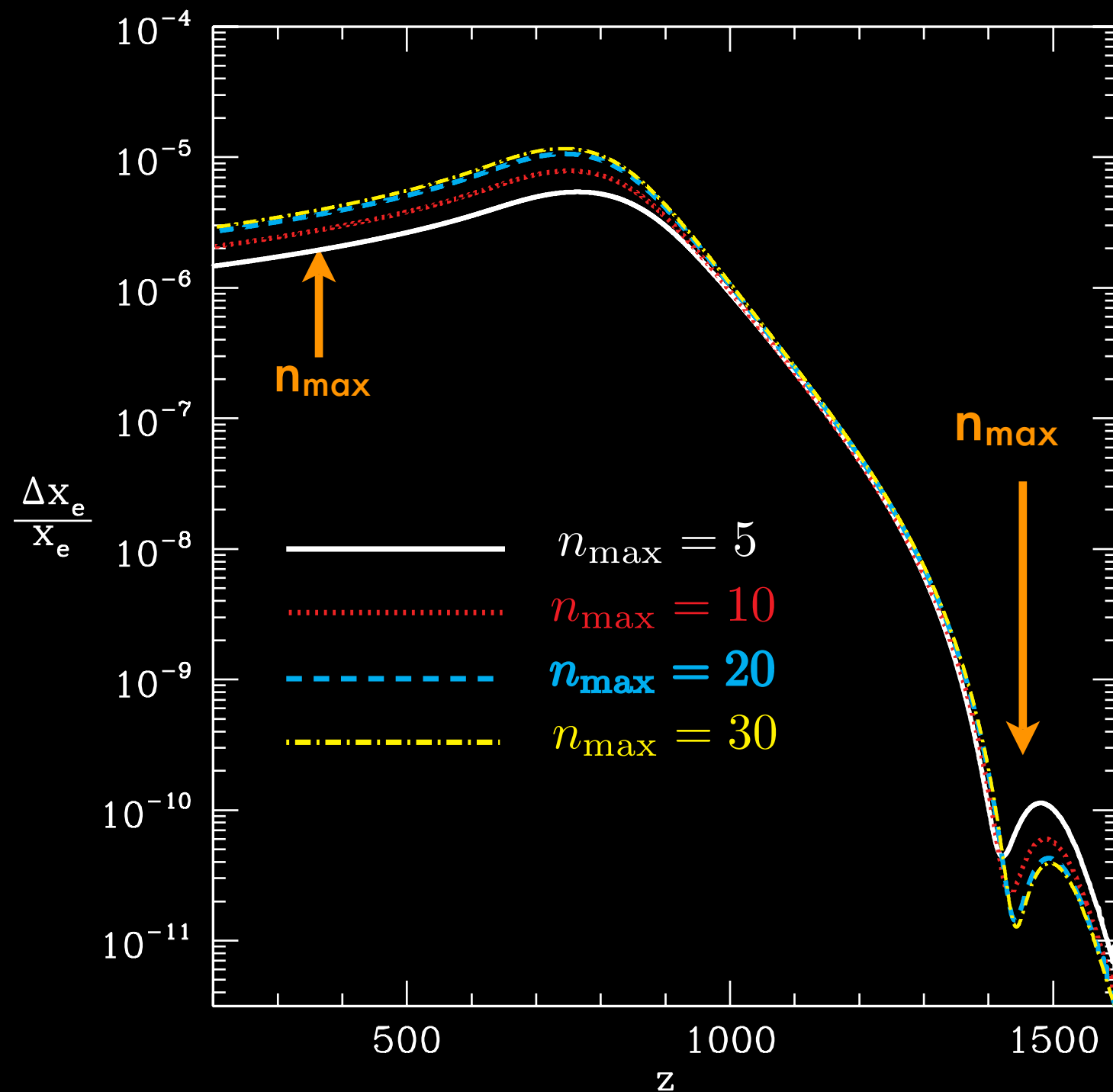


Dominant decay channel to gs, speeds up rec

$$R_{nd \rightarrow np}^{\text{quad}} = A_{nd \rightarrow 1s} \left(x_{nd} - \frac{5}{3}x_{np} \right)$$

All n , late times

RESULTS: RECOMBINATION WITH HYDROGEN

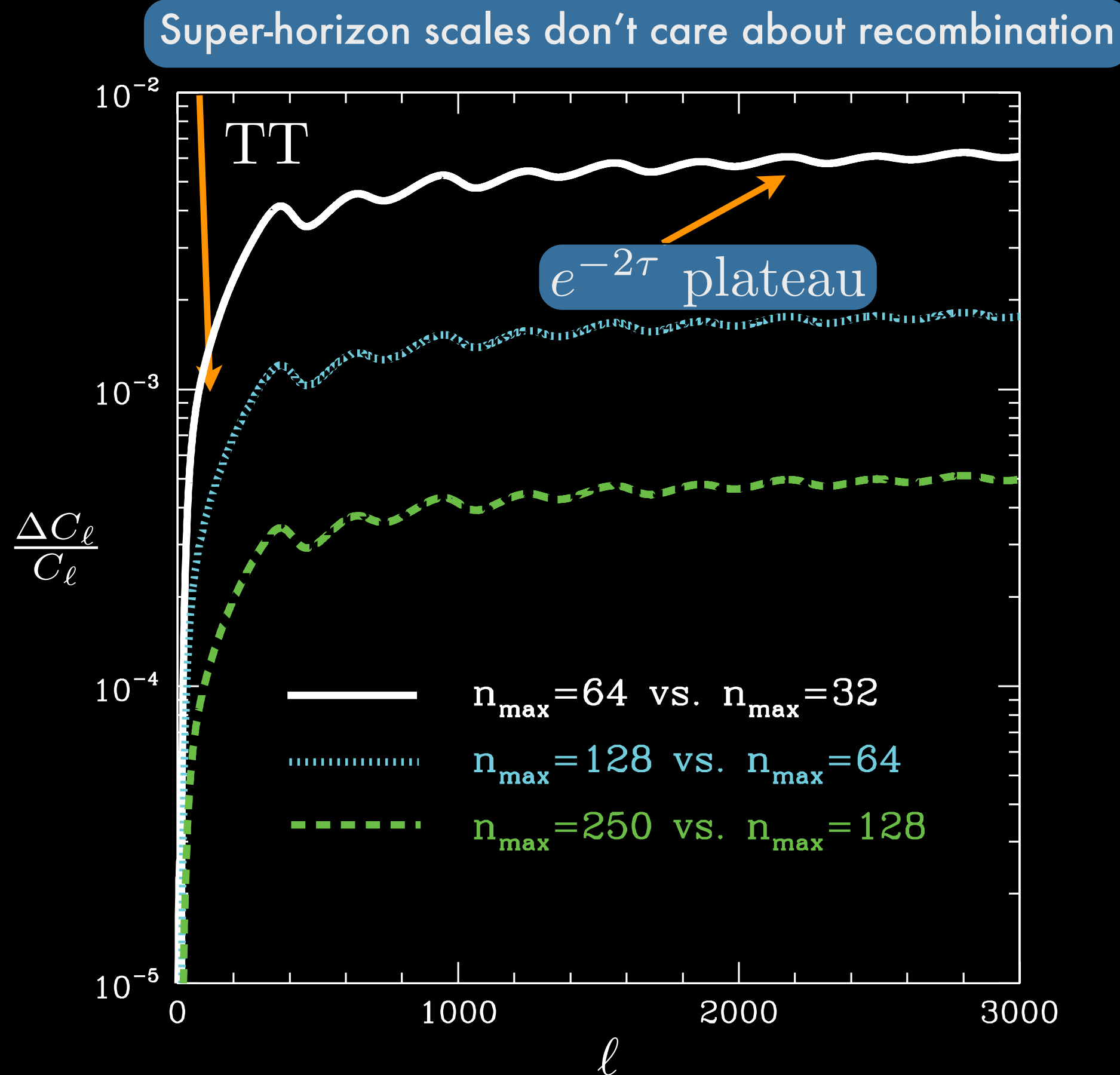


$$\Delta x_e \equiv x_e|_{\text{no } E2 \text{ transitions}} - x_e|_{\text{with } E2 \text{ transitions}}$$

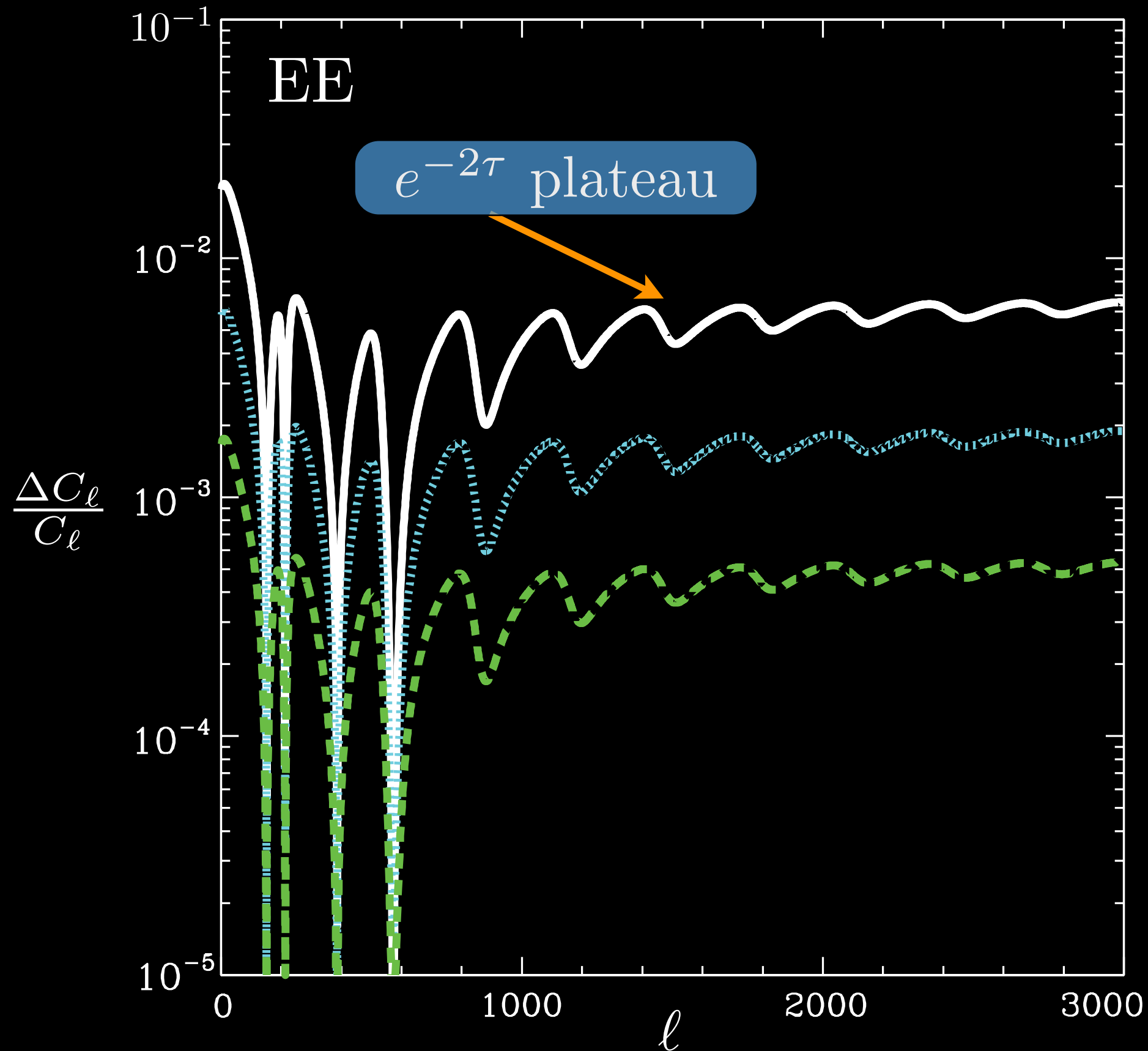
Negligible for Planck!

RESULTS: CMB ANISOTROPIES

RESULTS: TT C_ℓ s WITH HIGH-N STATES

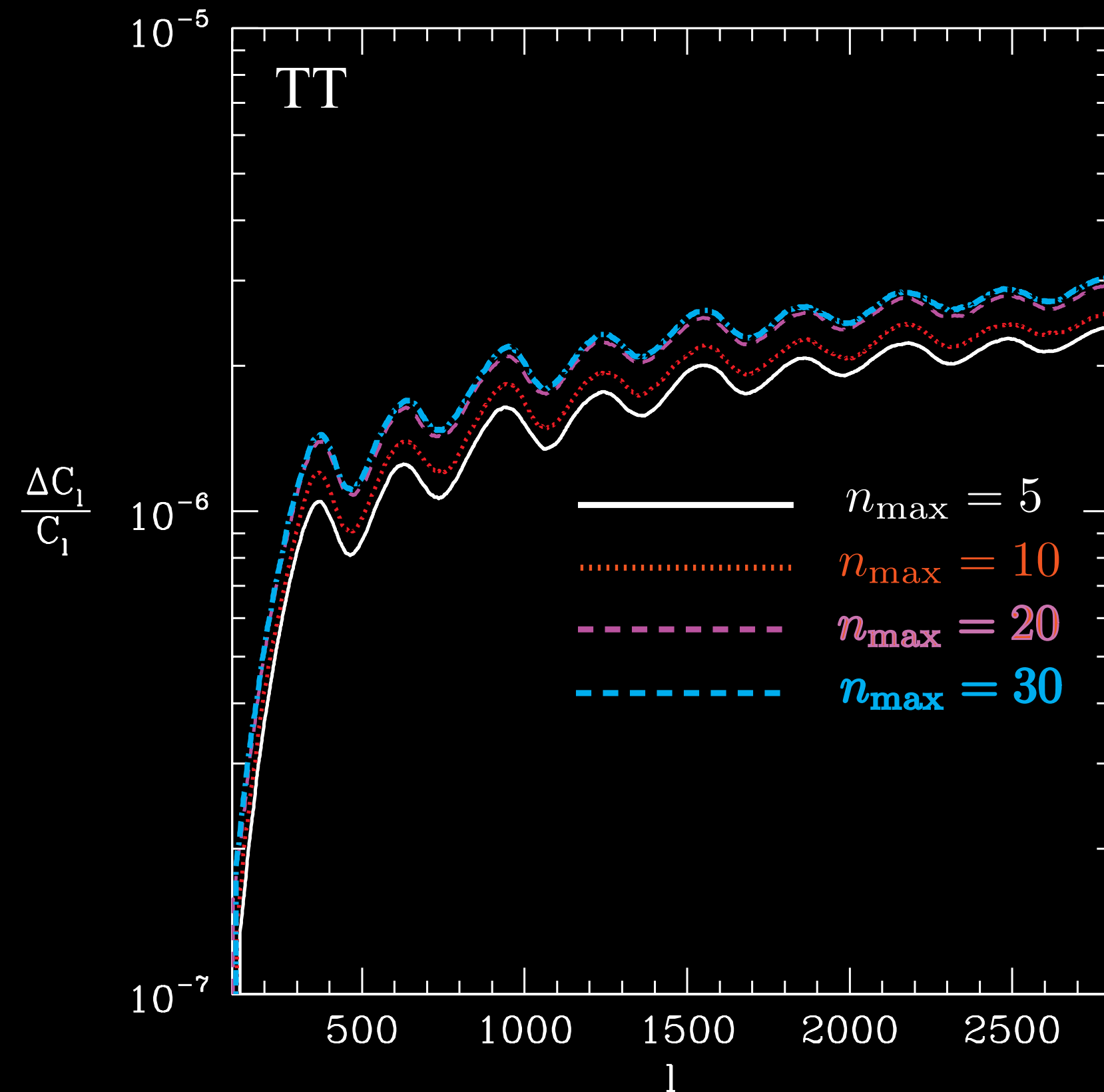


RESULTS: EE C_ℓ s WITH HIGH-N STATES



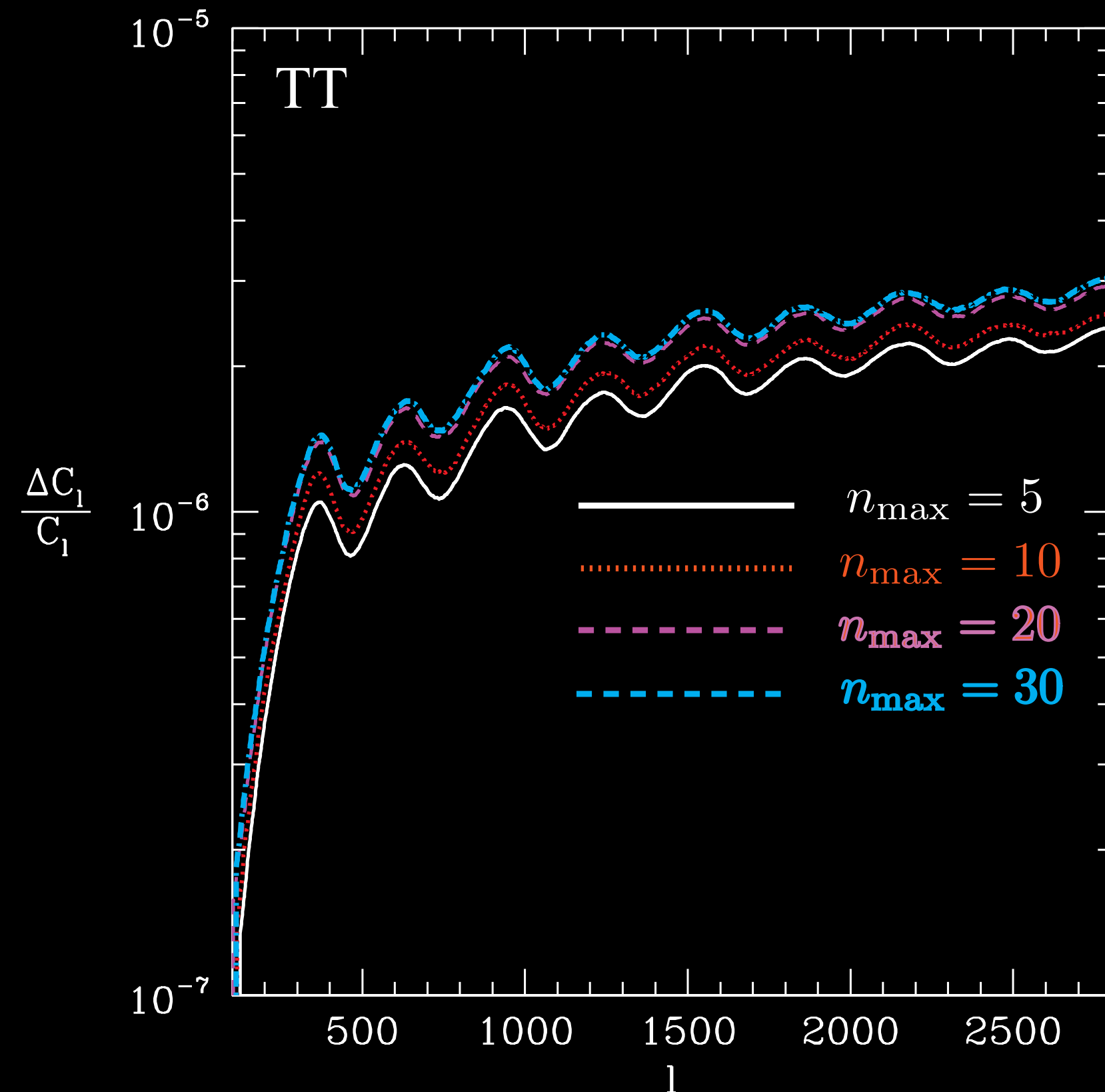
RESULTS: TEMPERATURE (TT) C_l s WITH HYDROGEN QUADRUPOLES,

Bulk of integral from late times, higher $n_{\text{max}} \rightarrow$ lower $x_e \rightarrow$ lower $\tau \rightarrow$ higher $e^{-2\tau} \rightarrow$ higher C_l



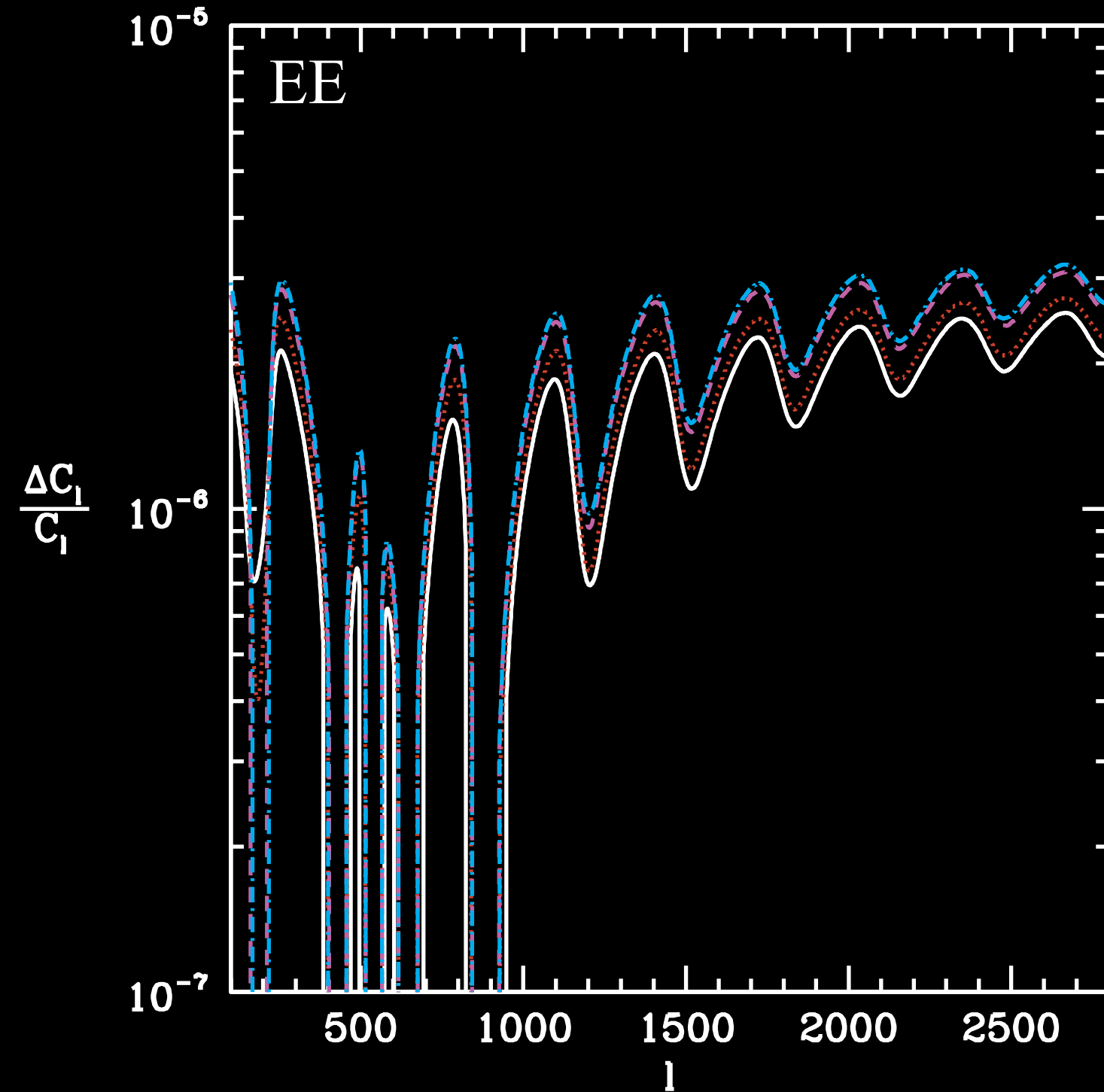
RESULTS: TEMPERATURE (TT) C_l s WITH HYDROGEN QUADRUPOLES,

Bulk of integral from late times, higher $n_{\text{max}} \rightarrow$ lower $x_e \rightarrow$ lower $\tau \rightarrow$ higher $e^{-2\tau} \rightarrow$ higher C_l



Overall effect is negligible for CMB experiments!

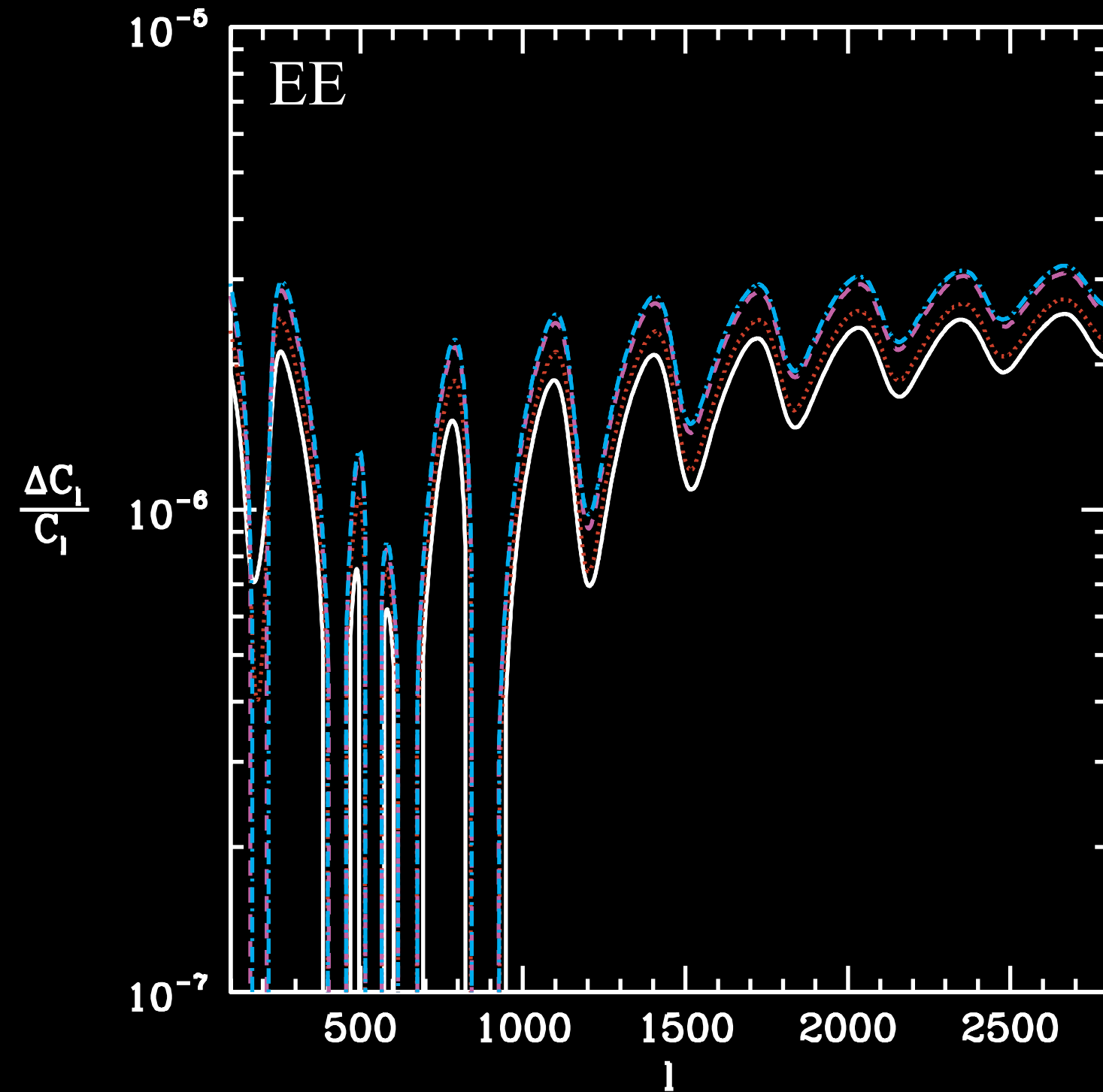
RESULTS: POLARIZATION (EE) C_l s WITH HYDROGEN QUADRUPOLES



$$\Delta C_l \equiv C_l|_{\text{with } E2 \text{ transitions}} - C_l|_{\text{no } E2 \text{ transitions}}$$

Bulk of integral from late times, higher $n_{\text{max}} \rightarrow$ lower $x_e \rightarrow$ lower $\tau \rightarrow$ higher $e^{-2\tau} \rightarrow$ higher C_l

RESULTS: POLARIZATION (EE) C_l s WITH HYDROGEN QUADRUPOLES

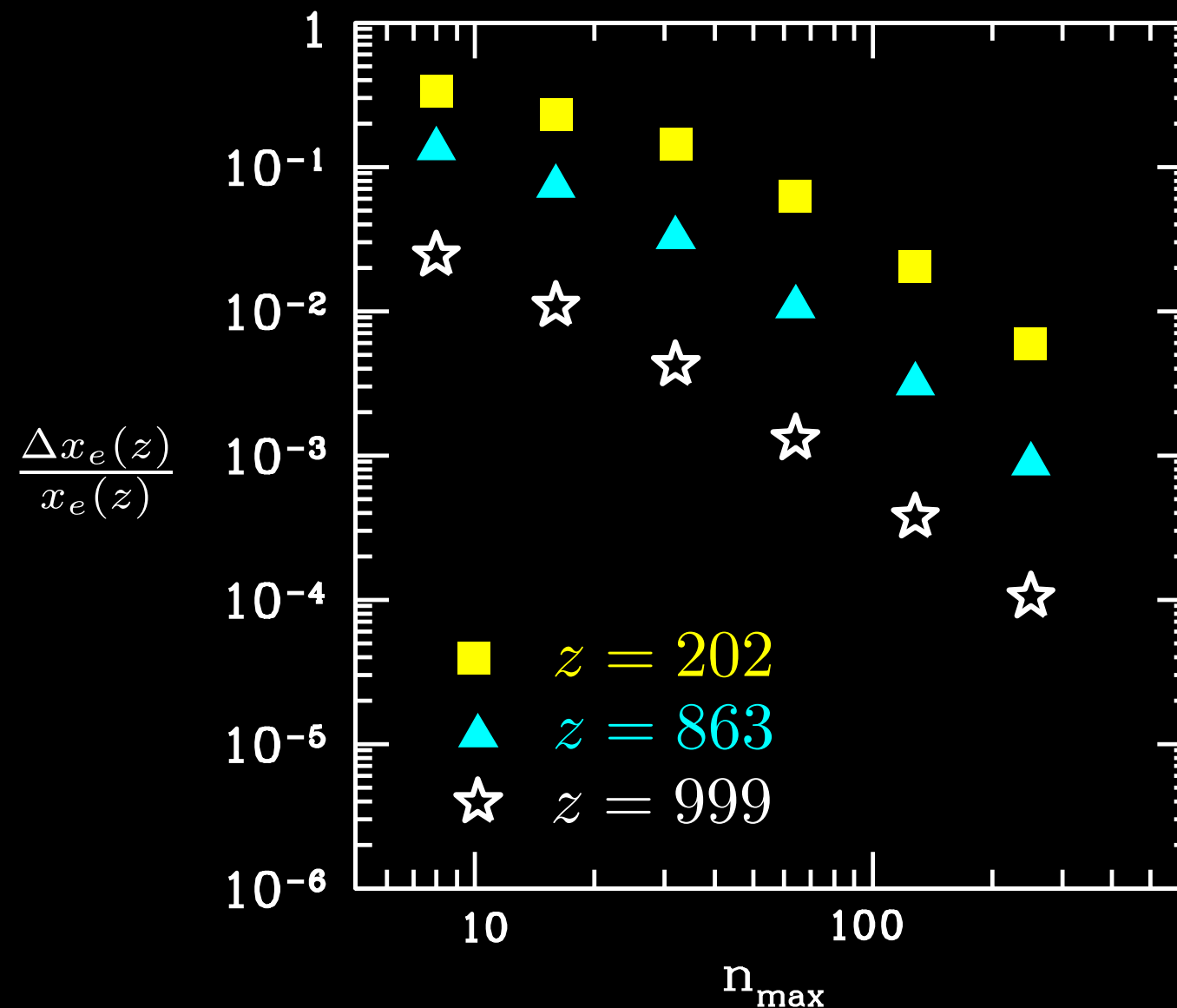


$$\Delta C_l \equiv C_l|_{\text{with } E2 \text{ transitions}} - x_e|_{\text{no } E2 \text{ transitions}}.$$

Overall effect is negligible for upcoming CMB experiments!

Bulk of integral from late times, higher $n_{\text{max}} \rightarrow$ lower $x_e \rightarrow$ lower $\tau \rightarrow$ higher $e^{-2\tau} \rightarrow$ higher C_l

CONVERGENCE



- * Relative error well described by power law at high n_{\max}

$$\Delta x_e / x_e \propto n_{\max}^{-1.9}$$

- * Can extrapolate to absolute error

THE UPSHOT FOR COSMOLOGY

- ✦ Can explore effect on overall Planck likelihood analysis

$$Z^2 = \sum_{ll', X, Y} F_{ll'} \Delta C_l^X \Delta C_l^Y$$

$$Z = 1.8 \text{ if } n_{\text{max}} = 64,$$

$$Z = 0.50 \text{ if } n_{\text{max}} = 128,$$

$$Z = 0.14 \text{ if } n_{\text{max}} = 250.$$

CONCLUSIONS

- * RecSparse: a new tool for MLA recombination calculations (*arXiv:0911.1359*)
- * Highly excited levels ($n \sim 64$ and higher) are relevant for Planck CMB data analysis
- * E2 transitions in H are not relevant for Planck CMB data analysis

FUTURE WORK

- * Include line-overlap
- * Develop cutoff method for excluded levels
- * Generalize **RecSparse** to calc. rec. line. spectra
- * Compute and include collisional rates
- * Monte-Carlo analyses
- * Cosmological masers

Bound-free rates

- * Using continuum wave functions, bound-free rates are obtained (Burgess 1957)
- * Bound-free matrix elements satisfy a convenient recursion relation:
- Matrix elements compared with Burgess 1965 (5 digits) and with WKB approximation (5%):
- At each temperature, thermal recombination/ionization rates obtained using 11-point Newton-Cotes formula, agreement with Burgess to 4 published digits

BB Rate coefficients: verification

- WKB estimate of matrix elements $\rho(n'l', nl) = a_0 n^2 \int_{-\pi}^{\pi} d\tau e^{i\Omega\tau} (1 + \cos\eta)$

Fourier transform of classical orbit!
Application of correspondence principle!

$$\Omega = \omega_n - \omega_{n'}$$

$$r = r_{\max} (1 + \cos \eta) / 2$$

$$\tau = \eta + \sin \eta$$

$$\rho^{\text{dipole}}(n, l, n', l') = \frac{n_c^2}{s} \left\{ J_{s-1}(s\epsilon) - \frac{1 \mp \sqrt{1 - \epsilon^2}}{\epsilon} J_s(s\epsilon) \right\}$$

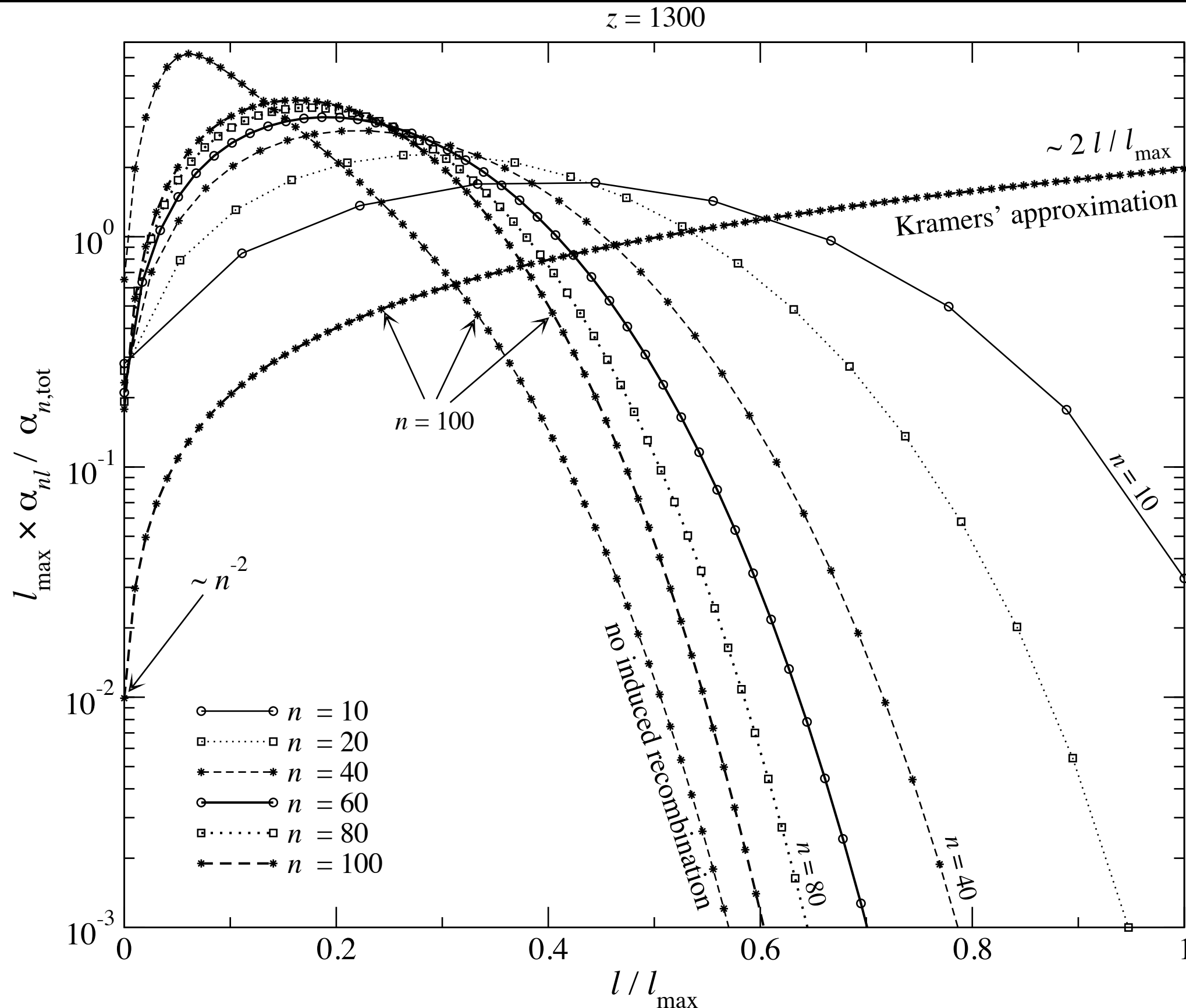
$$\epsilon = \left(1 - \frac{l(l+1)}{n^2} \right)^{1/2}$$

$$s = n - n'$$

- Radial matrix elements checked against WKB (10%), published rates of Brocklehurst (1971), Green, Rush, and Chandler (1967) (agreement to their published 4 digits)

DEVIATIONS FROM BOLTZMANN EQ: L-SUBSTATES

Chluba/Rubino-Martin/Sunyaev 2006



Quadrupole rates: basic formalism

$$\star A_{n_a, l_a \rightarrow n_b, l_b}^{\text{quad}} = \frac{\alpha}{15} \frac{1}{2l_a + 1} \frac{\omega_{ab}^5}{c^4} \left\langle l_a || C^{(2)} || l_b \right\rangle^2 \left({}^2 R_{n_b l_b}^{n_a l_a} \right)^2$$

- Reduced matrix element evaluated using Wigner 3J symbols:

$$\left\langle l_a || C^{(2)} || l_b \right\rangle = (-1)^{l_a} \sqrt{(2l_a + 1)(2l_b + 1)} \begin{pmatrix} l_a & 2 & l_b \\ 0 & 0 & 0 \end{pmatrix}$$

- Radial matrix element evaluated using operator methods

$${}^2 R_{n_b l_b}^{n_a l_a} \equiv \int_0^\infty r^4 R_{n_a l_a}(r) R_{n_b l_b}(r) dr$$

Quadrupole rates: Operator algebra

✱ Radial Schrödinger equation can be factored to yield:

$$^{-}\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 - l \left(\frac{d}{dr} + \frac{l+1}{r} \right) \right] \quad ^{+}\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 + l \left(\frac{d}{dr} - \frac{l-1}{r} \right) \right]$$

$$\begin{aligned} ^{-}\Omega_{nl} R_{nl}(r) &= R_{n \ l-1}(r) \\ ^{+}\Omega_{n \ l-1} R_{nl}(r) &= R_{nl}(r) \end{aligned} \quad A_{nl} = \frac{\sqrt{n^2 - l^2}}{nl}$$

✱ This algebra can be applied to radial matrix elements:

Quadrupole rates: Operator algebra

✱ Radial Schrödinger equation can be factored to yield:

$$^{-}\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 - l \left(\frac{d}{dr} + \frac{l+1}{r} \right) \right] \quad ^{+}\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 + l \left(\frac{d}{dr} - \frac{l-1}{r} \right) \right]$$

$$\begin{aligned} ^{-}\Omega_{nl} R_{nl}(r) &= R_{n \ l-1}(r) \\ ^{+}\Omega_{n \ l-1} R_{nl}(r) &= R_{nl}(r) \end{aligned} \quad A_{nl} = \frac{\sqrt{n^2 - l^2}}{nl}$$

✱ This algebra can be applied to radial matrix elements:

$$^2R_{n' \ l-1}^{n \ l-1} = \frac{1}{A_{nl}} \left\{ A_{n'l}^2 R_{n'l}^{nl} + 2^{(1)}R_{n' \ l-1}^{nl} \right\} \quad ^{(2)}R_{n' \ n'-1}^{n \ n'-1} = \frac{2nn'}{\sqrt{n^2 - n'^2}} ^{(1)}R_{n \ n'-1}^{nn'}$$

Diagonal!

Quadrupole rates: Operator algebra

✱ Radial Schrödinger equation can be factored to yield:

$$^{-}\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 - l \left(\frac{d}{dr} + \frac{l+1}{r} \right) \right] \quad ^{+}\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 + l \left(\frac{d}{dr} - \frac{l-1}{r} \right) \right]$$

$$\begin{aligned} ^{-}\Omega_{nl} R_{nl}(r) &= R_{n \ l-1}(r) \\ ^{+}\Omega_{n \ l-1} R_{nl}(r) &= R_{nl}(r) \end{aligned} \quad A_{nl} = \frac{\sqrt{n^2 - l^2}}{nl}$$

✱ This algebra can be applied to radial matrix elements:

$$l(2l+3)A_{n'l}^{(2)} R_{n' \ l-1}^{n \ l+1} = (2l+1)(l+2)A_{n \ l+2}^{(2)} R_{n'l}^{n \ l+2} + 2(l+1)A_{n' \ l+1}^{(2)} R_{n' \ l+1}^{n \ l+1} + 2(2l+1)(3l+5)^{(1)} R_{n'l}^{n \ l+1} \quad (1 \leq l \leq n' - 1)$$

$$^{(2)} R_{n' \ n'+1}^{n \ n'-1} = 0$$

$$^{(2)} R_{n' \ n'-1}^{n \ n'+1} = (-1)^{n-n'} 2^{2n'+4} \left[\frac{(n+n'+1)!}{(n-n'-2)!(2n'-1)!} \right]^{1/2} n' (nn')^{n'+3} \frac{(n-n')^{n-n'-3}}{(n+n')^{n+n'+3}}$$

Off-diagonal!