Cosmological Hydrogen Recombination: The effect of extremely high-n states

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in collaboration with Christopher M. Hirata

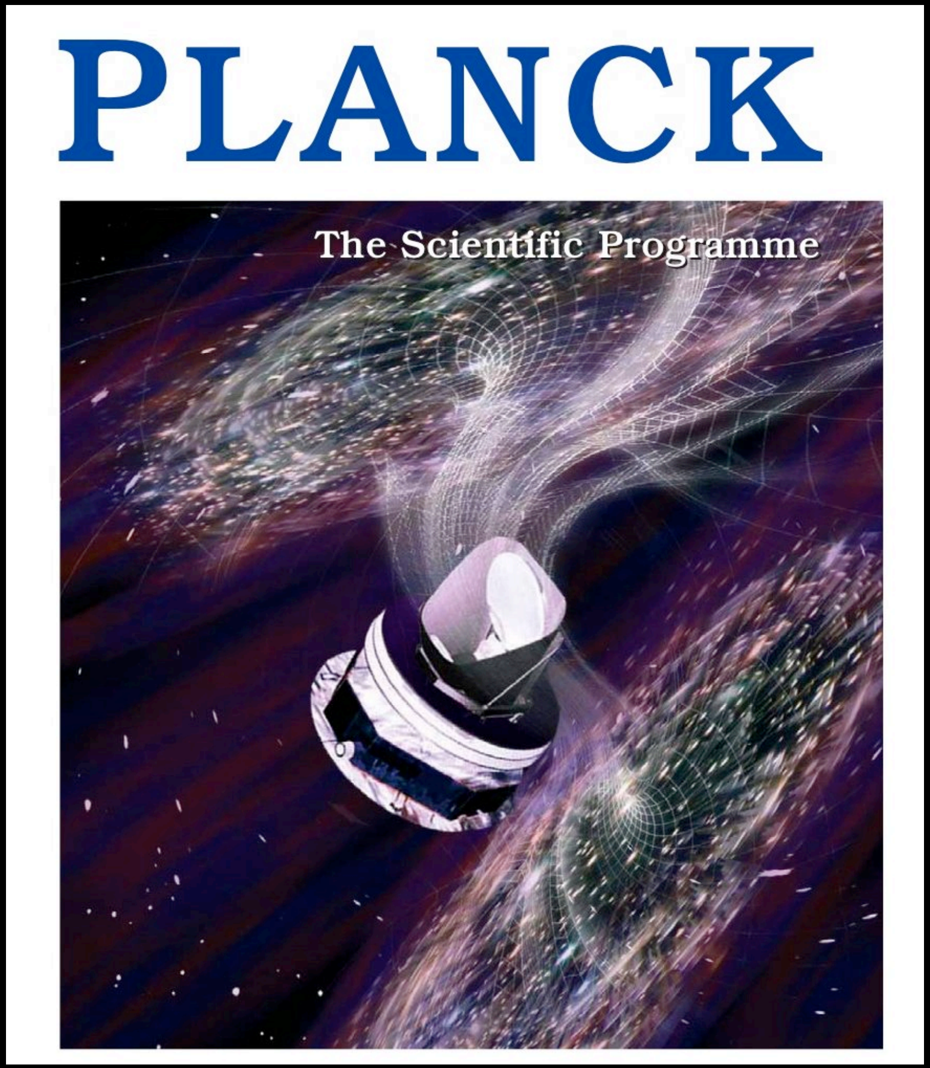
FermiLab Seminar

11/5/09

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

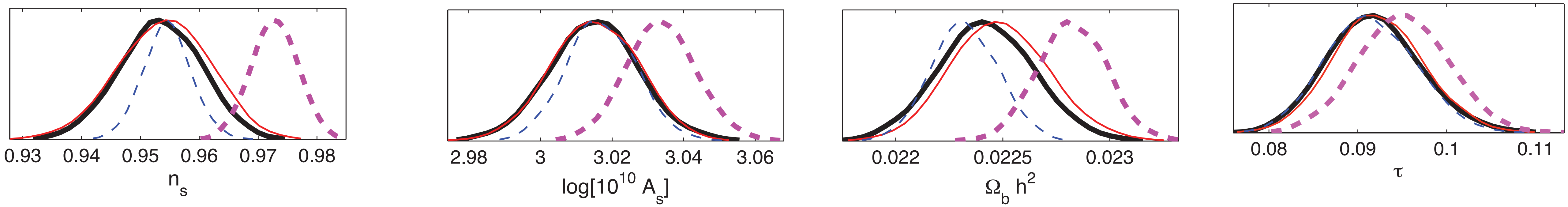


- Planck (launched May 2009) will make cosmic-variance limited CMB anisotropy measurements up to l~2500 (T), and l~1500 (E)

- 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

- Planck uncertainty forecasts using MCMC



$$\mathrm{P(k)}=\mathrm{A}_s\,(k\eta_0)^{n_s-1}$$

- 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

$$\mathrm{n}_s = 1 - 4\epsilon + 2\eta \qquad \epsilon = \frac{m_{\mathrm{pl}}^2}{16\pi}\left[\frac{V'(\phi)}{V(\phi)}\right]^2 \qquad \mathrm{A}_s^2 = \frac{32}{75}\frac{V}{m_{\mathrm{pl}}^4\epsilon}\bigg|_{k_{\mathrm{pivot}}=aH}$$

CAVEAT EMPTOR:

Need to do eV physics right to infer anything about 10^{15} GeV physics!

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RECOMBINATION, INFLATION, AND REIONIZATION

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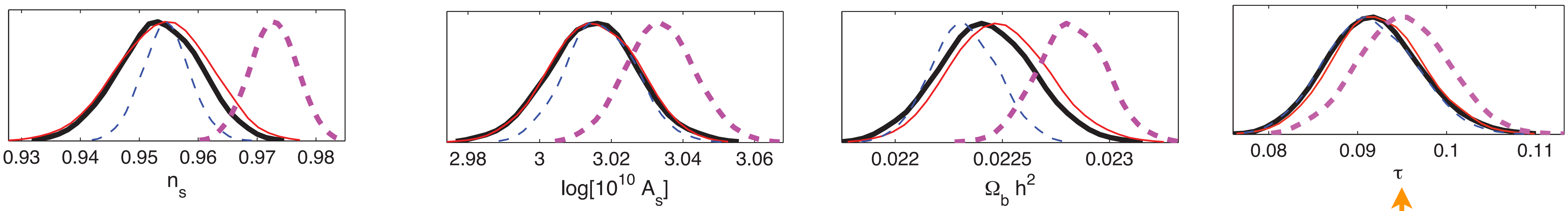


$$P(k) = A_s \, (k\eta_0)^{n_s - 1}$$

Bad recombination history yields biased inferences about reionization

WHO CARES?
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

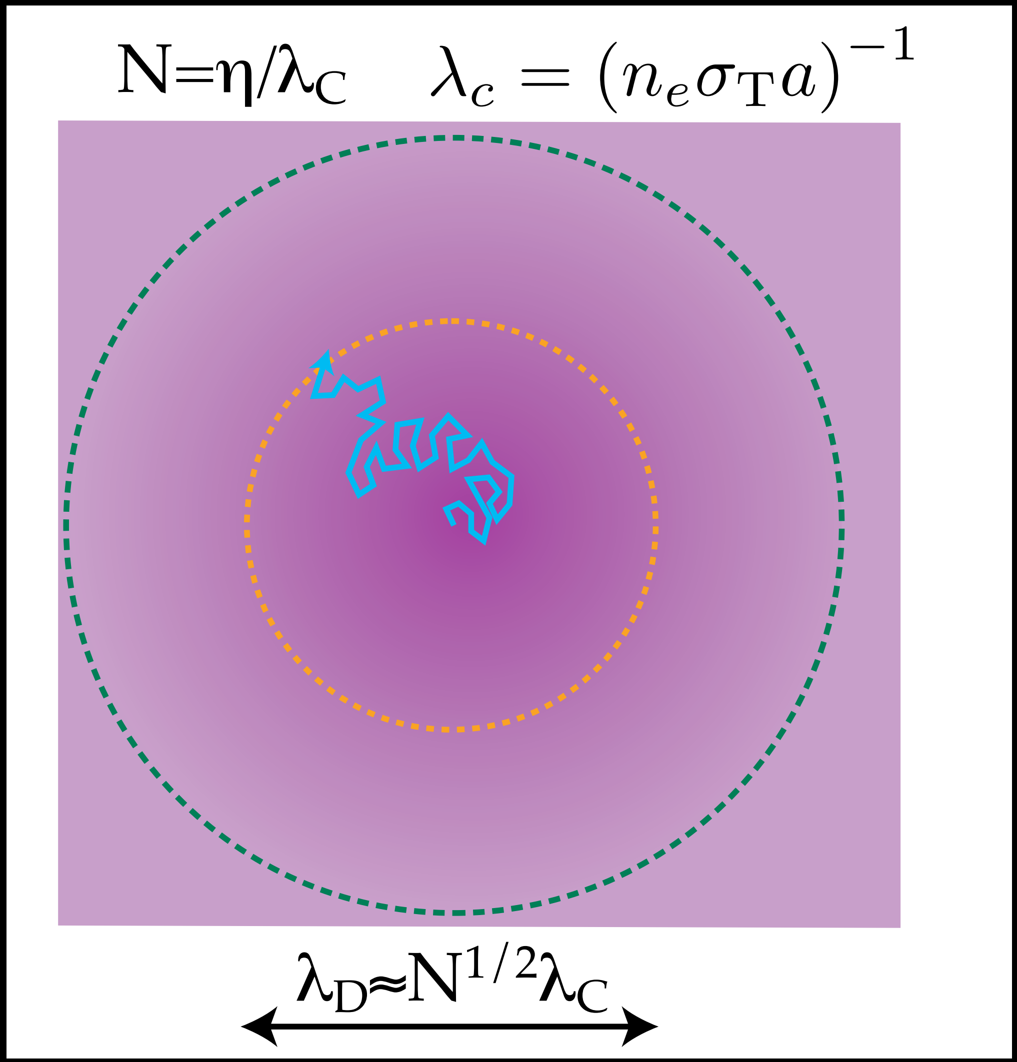
$$g(\tau) = \dot{\tau} e^{-\tau}$$

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

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

$$\tau(z) = \int_0^{\eta(z)} n_e \sigma_T a(\eta') d\eta'$$

WHO CARES?
THE SILK DAMPING TAIL

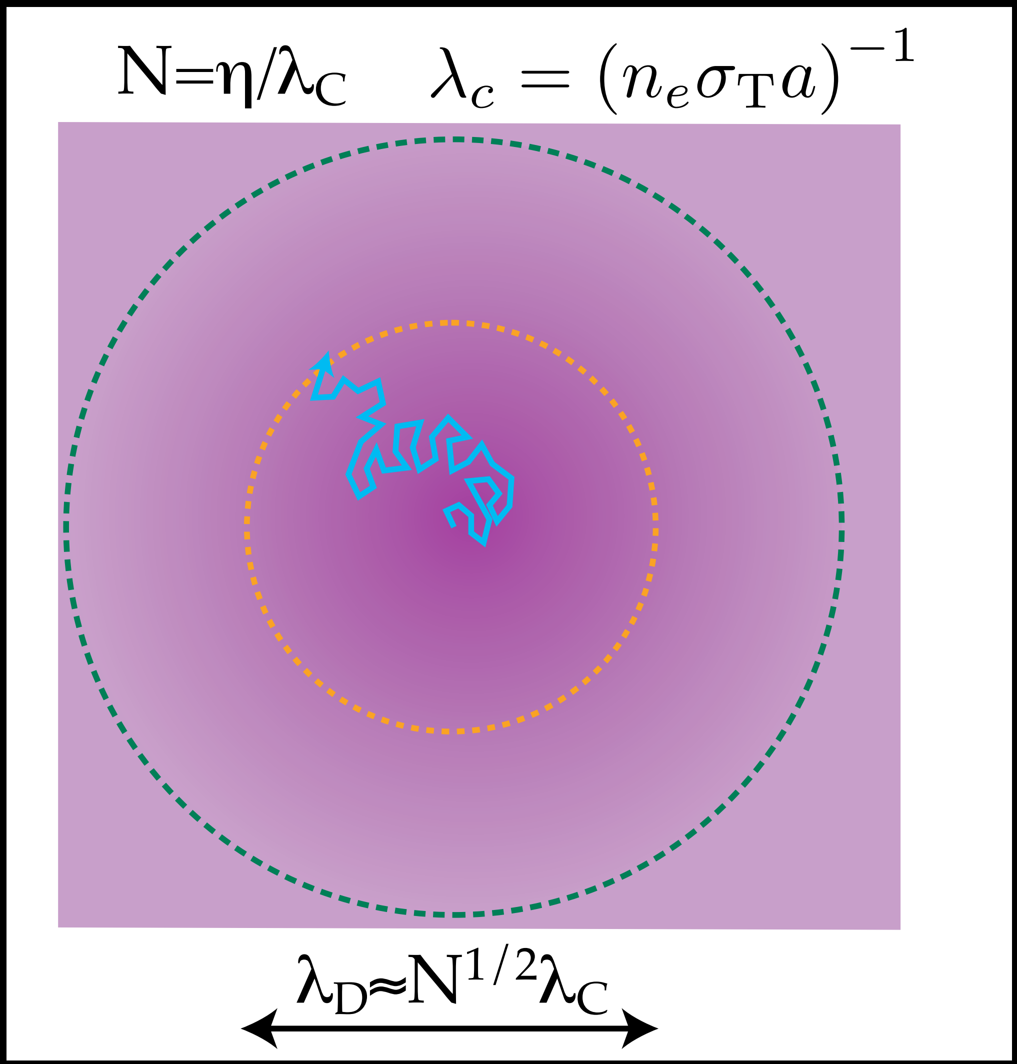


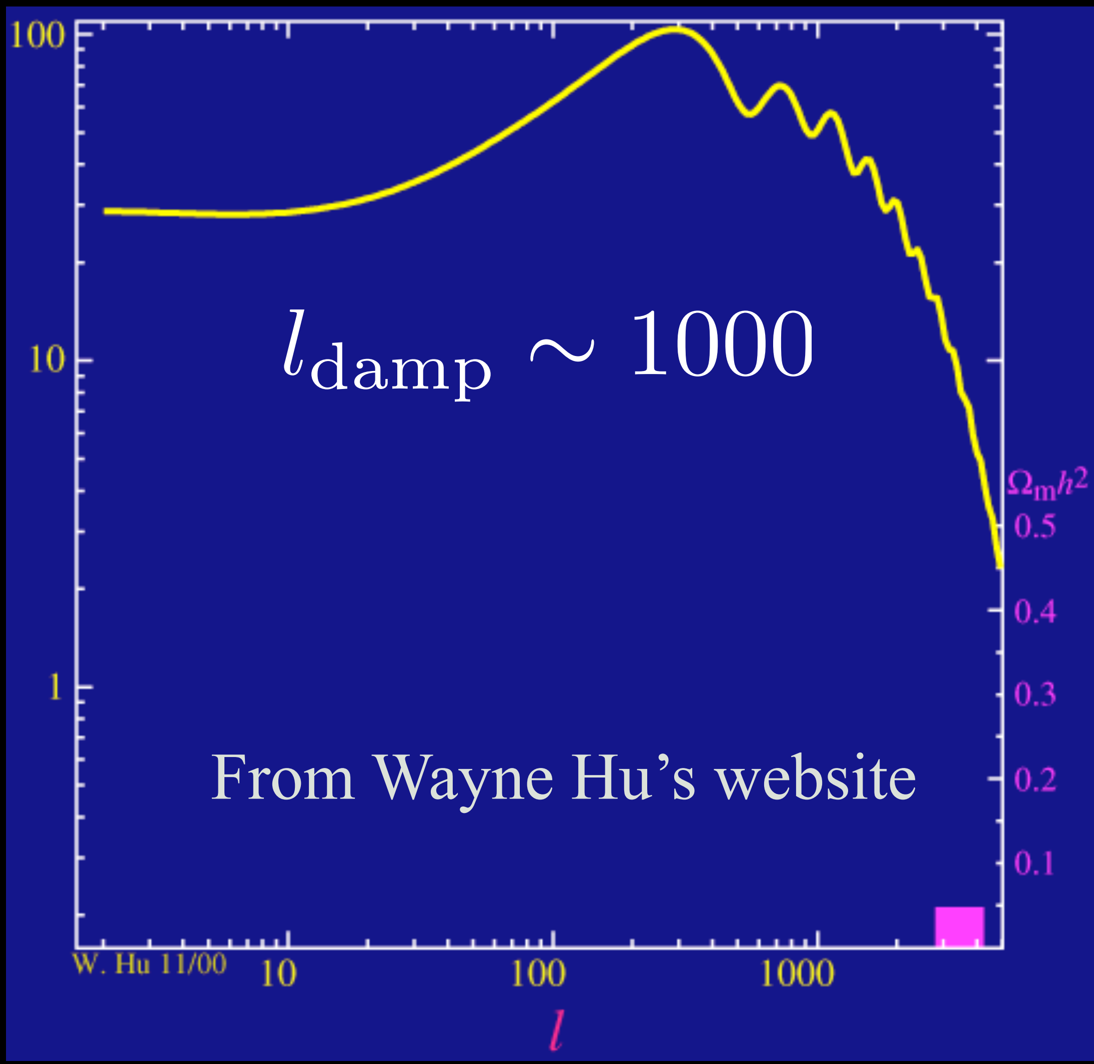
$$l_{\rm damp} \sim 1000$$

From Wayne Hu's website

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

Who Cares? The Silk Damping Tail





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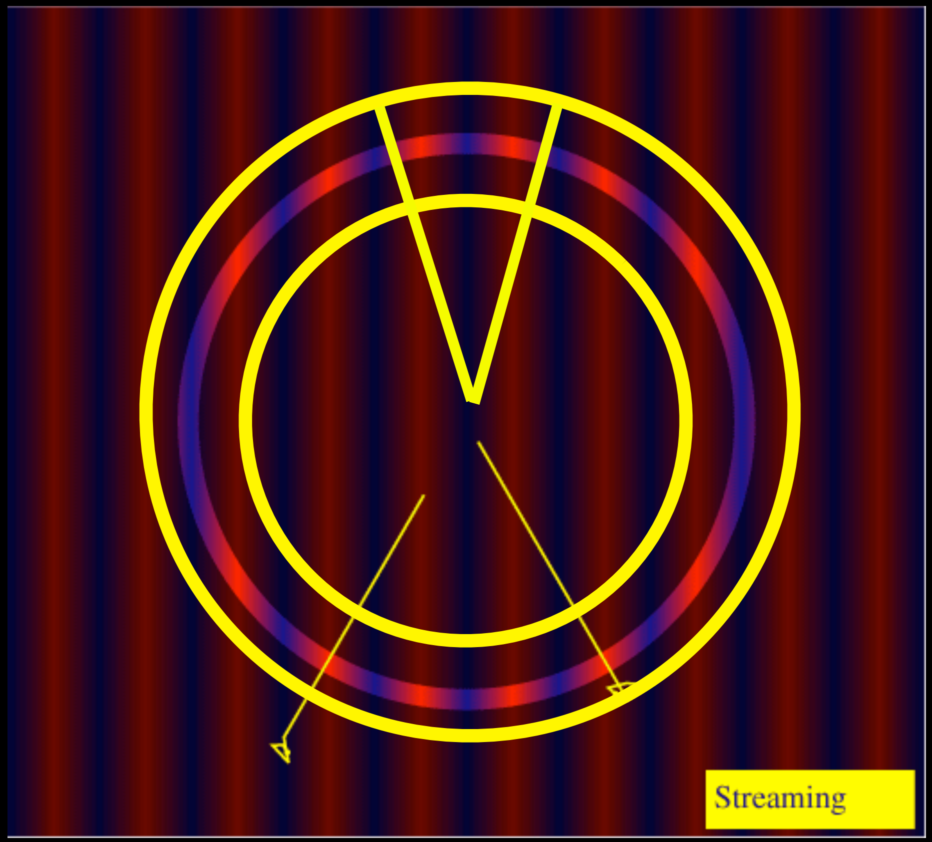
WHO CARES? FINITE THICKNESS OF THE SLSS



* Additional damping of form

$$|\Theta_l\left(\eta_0, k\right)| \rightarrow |\ \Theta_l\left(\eta_0, k\right)|\, e^{-\sigma^2 \eta_{\rm rec}^2 k^2}$$

WHO CARES? CMB POLARIZATION

- From Wayne Hu's website

- Need to scatter quadrapole to polarize CMB

$$\Theta_l^P(k) = \int d\eta \dot{\tau} e^{-\tau(\eta)} \Theta_{T,2}(k,\eta) \frac{l^2}{(k\eta)^2} j_l(k\eta)$$

- Need time to develop a quadrapole

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

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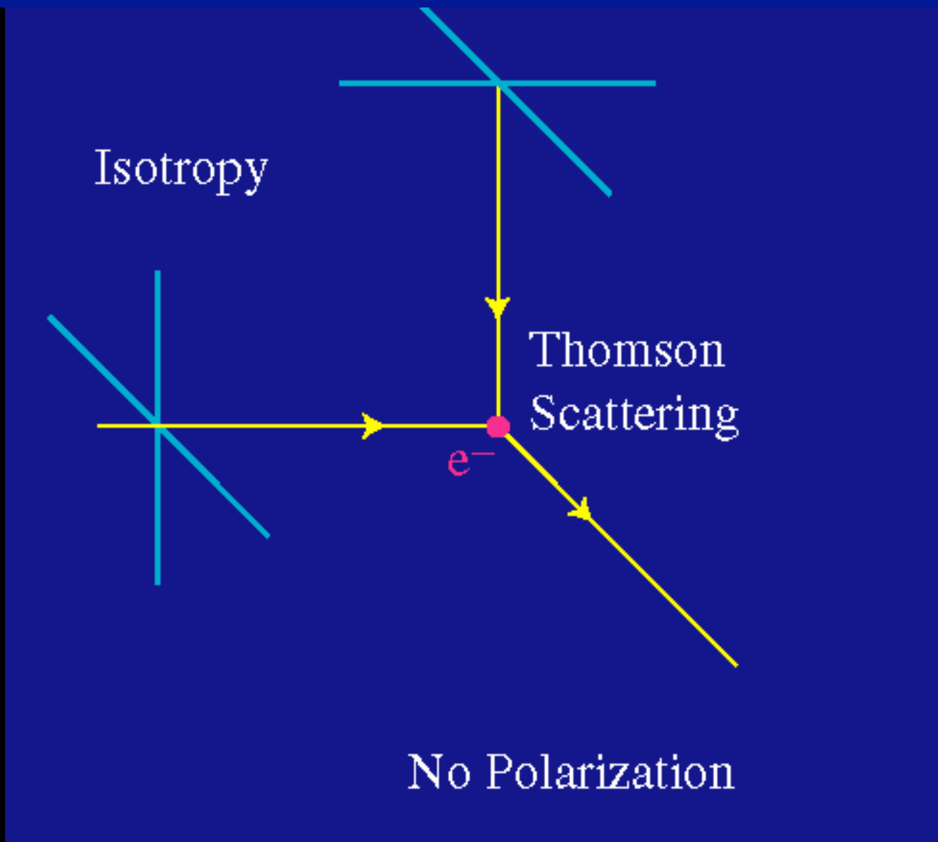
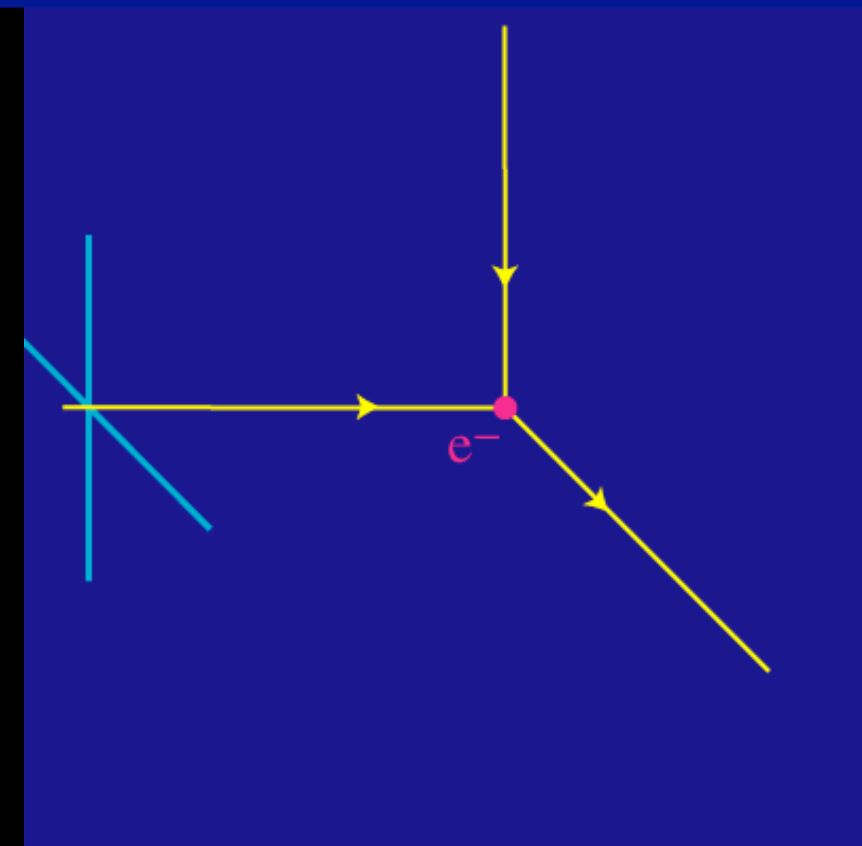


✳ From Wayne Hu's website



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WHO CARES?
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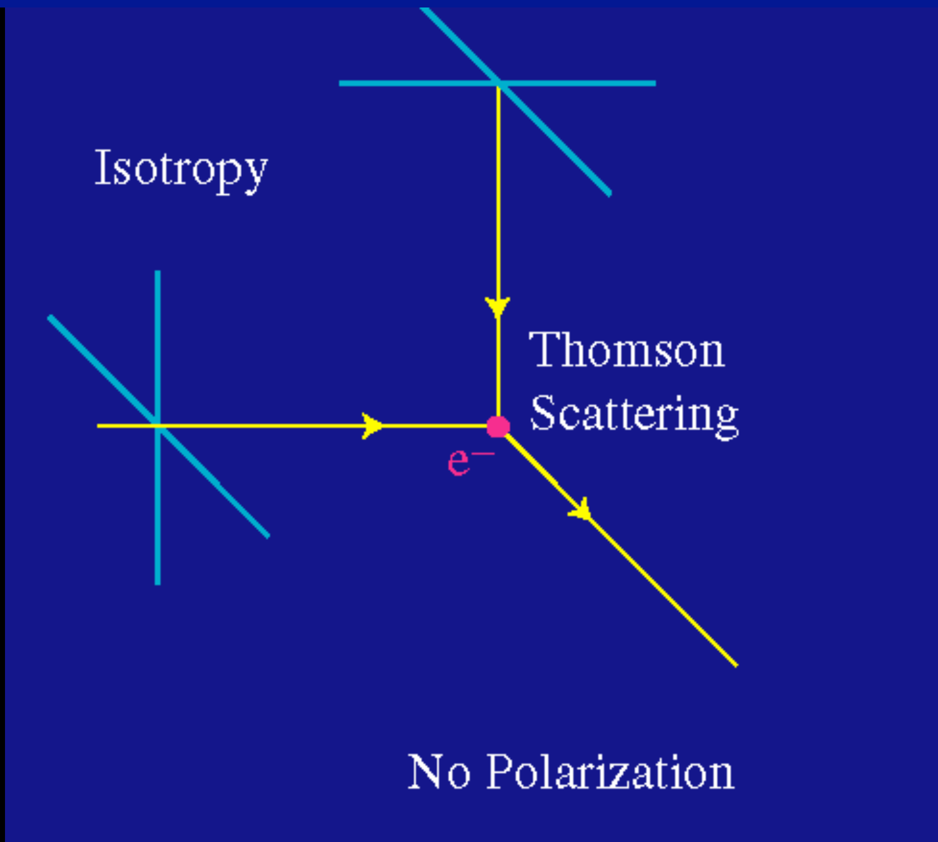

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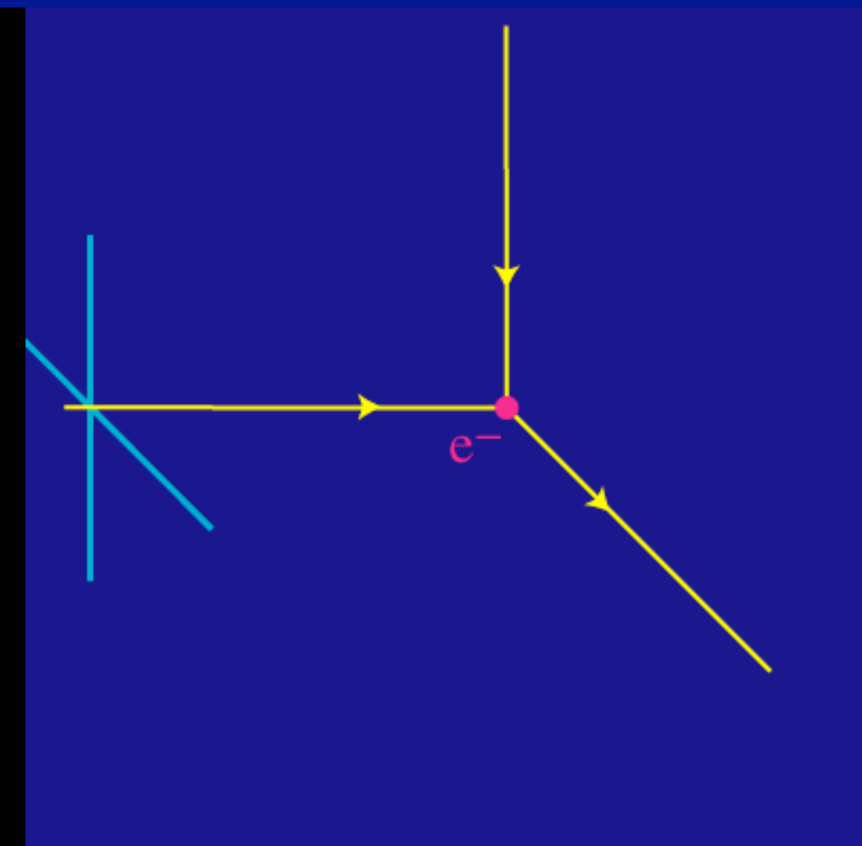

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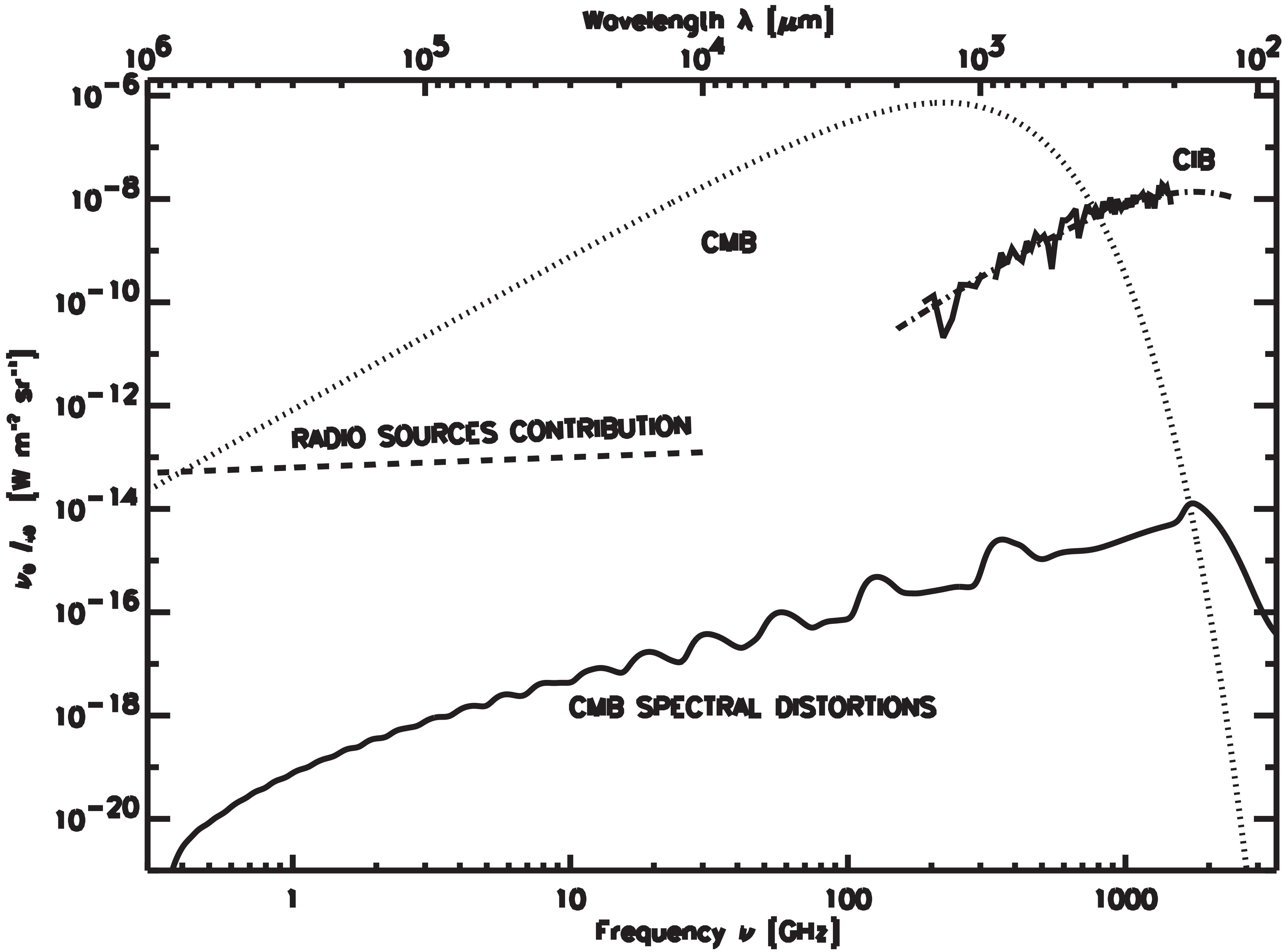
WHO CARES?
SPECTRAL DISTORTIONS FROM RECOMBINATION



SAHA EQUILIBRIUM IS INADEQUATE

$$p + e^- \leftrightarrow H^{(n)} + \gamma^{(nc)}$$

✳ Chemical equilibrium does reasonably well predicting "moment of recombination"

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

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

✳Further evolution falls prey to reaction freeze-out

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

BOTTLENECKS/ESCAPE ROUTES

BOTTLENECKS

✳ Ground state recombinations are ineffective

$$\tau^{-1}_{c\rightarrow 1s} = 10^{-1}\ \mathrm{s}^{-1} \gg H \simeq 10^{-12}\ \mathrm{s}^{-1}$$

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

$$\tau^{-1}_{2p\rightarrow 1s} = 10^{-2}\ \mathrm{s}^{-1} \gg H \simeq 10^{-12}\ \mathrm{s}^{-1}$$

ESCAPE ROUTES (e.g. n=2)

✳ Two-photon processes

$$H^{2s} \rightarrow H^{1s} + \gamma + \gamma \qquad \boldsymbol{\Lambda}_{\mathrm{2s}\rightarrow \mathrm{1s}} = \mathbf{8.22}\ \mathrm{s}^{-1}$$

✳ Redshifting off resonance

$$R \sim \left(n_{\mathrm{H}}\lambda_\alpha^3\right)^{-1}\left(\frac{\dot{a}}{a}\right)$$

THE PEEBLES PUNCHLINE

✳ Only n=2 bottlenecks are treated

✳Net Rate is suppressed by   bottleneck vs. escape factor

$$-\frac{dxe}{dt} = \mathcal{S} \sum_{n,l>1s} \alpha_{nl}\left(T\right) \left\{ n x_e^2 - x_{1s} e^{-\frac{B_1}{kT}} \left(\frac{2\pi m_e kT}{h^2}\right)^{3/2} \right\}$$

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The Peebles Model

- Net Rate is suppressed by bottleneck vs. escape factor

$$\mathcal{C} = \frac{\frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + \Lambda_{2s\to 1s}}{\frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + (\Lambda_{2s\to 1s} + \beta_c)}$$

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Redshifting term

13

THE PEEBLES MODEL

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2γ term

13

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Ionization Term

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Ionization Term

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

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

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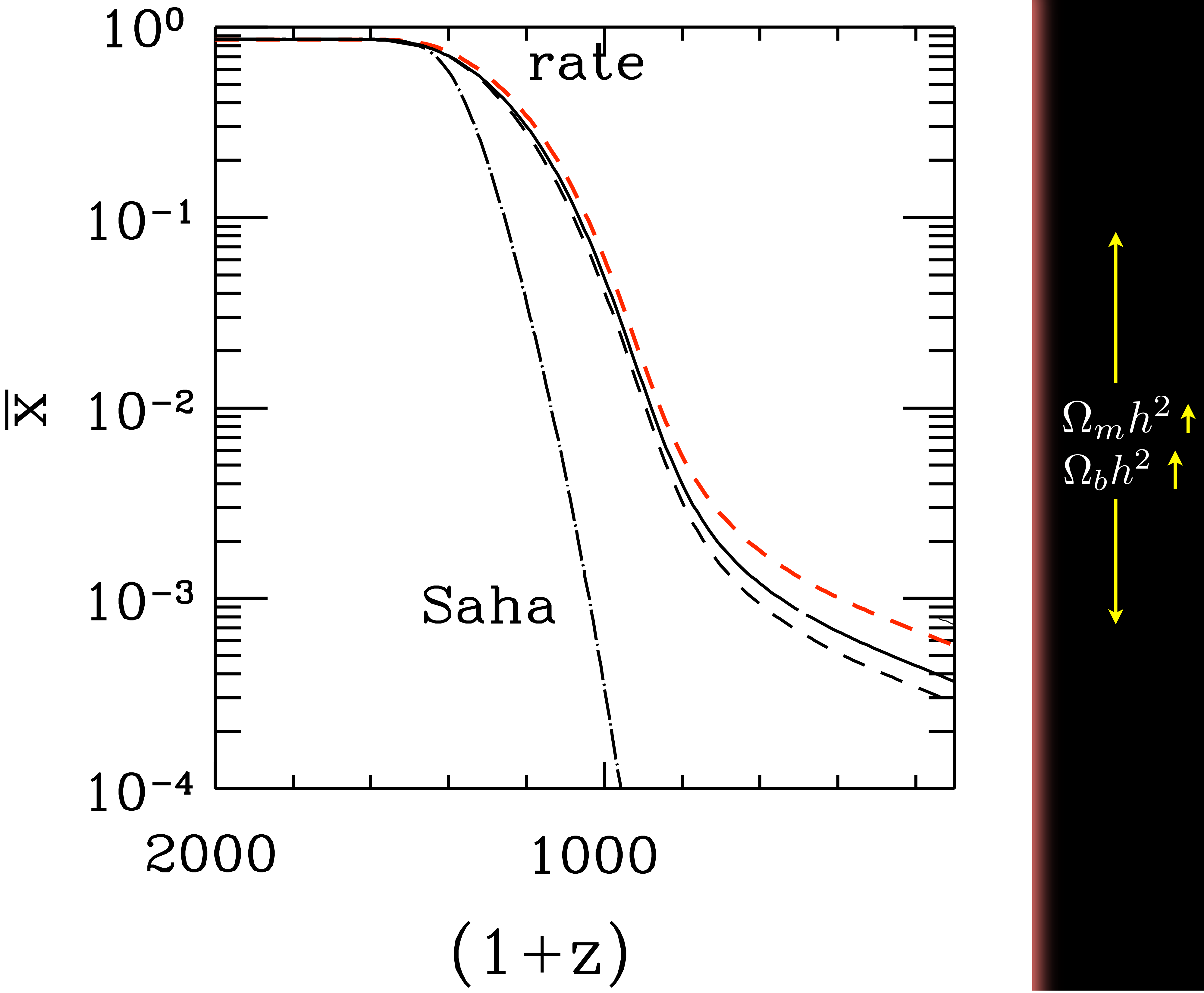
THE PEEBLES MODEL

- 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

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

✳Matter in eq. with radiation due to Thompson scattering

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

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Seager/Scott/Sasselov 2000/RECFAST!

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Non-eq rate equations

✳ Matter in eq. with radiation due to Thompson scattering

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BREAKING EQUILIBRIUM

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

$$t_{\rm compute} \sim \mathcal{O}\,(\text{years}) \;\; \text{for } \mathrm{n}_{\rm max} = 300$$

How to proceed if we want 0.01% accuracy in $x_e(z)$?

THESE ARE REAL STATES

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

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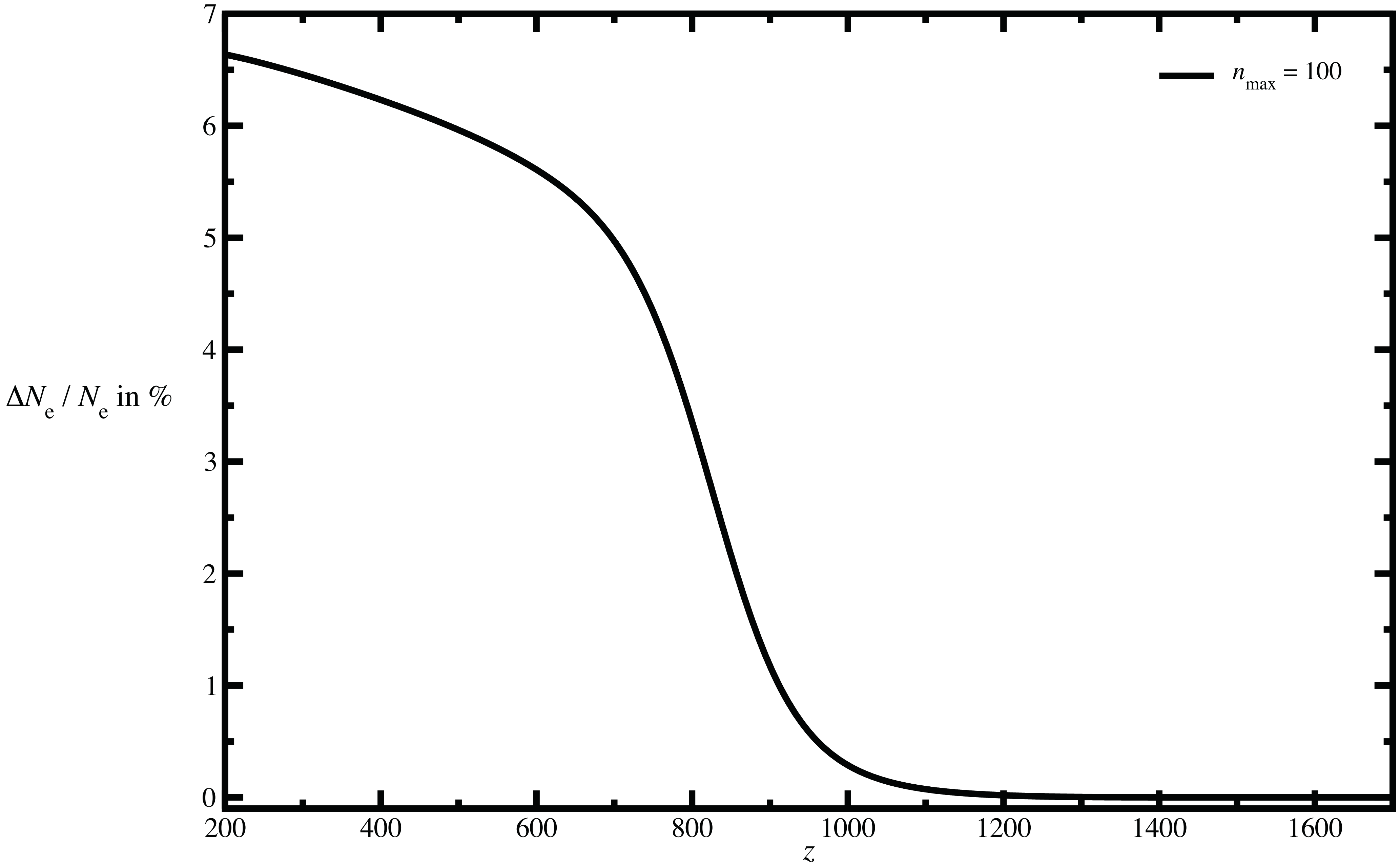
THE EFFECT OF RESOLVING L- SUBSTATES

Resolved l vs unresolved l



- ‘Bottlenecked’ l-substates decay slowly to 1s: Recombination is slower; Chluba al. 2006

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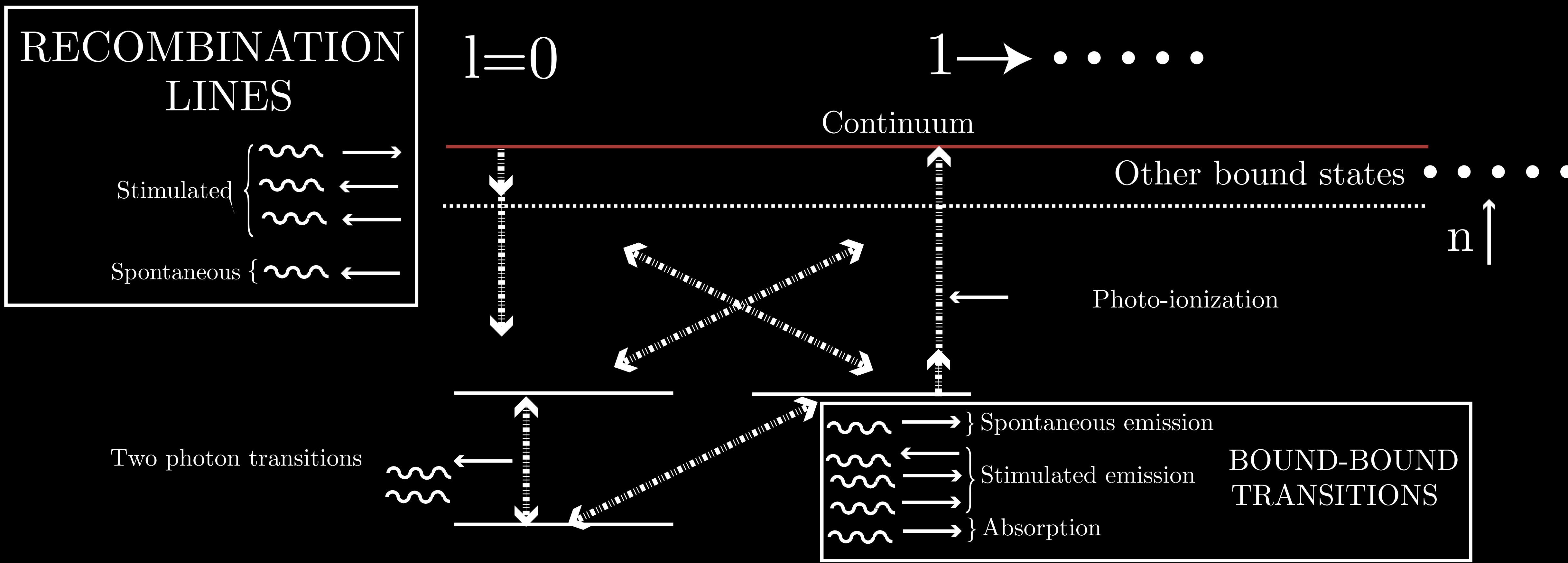
RECSPARSE AND THE MULTI-LEVEL ATOM



- We implement a multi-level atom computation in a new code, RecSparse!
- Bound-bound rates evaluated using Gordon (1929) formula and verified using WKB
- Bound-free rates tabulated and integrated at each T_m
- Boltzmann eq. solved for T_m (T_γ)

The multi-level atom (MLA)

- Two photon transitions between n=1 and n=2 are included:

$$\dot{x}_{2s\to 1s,2\gamma} = -\dot{x}_{1s\to 2s,2\gamma} = \Lambda_{2s}(-x_{2s} + x_{1s}e^{-E_{2s\to 1s}/T_\gamma})$$

- Net recombination rate:

$$x_e \simeq 1 - x_{1s} \to \dot{x}_e \simeq -\dot{x}_{1s} = -\dot{x}_{1s\to 2s}$$
$$+\sum_{n,l>1s} A^{l0}_{n1} P^{l0}_{n1} \left\{ \frac{g_{nl}}{2} f^+_{n1} x_{1s} - (1+f^+_{n1}) x_{nl} \right\}$$

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2s-1s decay rate

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Einstein coeff.

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Occ. number blueward of line

20

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Escape probability

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Lyman series current to ground state

RADIATION FIELD: BLACK BODY +

- Escape probability treated in Sobolev approx.

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

$$\tau_s = \frac{c^3 n_{\rm H}}{8\pi H \nu^3_{nn'}} A^{ll'}_{nn'} \left[\frac{g^{l'}_{n'}}{g^l_n} x^l_n - x^{l'}_{n'}\right]$$

$$\mathcal{R}(\nu,\nu') = \phi(\nu)\phi(\nu')$$

$$\frac{v_{\rm th}}{H(z)} \ll \lambda$$

- Excess line photons injected into radiation field
- Ongoing work by collabs and others uses FP eqn. to obtain evolution of $f(\nu)$ more generally, including:
  - Atomic recoil/diffusion,
  - Time-dependence of problem,
  - Coherent scattering,
  - Overlap of higher-order Lyman lines, $\longrightarrow$ Analytic corr. to Sobolev, soon to be in RecSparse
  - Higher 2γ decay
- Ultimate goal is to combine all new atomic physics effect in one fast recombination code

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

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$$\vec{x} = \begin{pmatrix} \vec{x}_0 \\ \vec{x}_1 \\ \ldots \\ \vec{x}_{n_{\max}-1} \end{pmatrix}$$

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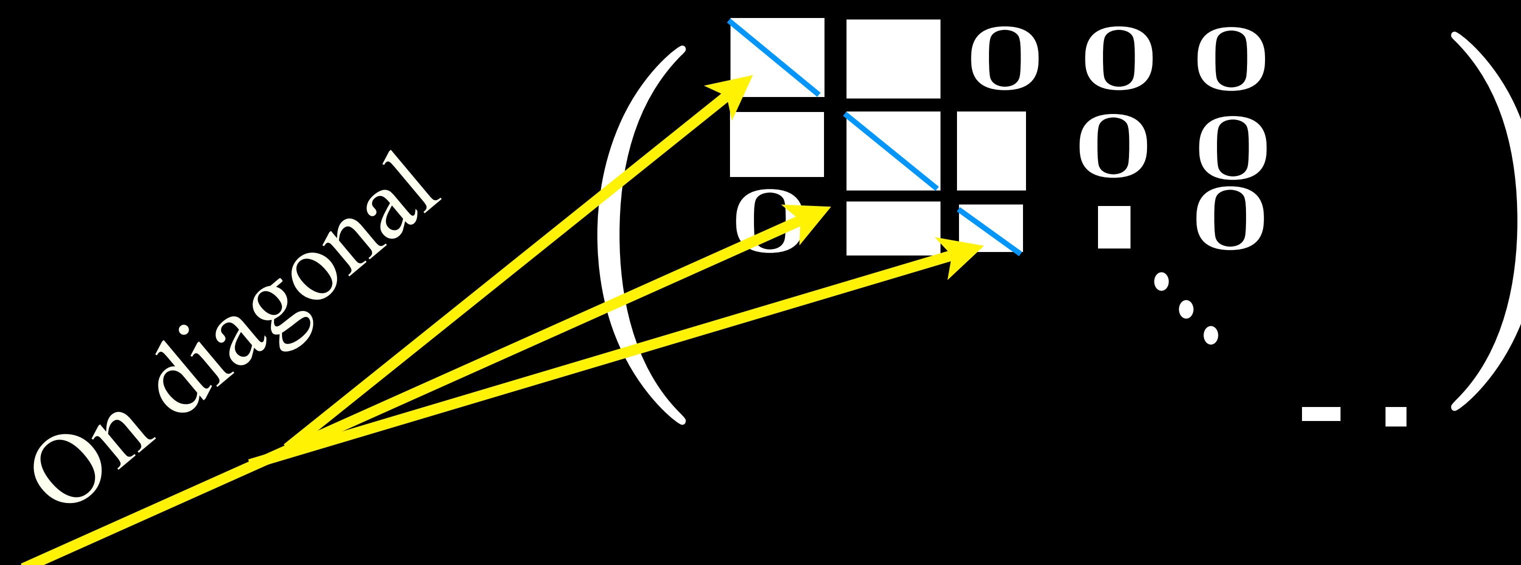

For state l, includes BB transitions out of l to all other l'',
photo-ionization, 2γ transitions to ground state

Steady-state for excited levels

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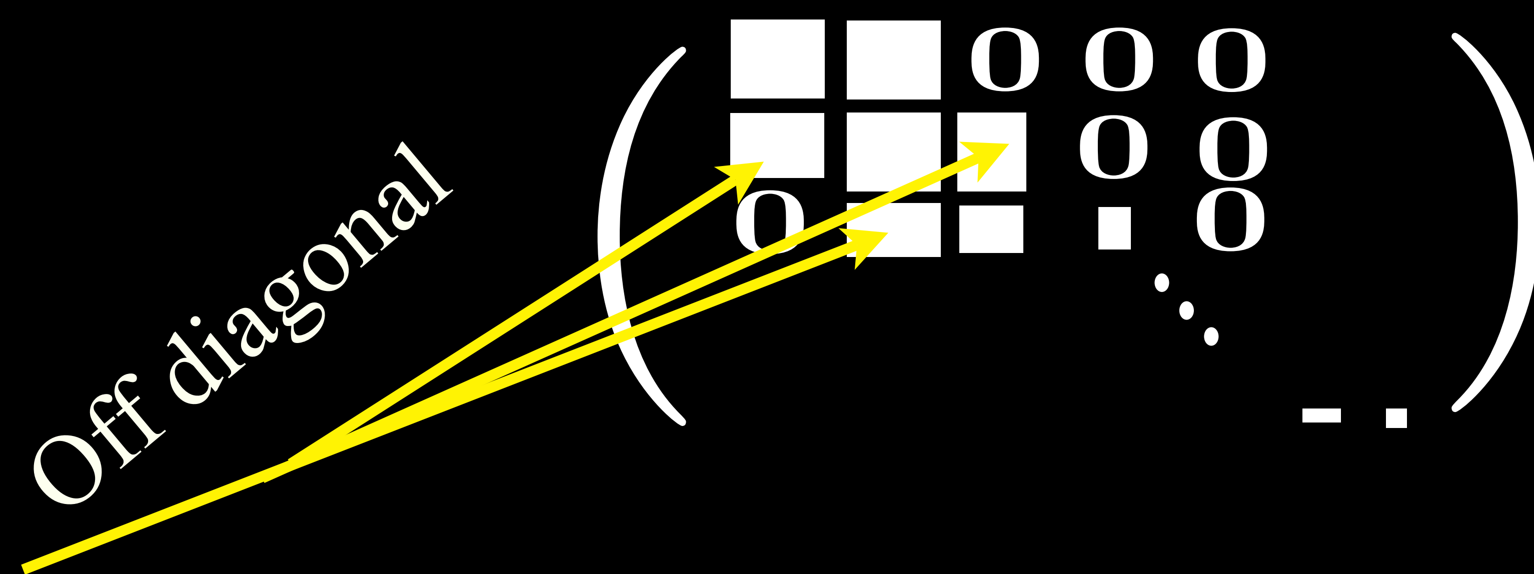

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STEADY-STATE FOR EXCITED LEVELS

* Evolution equations may be re-written in matrix form

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

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

STEADY-STATE FOR EXCITED LEVELS

For n>1, $t_{\rm rec}^{-1} \sim 10^{-12} s^{-1} \ll \mathbf{R}$, $\vec{s} \rightarrow \vec{x} \simeq \mathbf{R}^{-1}\vec{s}$

$\mathbf{R} \lesssim 1\ \mathrm{s}^{-1}$ (e.g. Lyman-α)

- Evolution equations may be re-written in matrix form

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

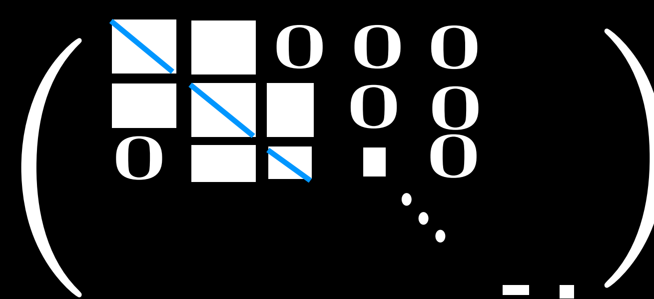
RAPID MATRIX INVERSION: SPARSITY TO THE RESCUE

- 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: $\Delta l = \pm 1$

  $\mathrm{M}_{l,\mathbf{l-1}}\vec{x}_{\mathbf{l-1}} + \mathbf{M}_{l,l}\vec{x}_l + \mathbf{M}_{l,\mathbf{l+1}}\vec{x}_{\mathbf{l+1}} = \vec{s}_l$



$$\begin{pmatrix} \vec{x}_0 \\ \vec{x}_1 \\ \cdots \\ \vec{x}_{n_{\max}-1} \end{pmatrix} = \vec{s}_l$$

- 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 10^{-8} precision, with computation time ~ $n_{\max}^{2.5}$: 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-σ 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.
- ***Unfinished business***: *Are other forbidden transitions in hydrogen important, particularly for Planck data analysis?*

QUADRUPOLE TRANSITIONS AND RECOMBINATION

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

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

- Coupling to ground state will overwhelmingly dominate:

$$\frac{A^{\text{quad}}_{n,2\to 1,0}}{A^{\text{quad}}_{n,2\to m,0}} \propto \frac{\omega^5_{n1}}{\omega^5_{nm}} = \left(\frac{1-\frac{1}{n^2}}{\frac{1}{m^2}-\frac{1}{n^2}}\right)^5 \geq 1024 \text{ if } m \geq 2$$

- Magnetic dipole rates suppressed by several more orders of magnitude

- Hirata, Switzer, Kholupenko, others have considered other `forbidden' processes, two-photon processes in H, E2 transitions in He

QUADRUPOLE TRANSITIONS AND RECOMBINATION

- Rates obtained using algebra of Coulomb w.f. (Hey 1995) and checked with WKB

- 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 $A_{nd\rightarrow 1s} x_{nd}$.

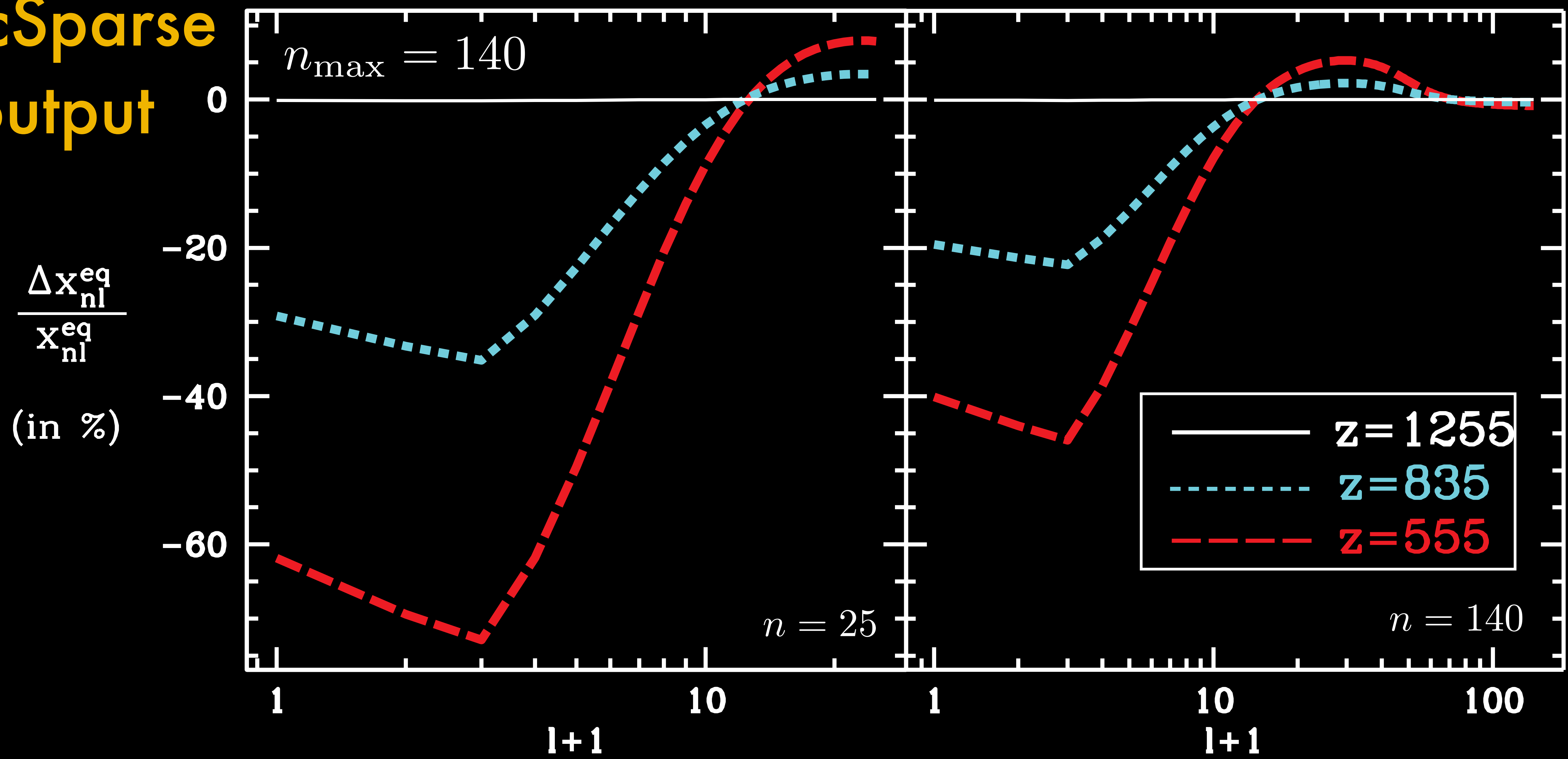
- Same sparsity pattern of rate matrix, similar to l-changing collisions

- Detailed balance yields net rate $$R^{\mathrm{quad}}_{nd\rightarrow np} = A_{nd\rightarrow 1s}\left(x_{nd} - \frac{5}{3} x_{np}\right)$$

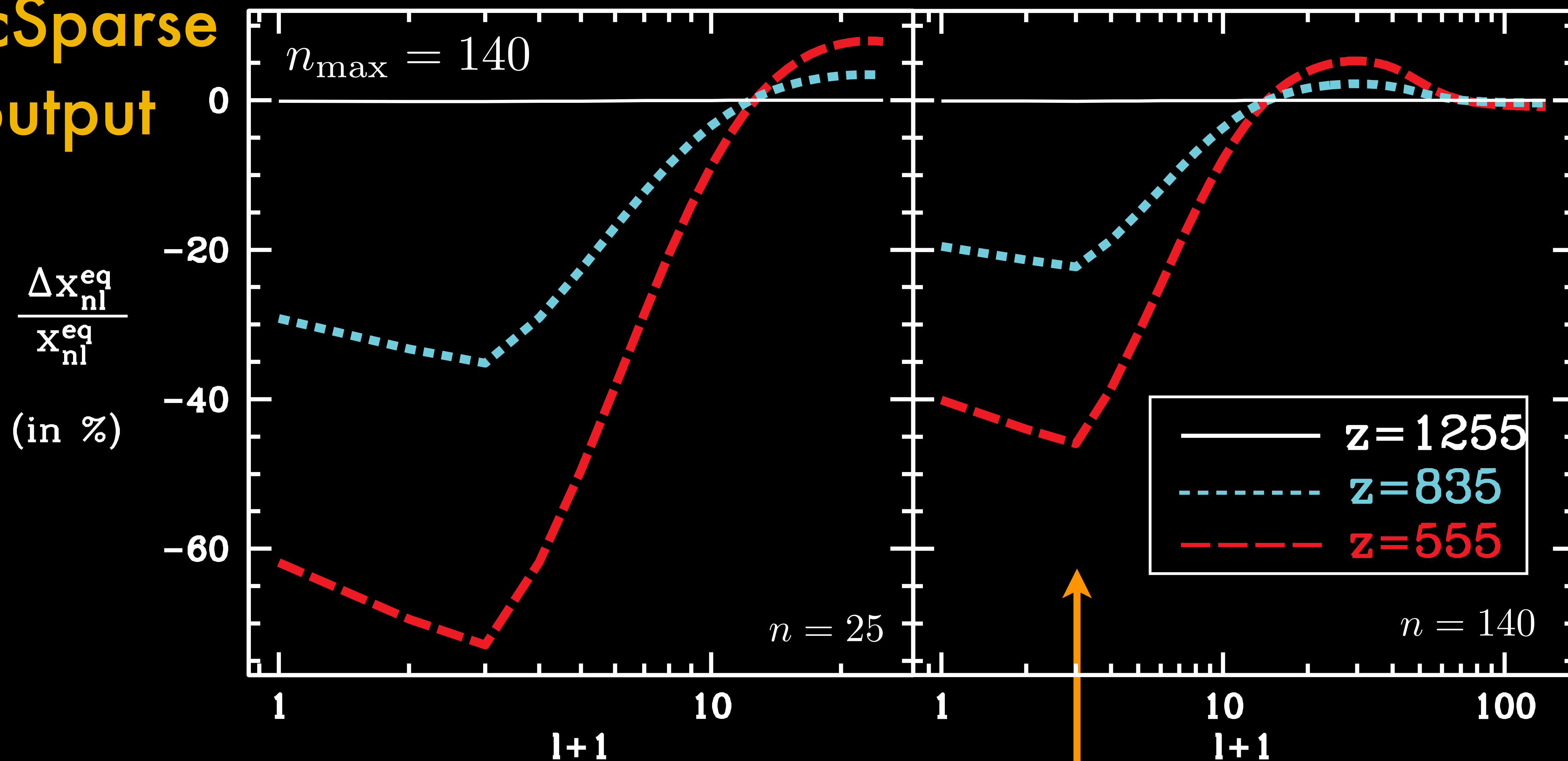
RESULTS: STATE OF THE GAS

DEVIATIONS FROM BOLTZMANN EQ: L-SUBSTATES

RecSparse output



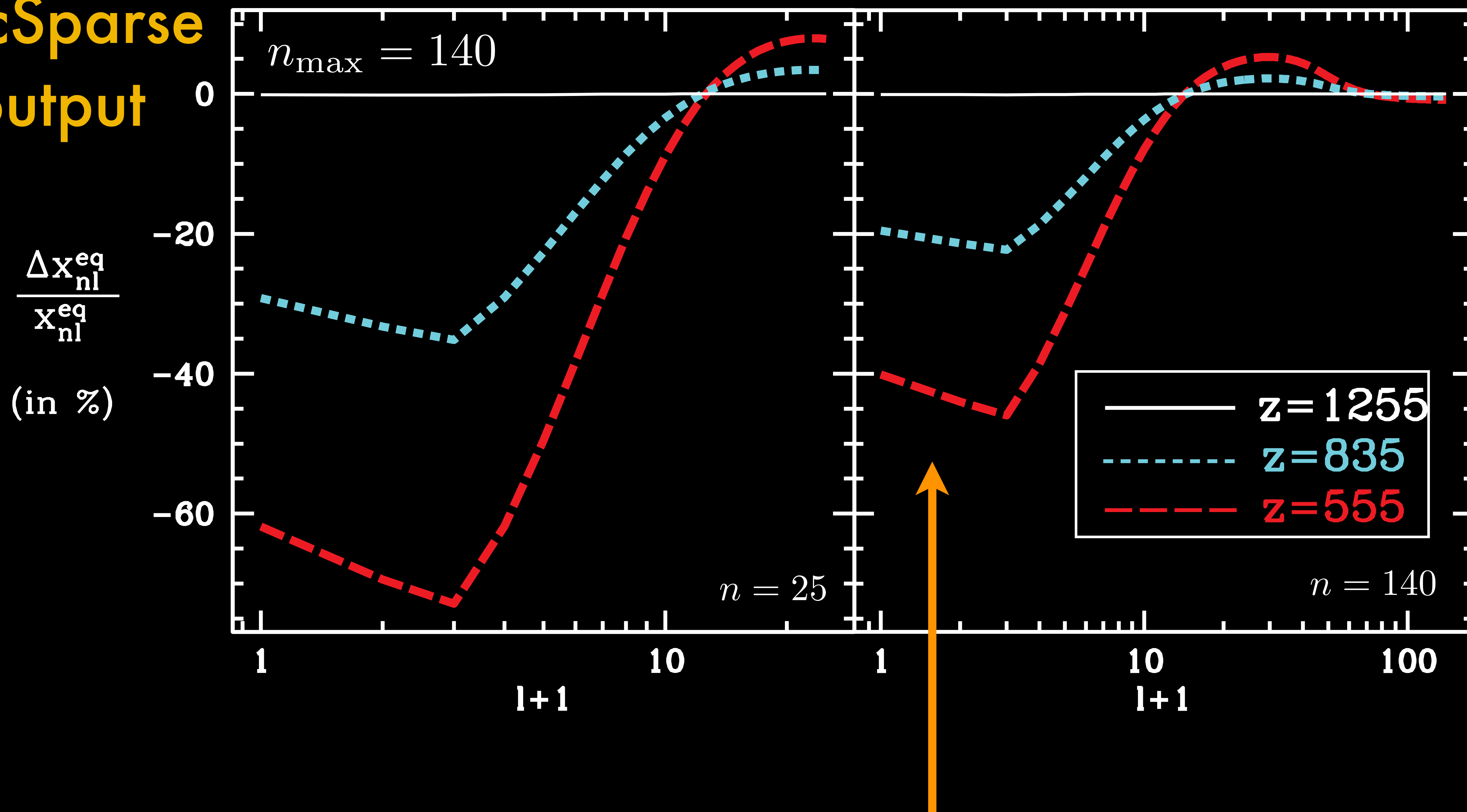
RecSparse output



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

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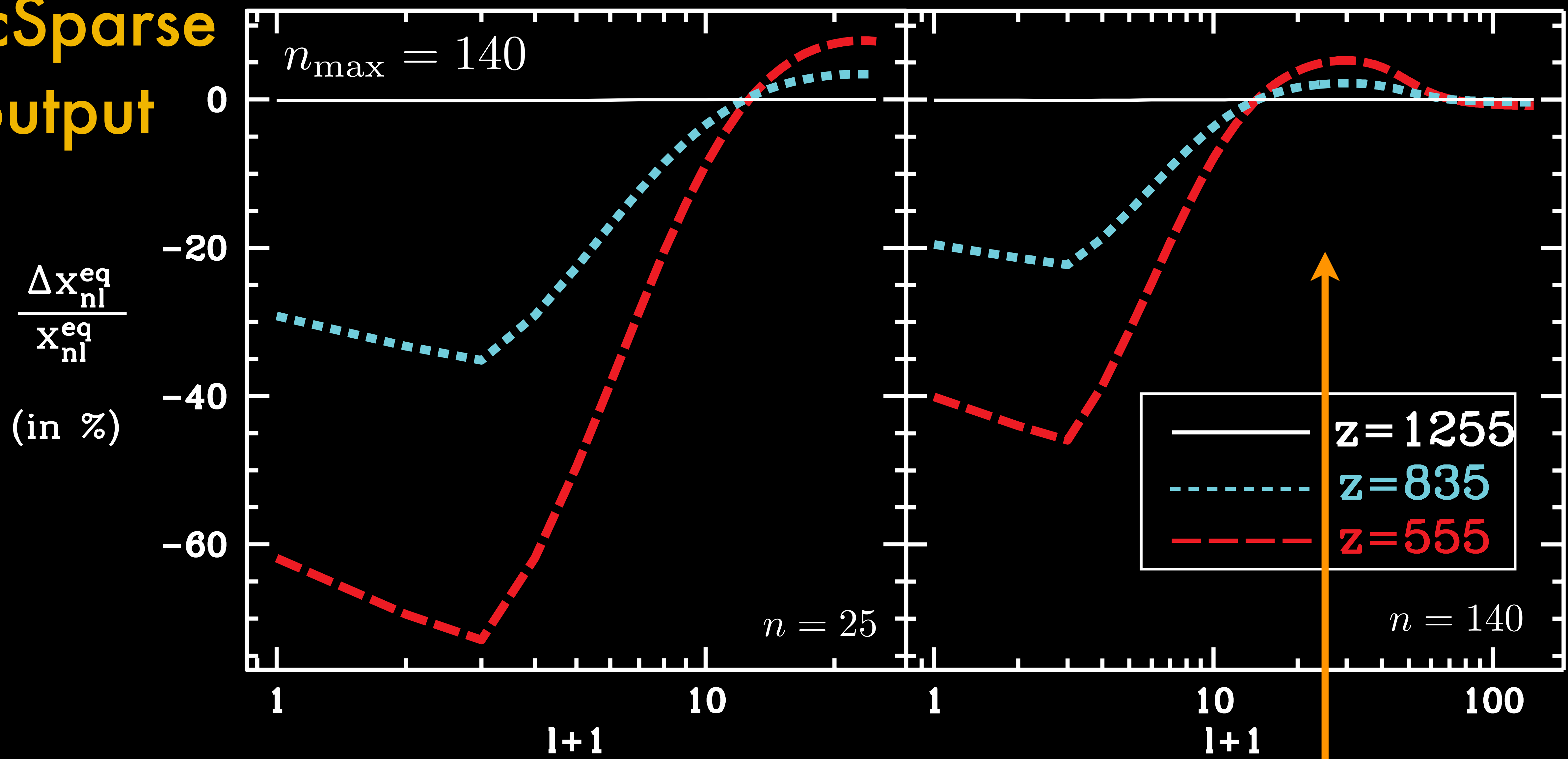
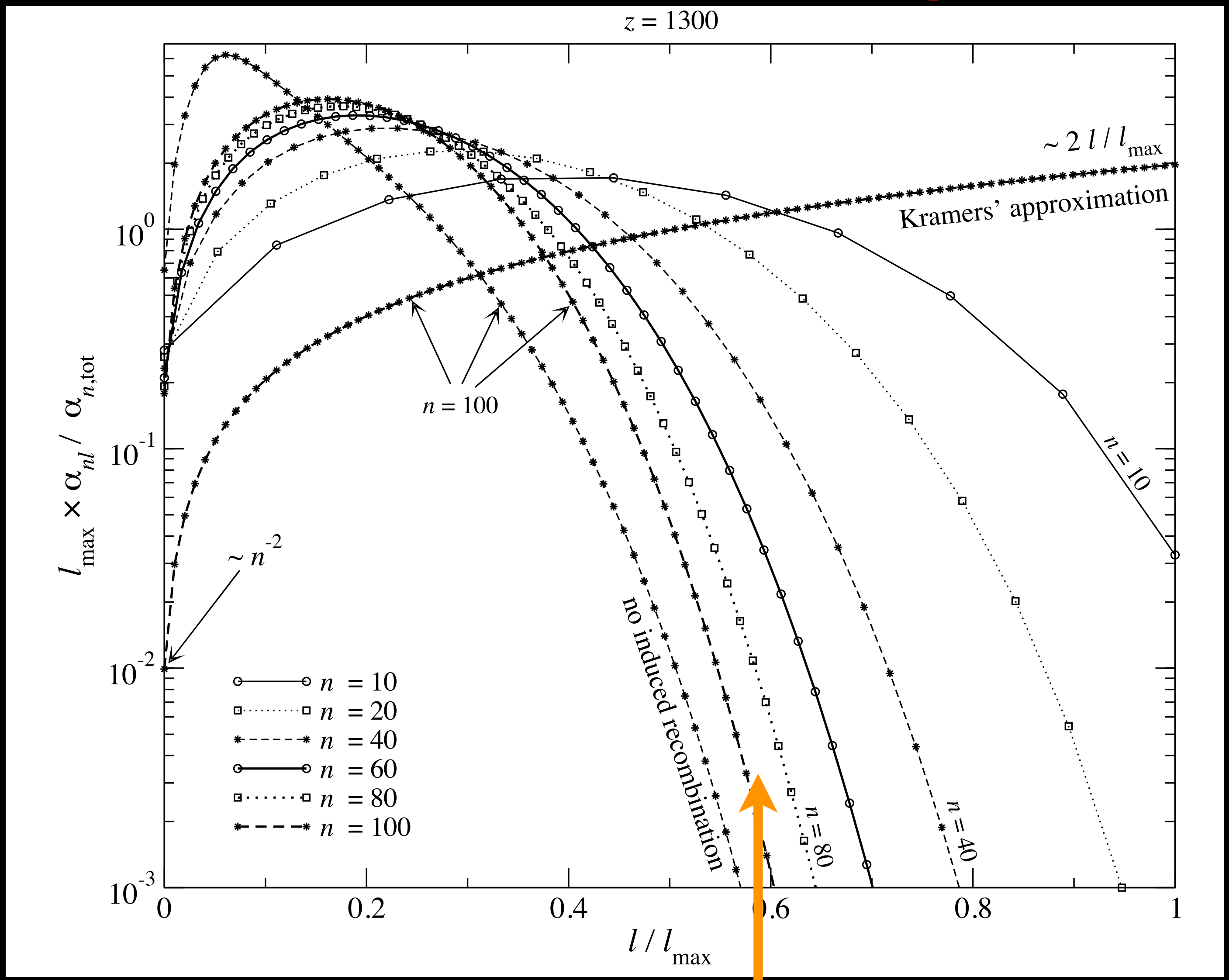
RecSparse output

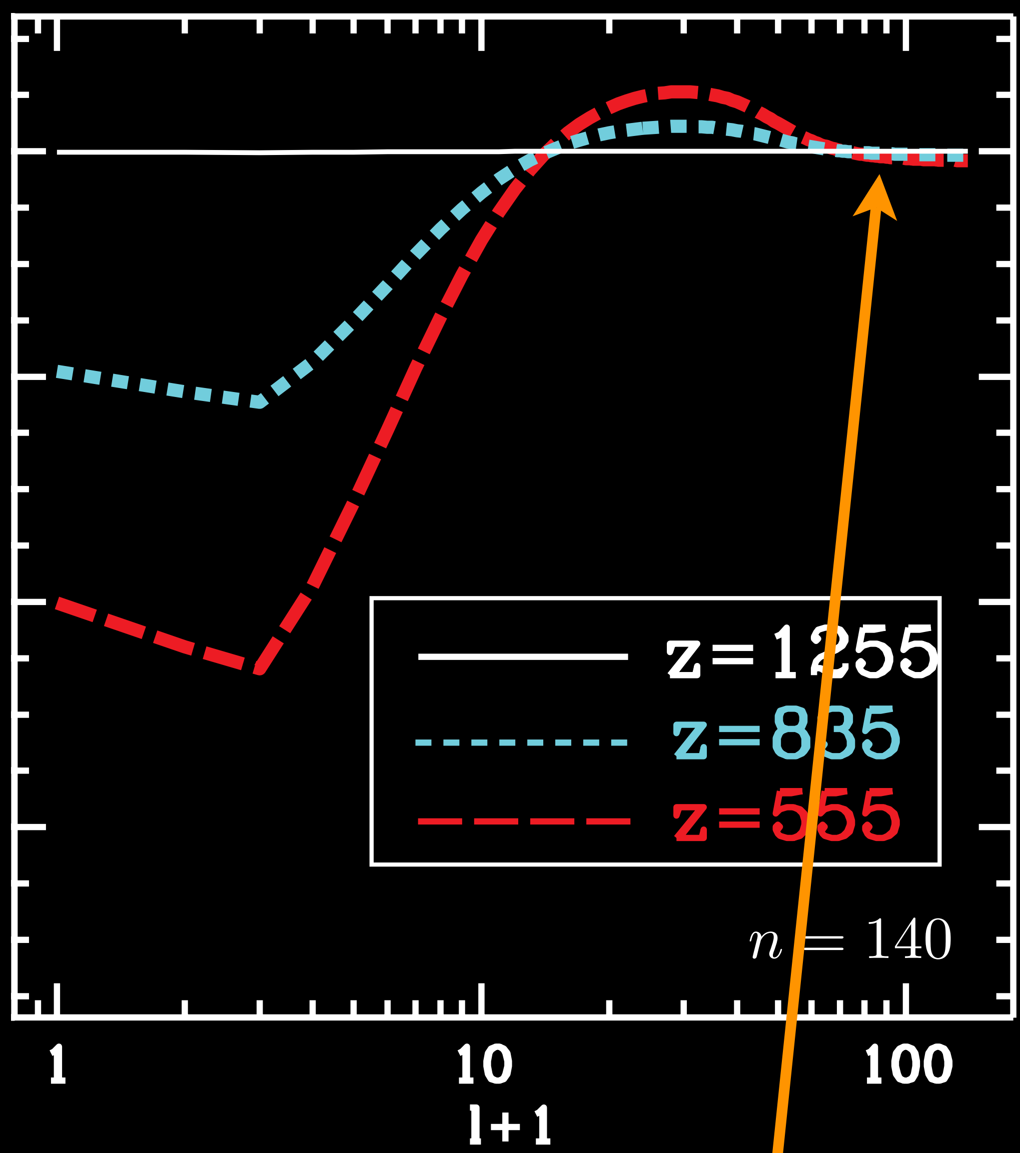


Higher l are bottlenecked by $\Delta l = \pm 1$ (over-pop)

DEVIATIONS FROM BOLTZMANN EQ: L-SUBSTATES

Chluba/Rubino-Martin/Sunyaev 2006

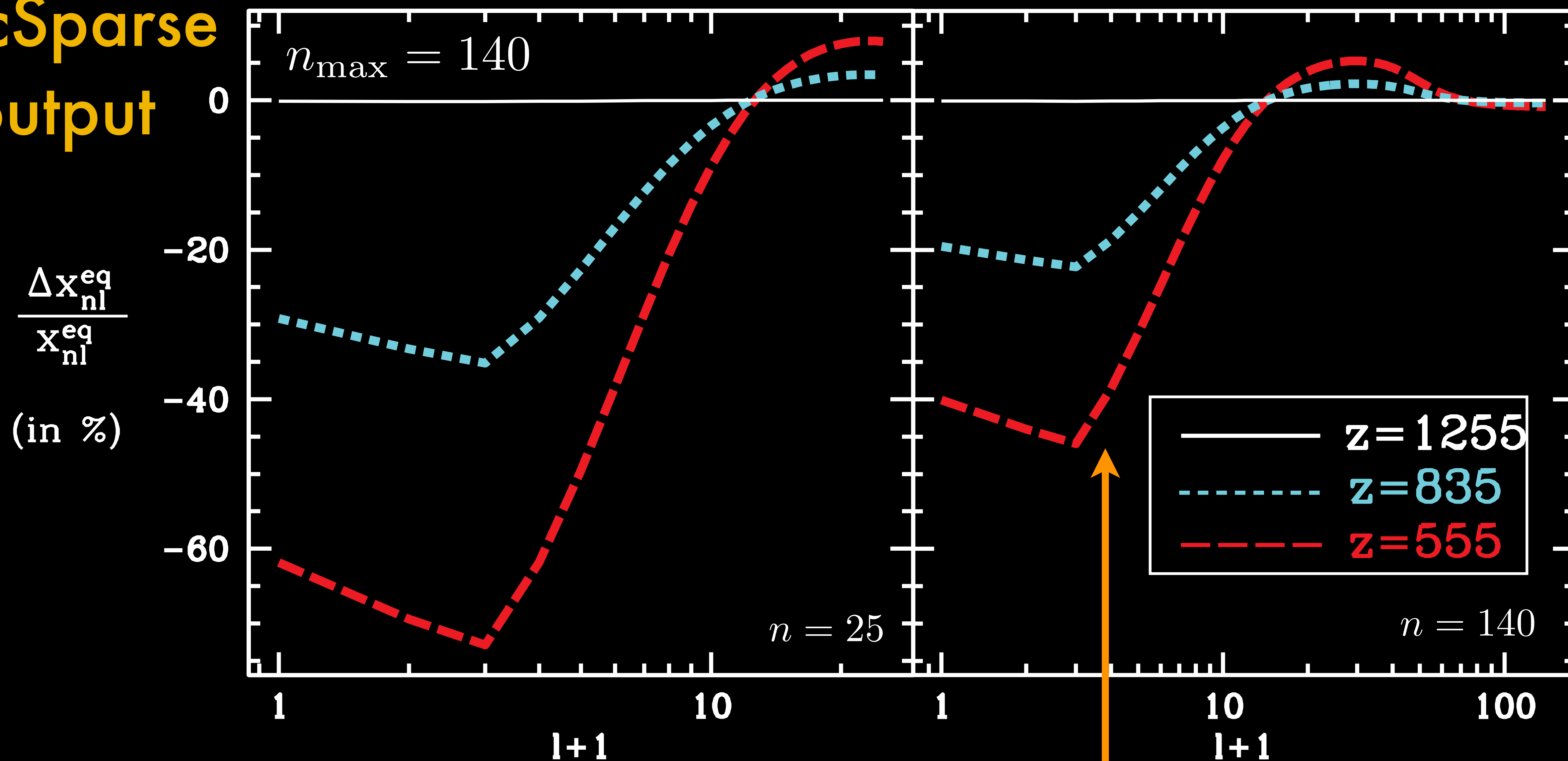




Highest l states recombine inefficiently, and are under-populated

DEVIATIONS FROM BOLTZMANN EQ: L-SUBSTATES

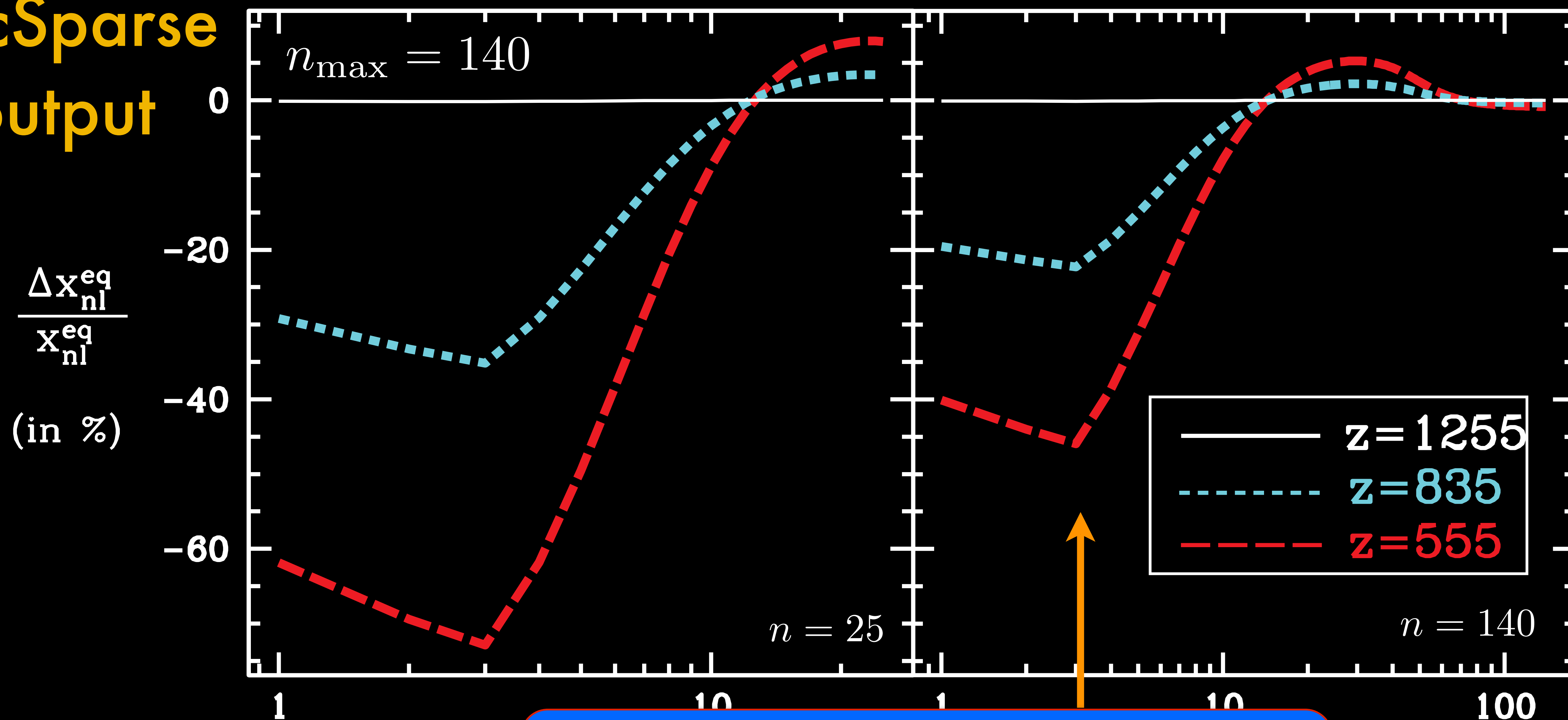
RecSparse output



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

DEVIATIONS FROM BOLTZMANN EQ: L-SUBSTATES

RecSparse output



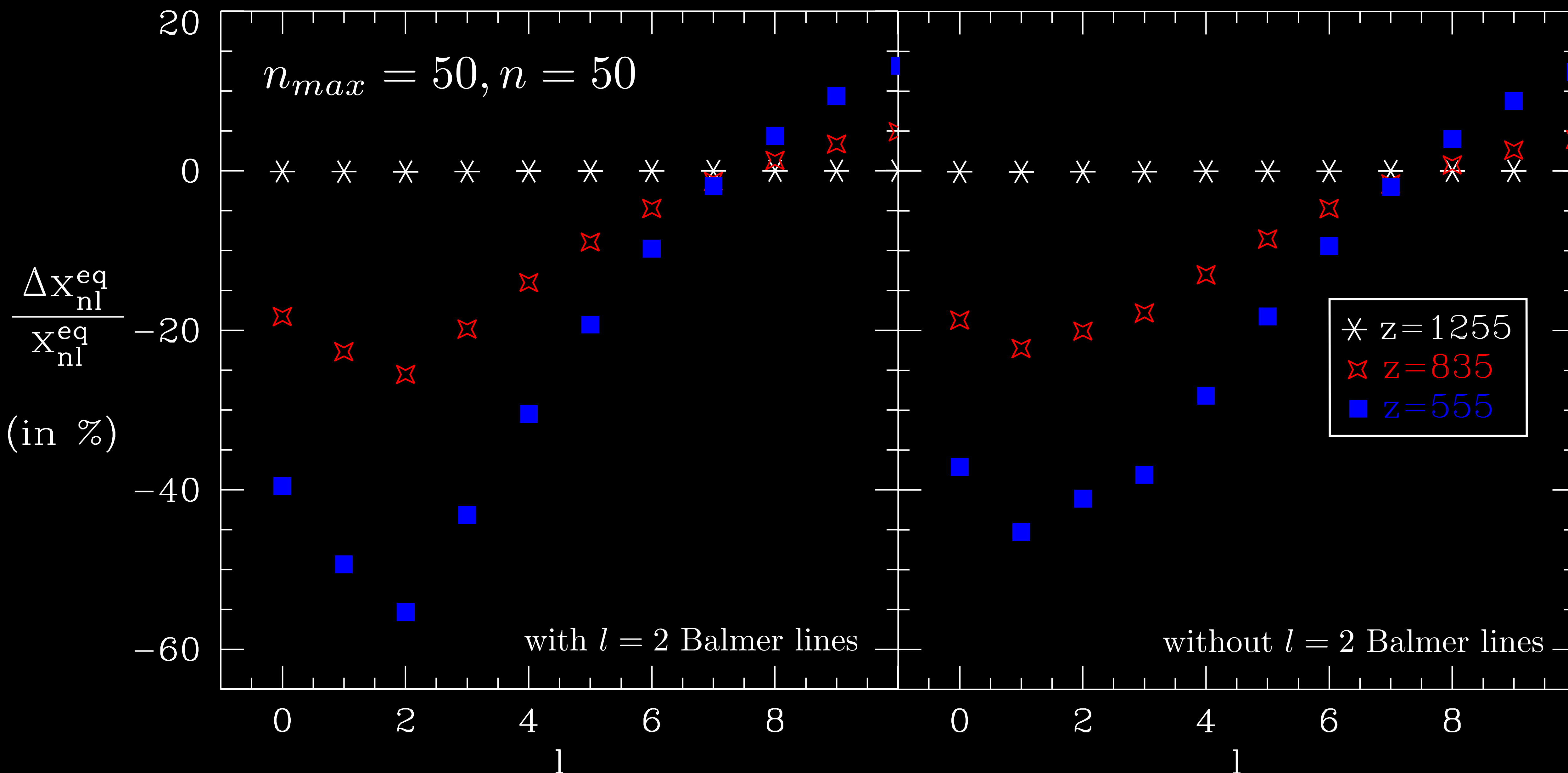
Why the feature at l=2?

WHAT IS THE ORIGIN OF THE L=2 DIP?

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

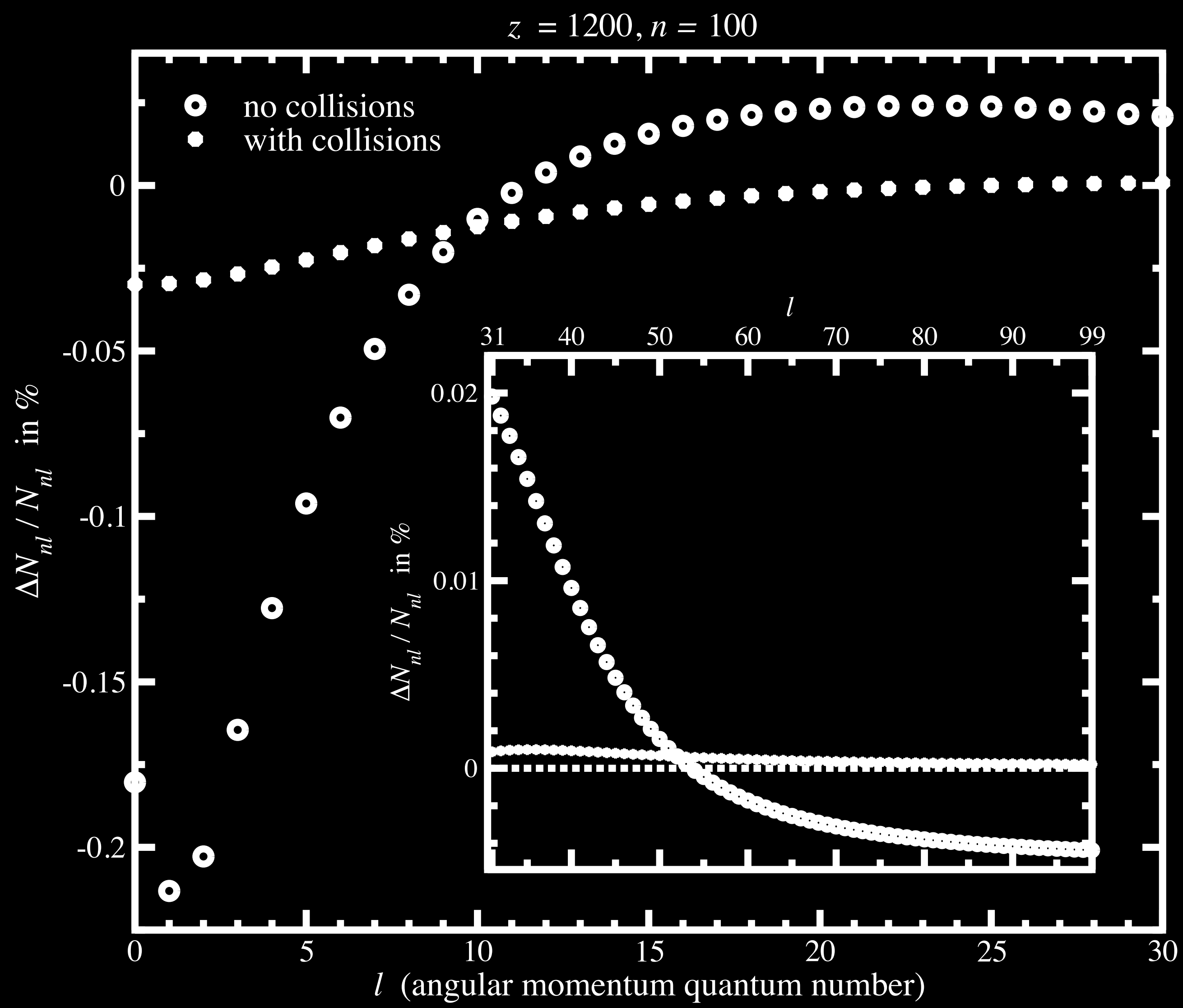
- l=2 depopulates more rapidly than l=1 for higher (n>2) excited states
- We can test if this explains the dip at l=2 by running the code with these Balmer transitions the blip should move to l=1

L-SUBSTATE POPULATIONS, BALMER LINES OFF



Dip moves as expected when Balmer lines are off!

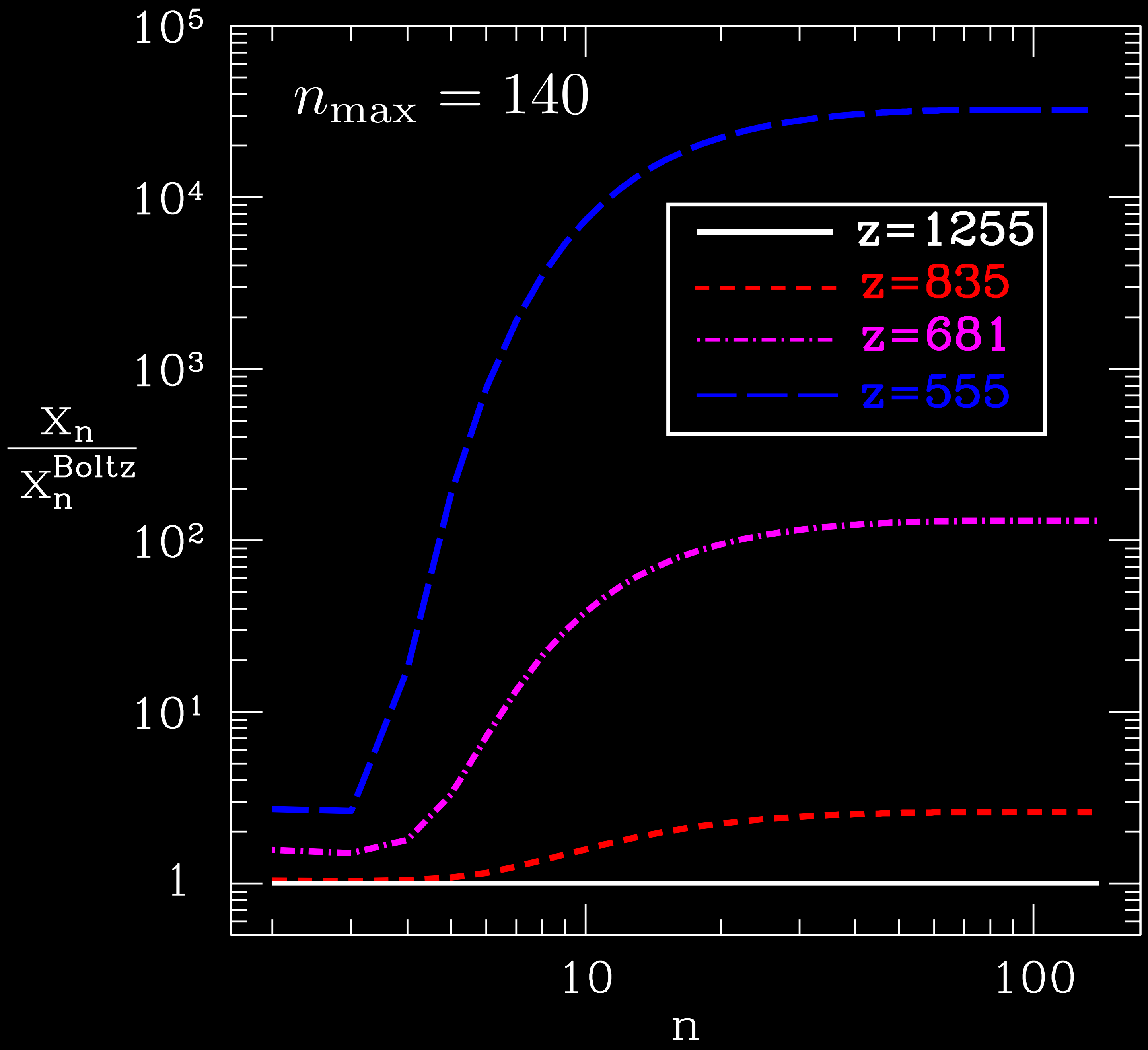
ATOMIC COLLISIONS



$n_{\max} = 100$

- l-changing collisions bring l-substates closer to statistical equilibrium (SE)
- Being closer to SE speeds up rec. by mitigating high-l bottleneck (Chluba, Rubino Martin, Sunyaev 2006)
- Theoretical collision rates unknown to factors of 2!
  - $b < a_0 n^2 \rightarrow$ multi-body QM!
    $t_{\rm pass} < t_{\rm orbit} \rightarrow$ Impulse approximation breaks down!
- Next we'll include them to see if we need to model rates better

DEVIATIONS FROM BOLTZMANN EQUILIBRIUM: DIFFERENT N-SHELLS



$$\alpha_n n_e > \sum_{n'l}^{n'<n} A_{nn'}^{ll\pm1}$$

- ✶ No inversion relative to n=2 (just-over population)
- ✶ Population inversion seen between some excited states: Does radiation stay coherent? Does recombination mase? Stay *tuned*
- ✶ Dense regions may mase more efficiently: maser spots as probe of l.s.s at early times? (Spaans and Norman 1997)

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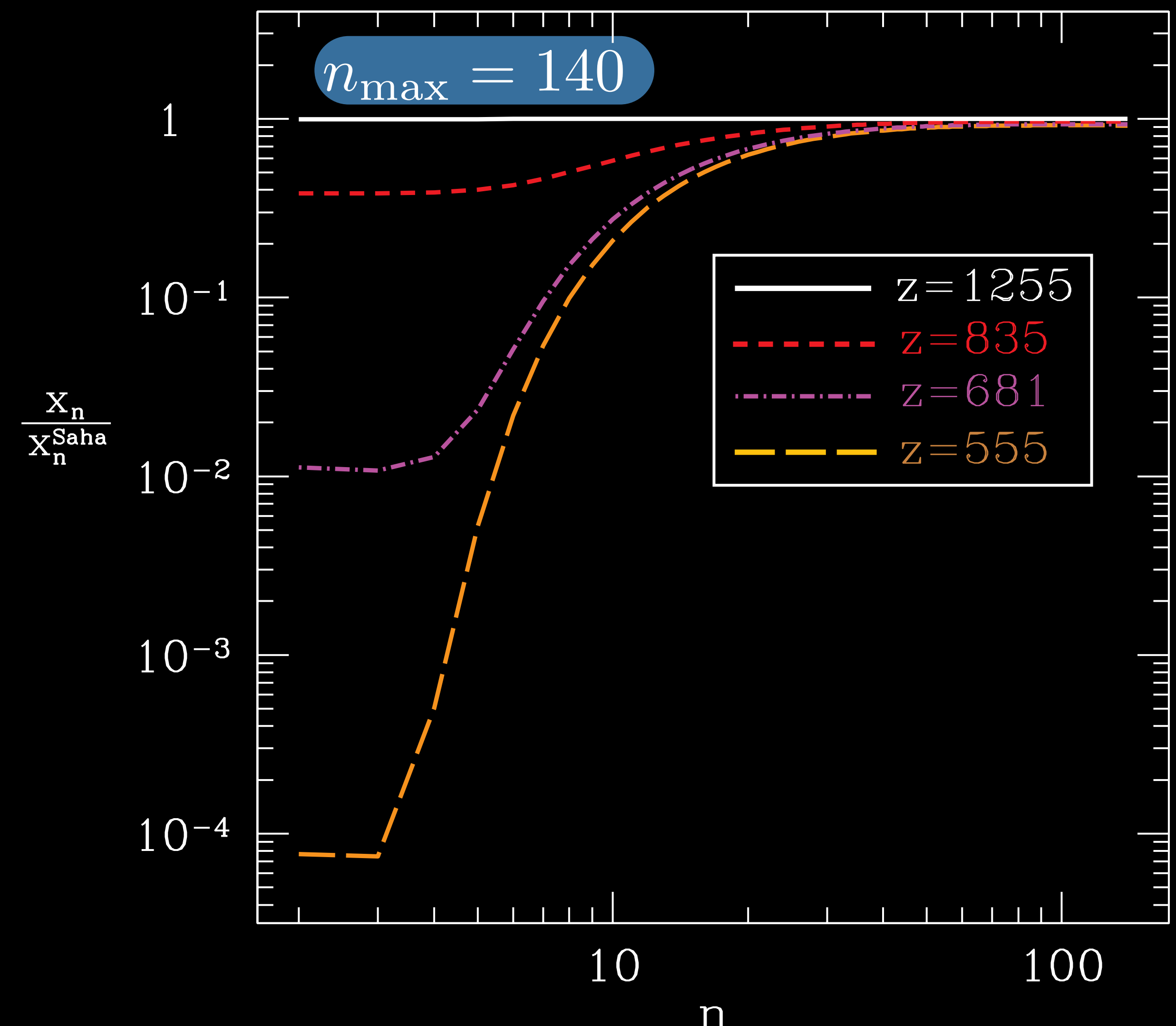
DEVIATIONS FROM SAHA EQUILIBRIUM

HUGE DEVIATIONS FROM SAHA EQ!



- n=1 suppressed due to freeze-out of x_e
- Remaining levels 'try' to remain in Boltzmann eq. with n=2
- Super-Boltz effects and two-γ transitions (n=1$\longrightarrow$ n=2) yield less suppression for n>1
- Effect larger at late times (low z) as rates fall

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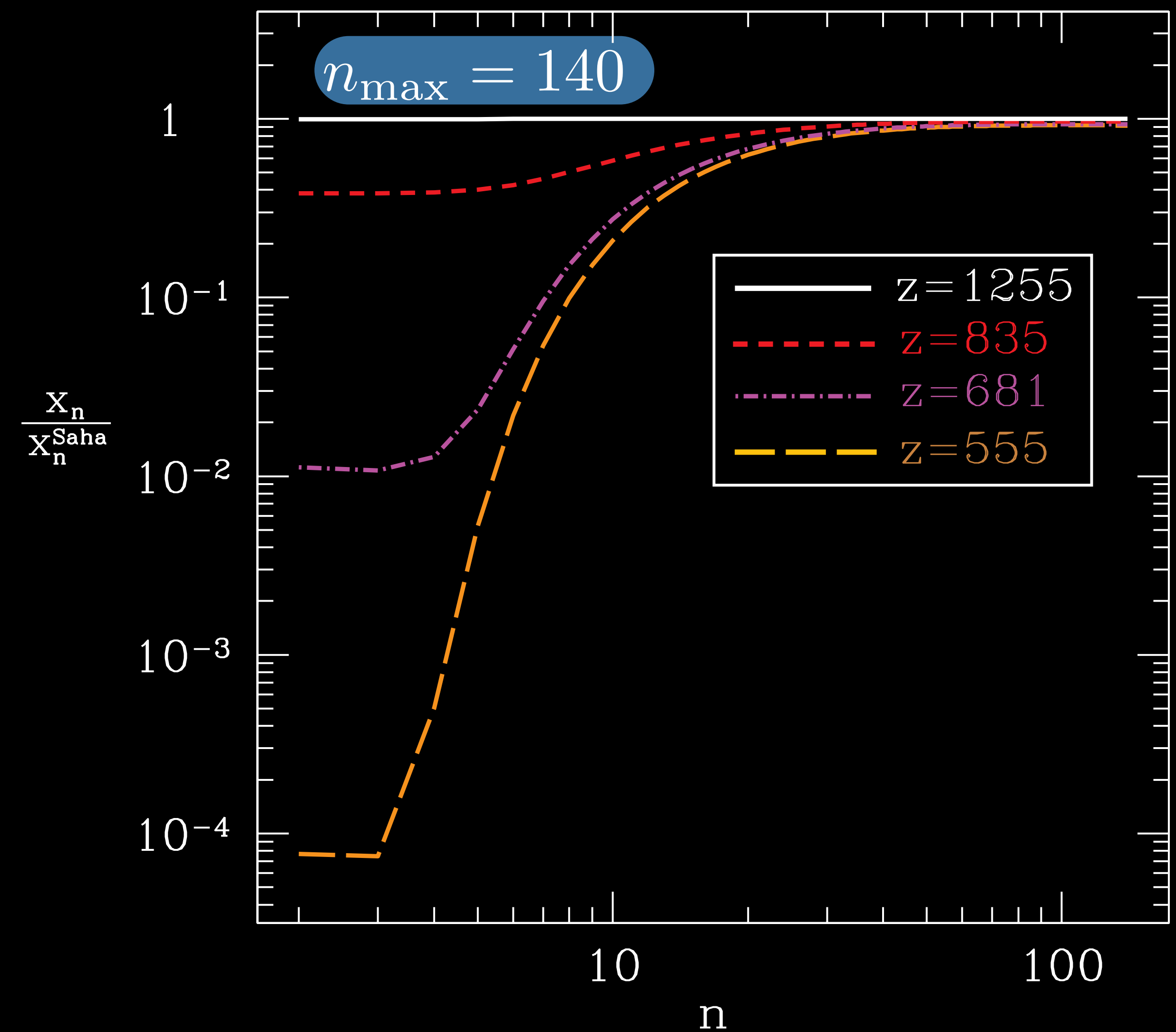
DEVIATIONS FROM SAHA EQUILIBRIUM

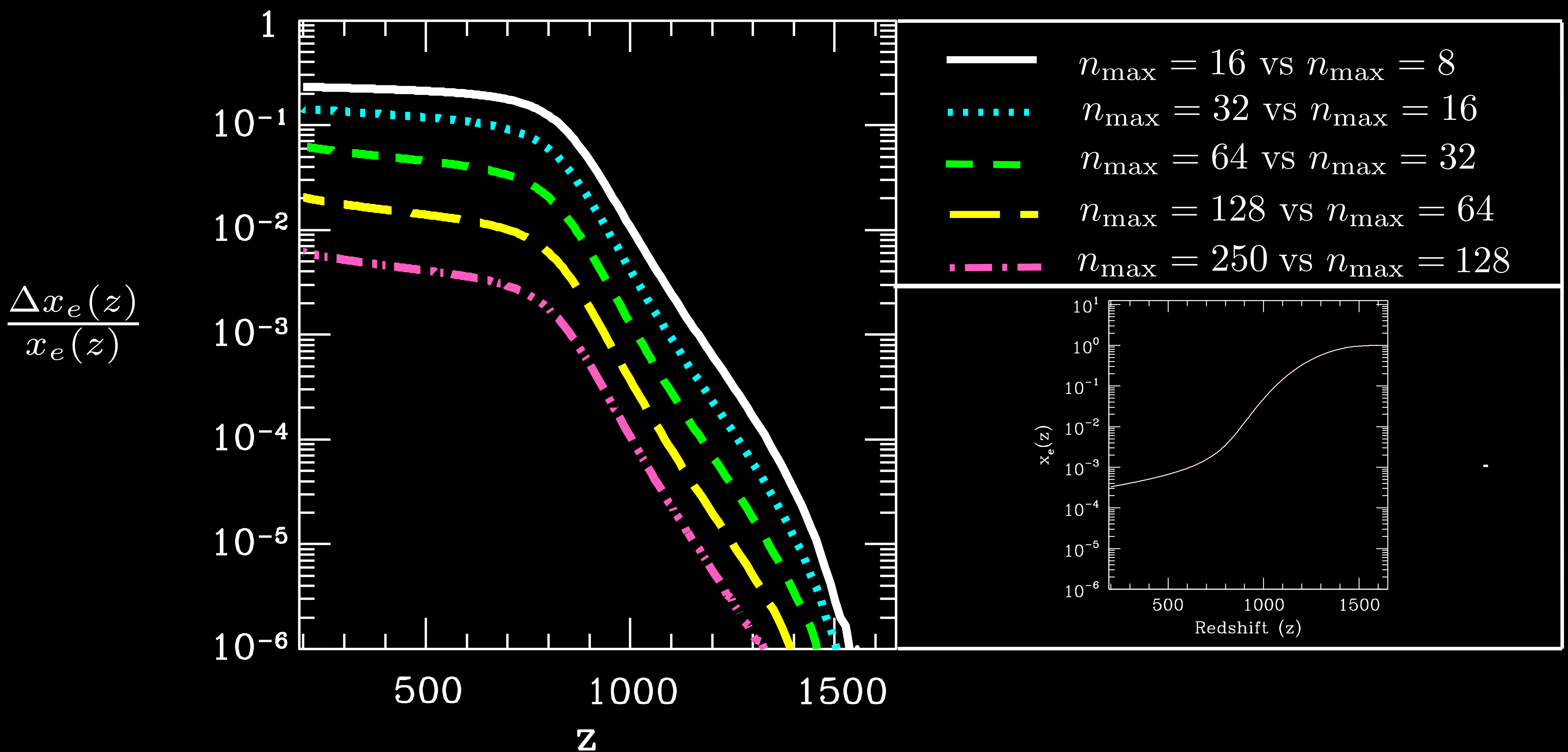
HUGE DEVIATIONS FROM SAHA EQ!



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

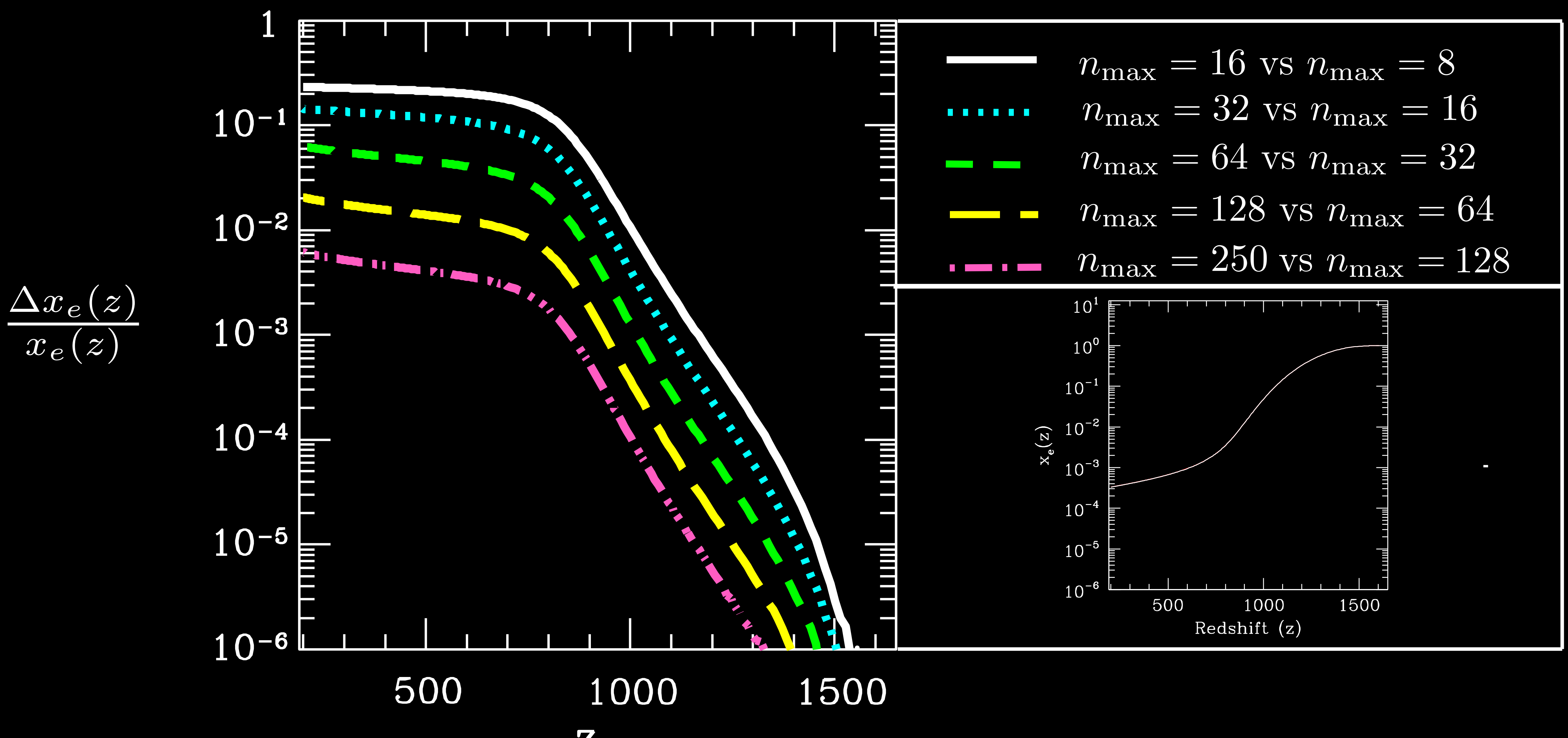
RESULTS: RECOMBINATION HISTORIES

RESULTS: RECOMBINATION HISTORIES INCLUDING HIGH-N



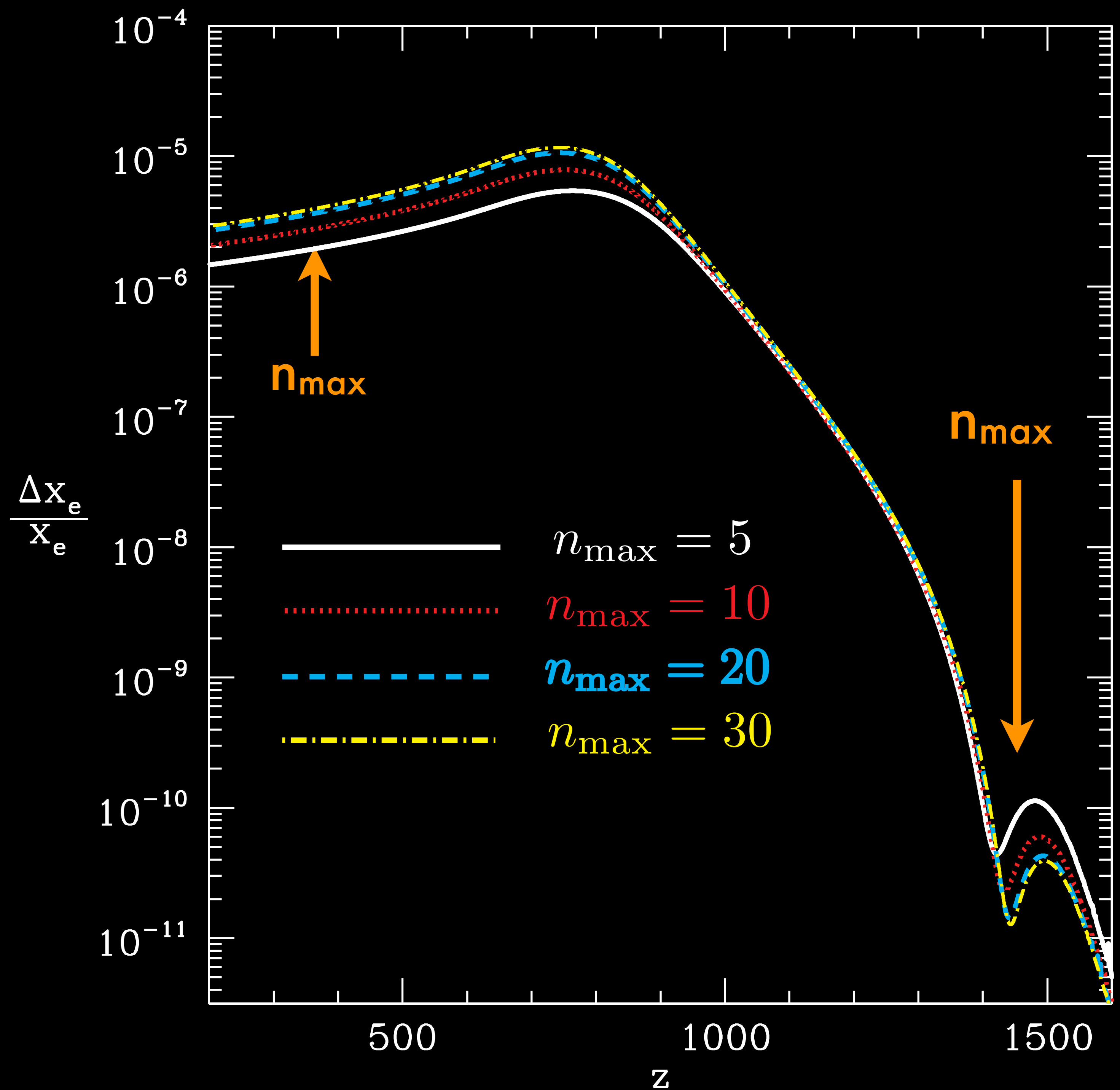
- ✴ $x_e(z)$ falls with increasing $n_{\max} = 10 \to 200$, as expected.
- ✴ Rec Rate>downward BB Rate> Ionization, upward BB rate
- ✴ For $n_{max} = 100$, code computes in only 2 hours

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}=250 and n_{max}=300 under way to further test convergence (more time consuming)

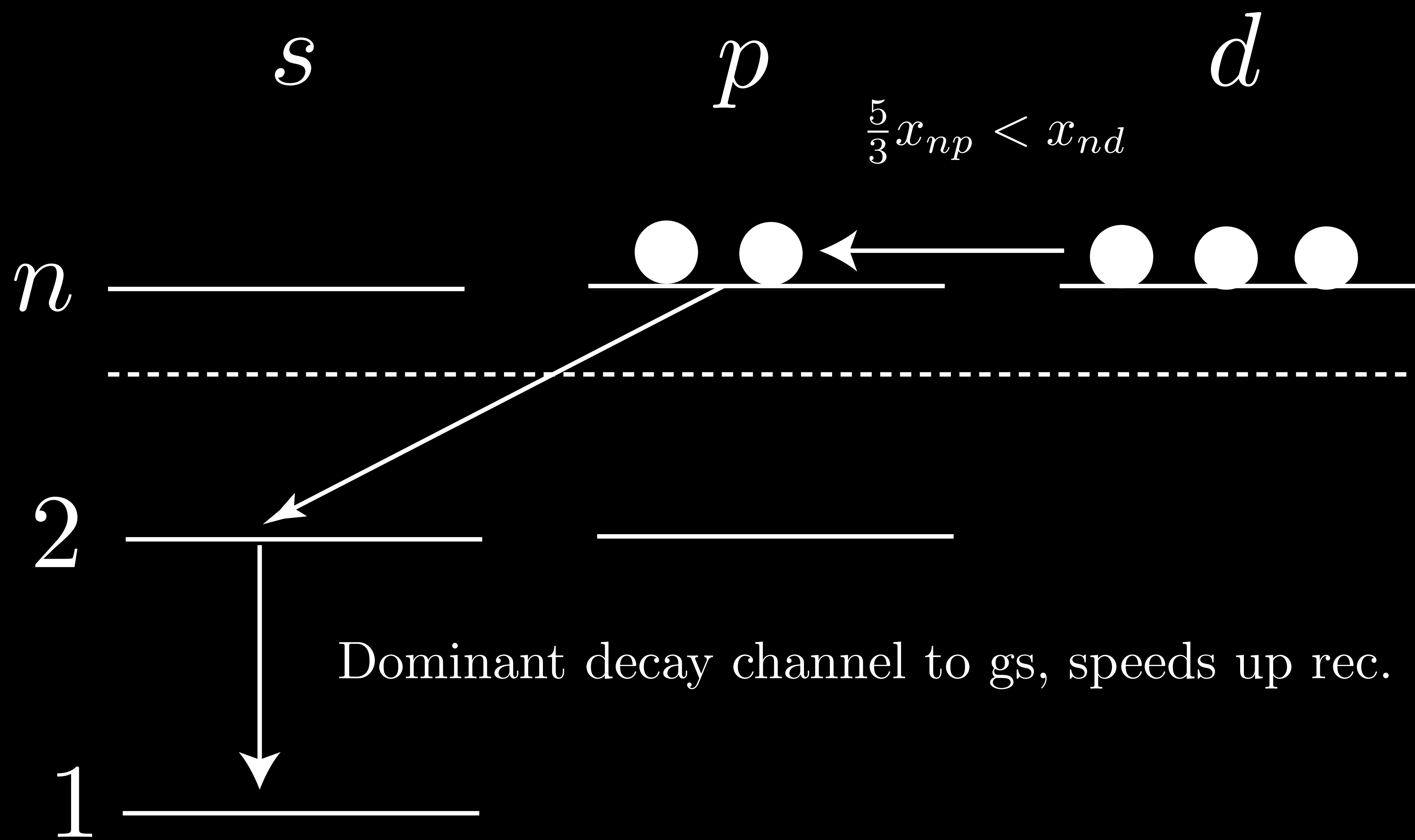
RESULTS: RECOMBINATION WITH HYDROGEN



$$\Delta x_e \equiv x_e\big|_{\rm no\ \it E2 \rm\ transitions} - x_e\big|_{\rm with\ \it E2 \rm\ transitions}$$

Negligible for Planck!

BUILDING INTUITION FOR THE EFFECT OF E2 TRANSITIONS



$$R^{\mathrm{quad}}_{nd\to np} = A_{nd\to 1s}\left(x_{nd} - \frac{5}{3}x_{np}\right)$$

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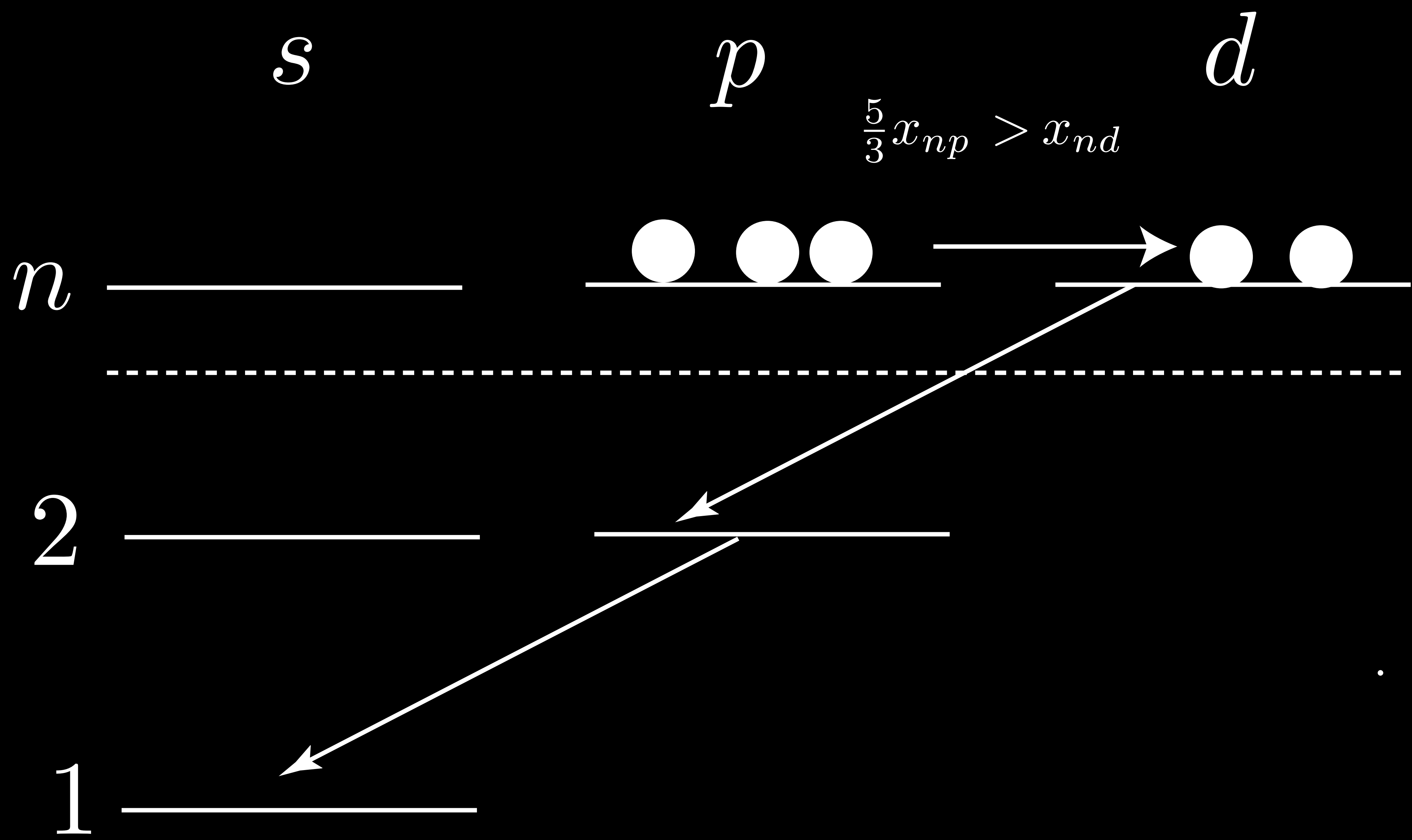
BUILDING INTUITION FOR THE EFFECT OF E2 TRANSITIONS

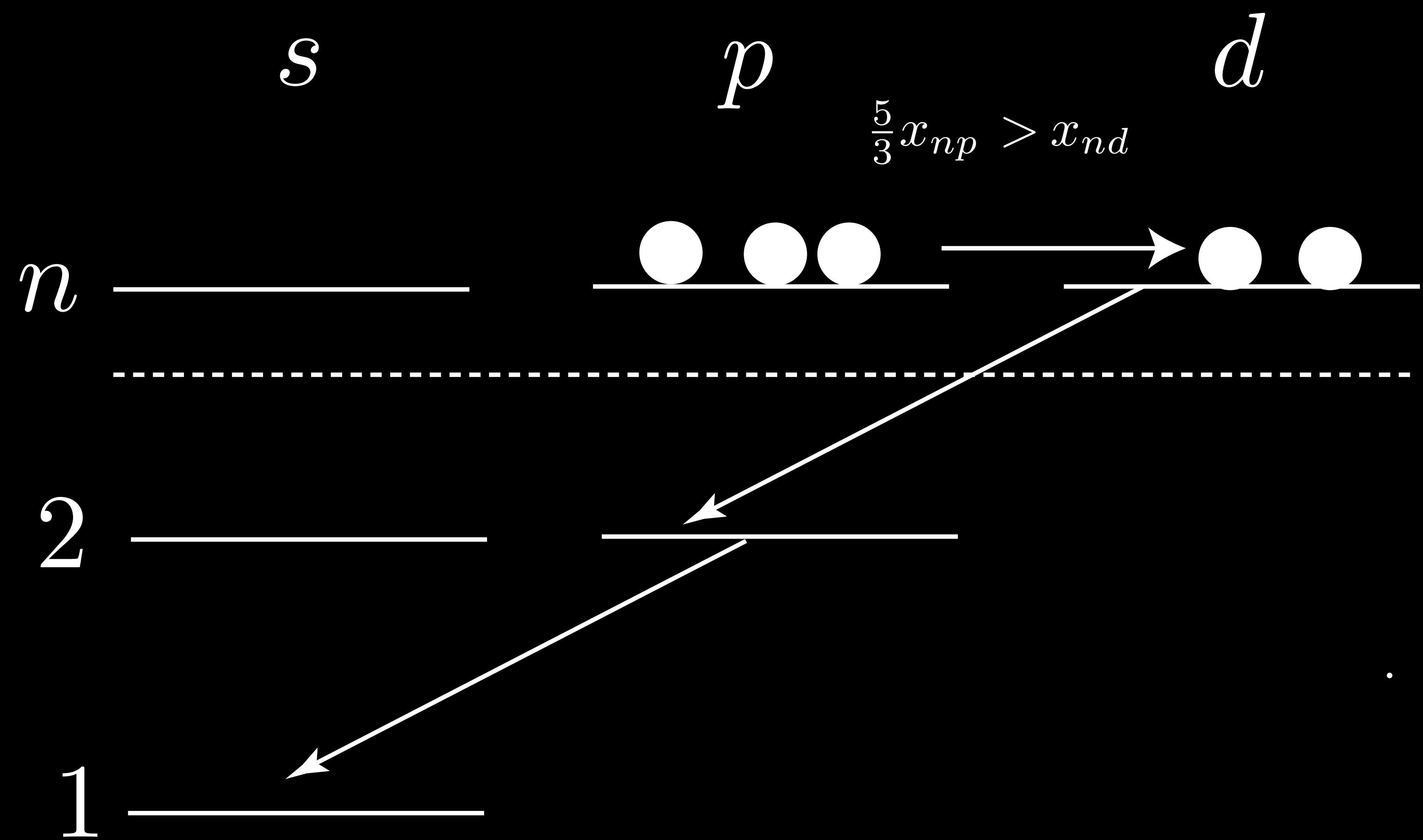


Sub-Dominant decay channel to gs, slows rec down rel. to $n < 5$

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

$n \geq 5$, early times

BUILDING INTUITION FOR THE EFFECT OF E2 TRANSITIONS

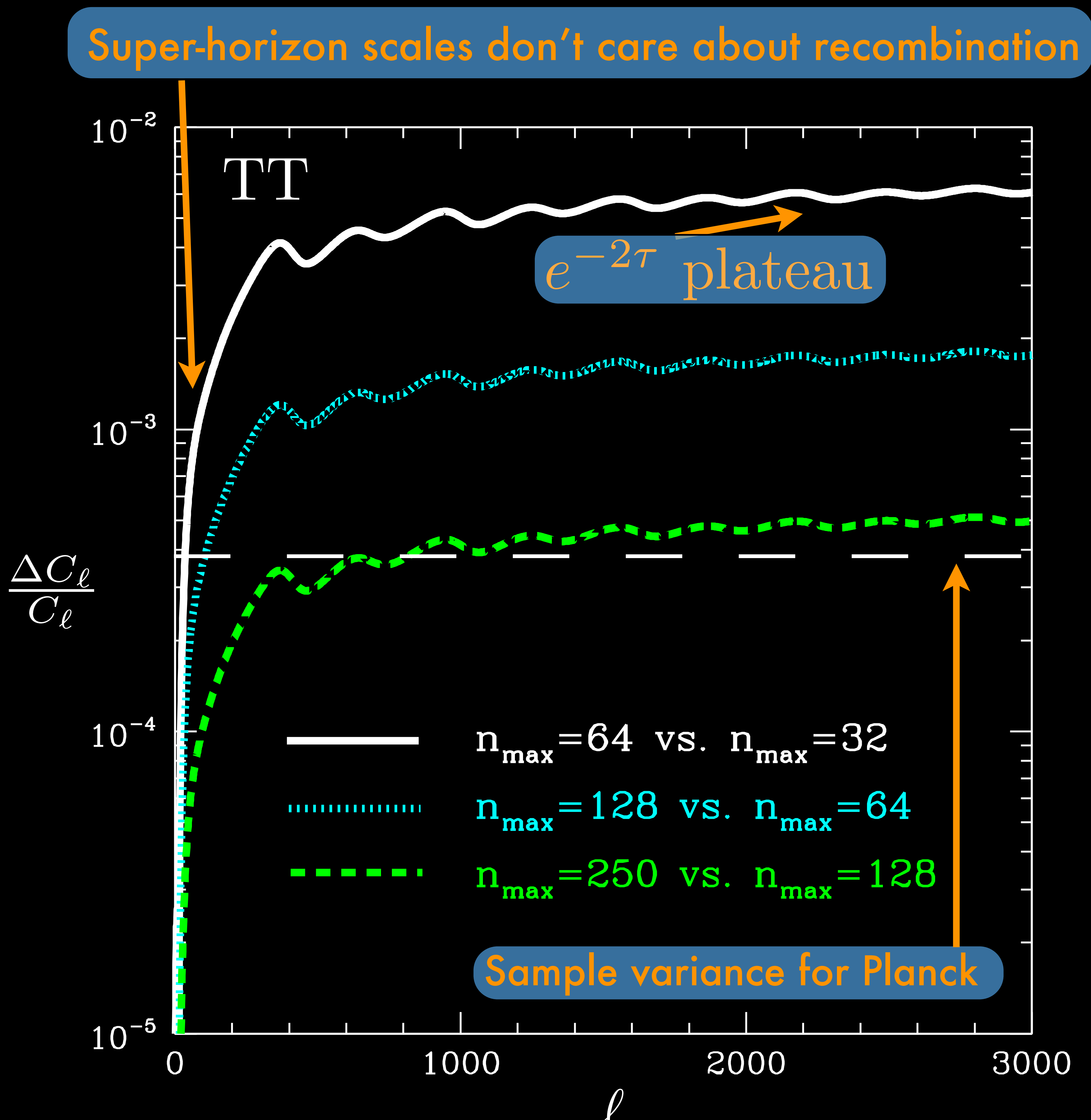


Dominant decay channel to gs, speeds up rec

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

All n, late times

RESULTS: TT $C_l s$ WITH HIGH-N STATES



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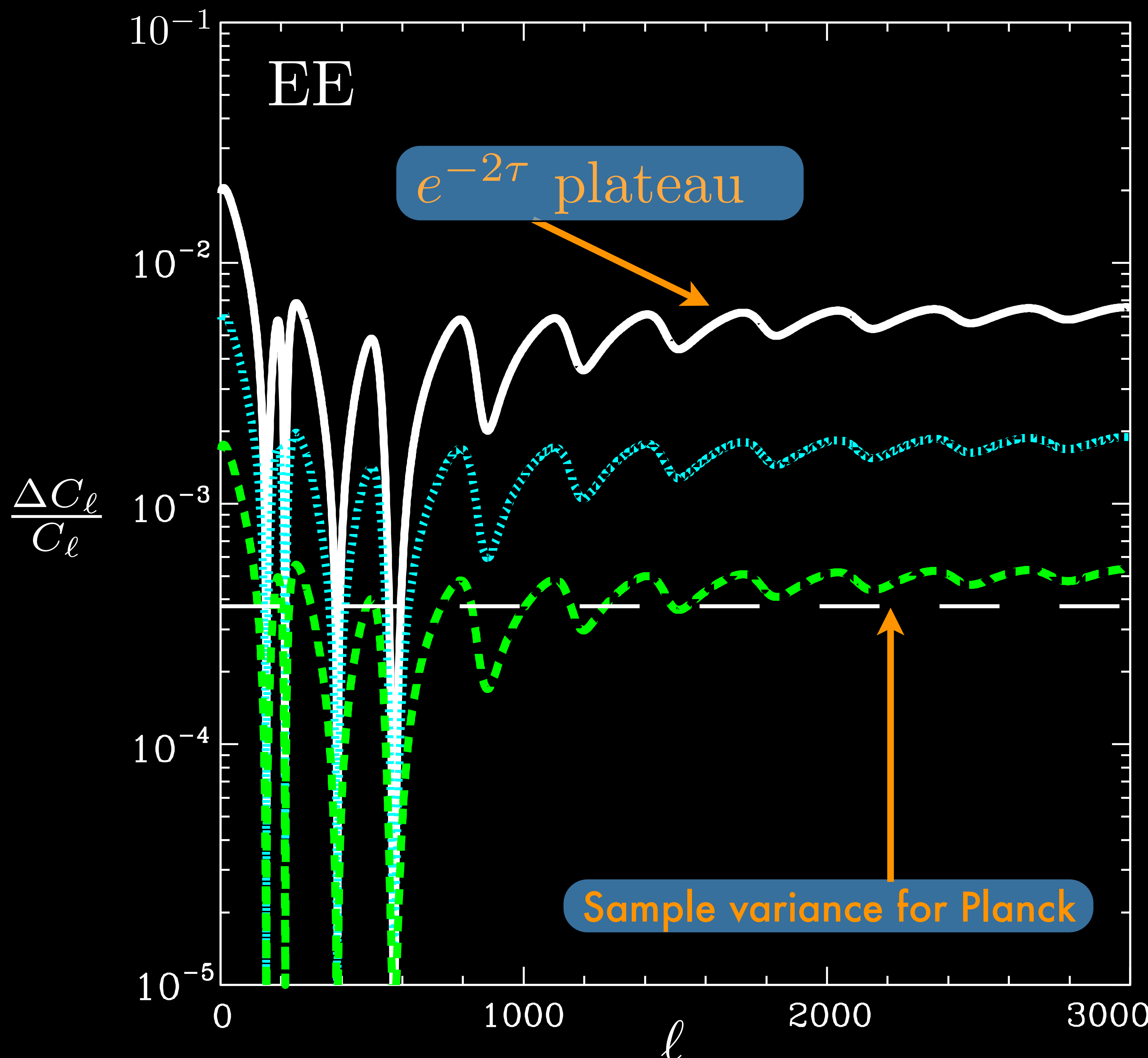
RESULTS: EE $C_l s$ WITH HIGH-N STATES



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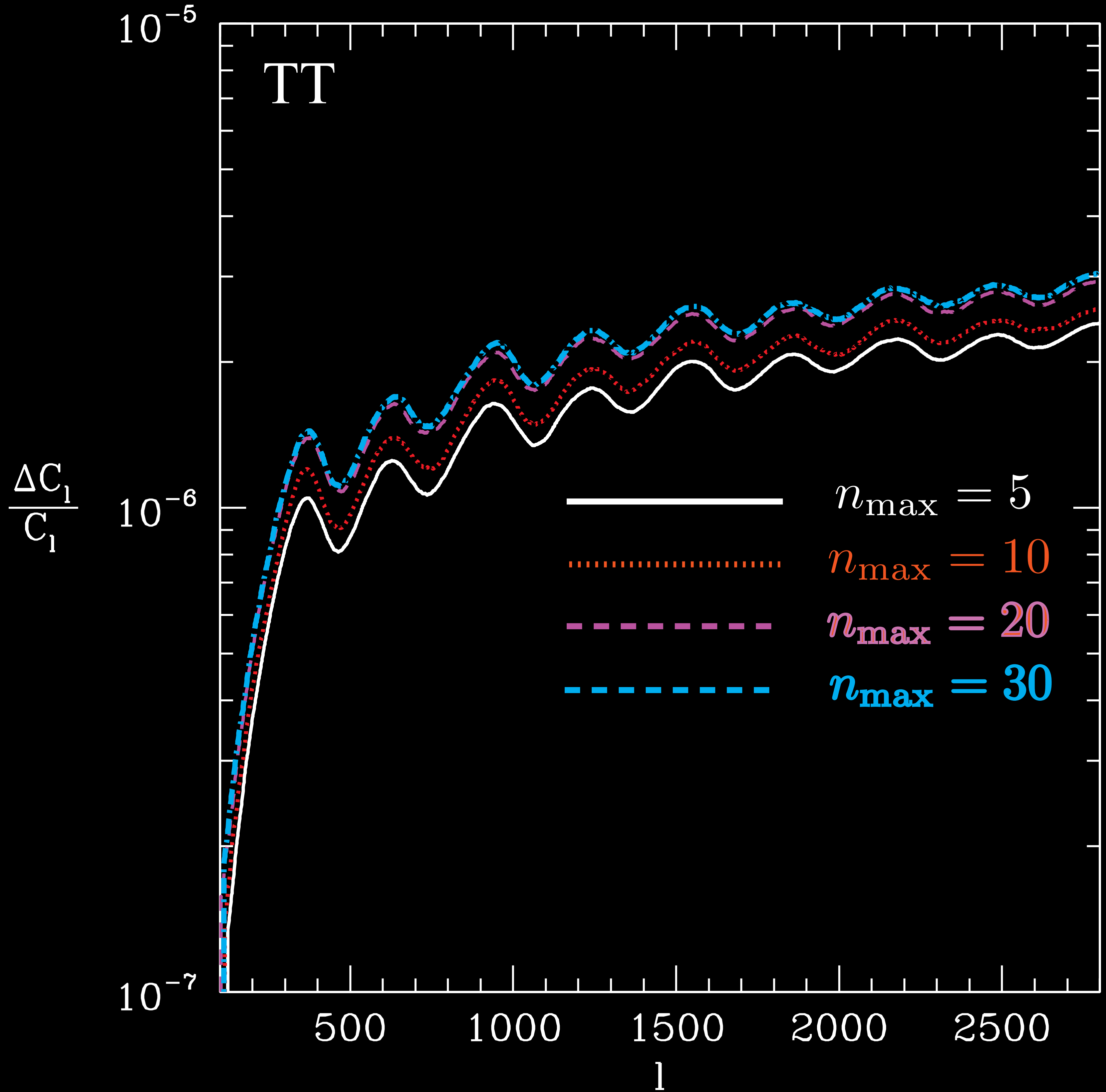
RESULTS: TEMPERATURE (TT) $C_l s$ WITH HYDROGEN QUADRUPOLES,

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



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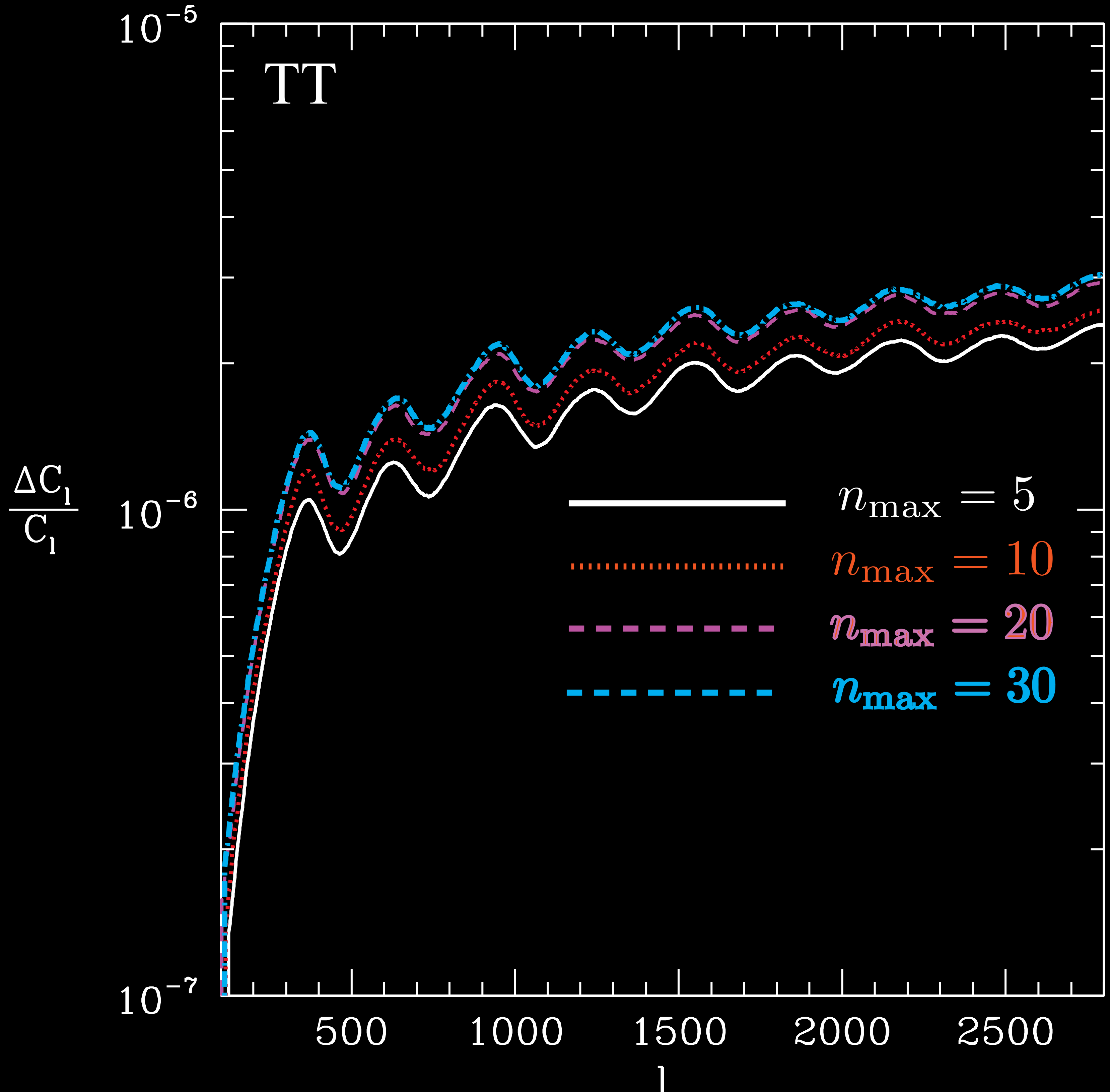
RESULTS: TEMPERATURE (TT) C_ls WITH HYDROGEN QUADRUPOLES,

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



Overall effect is negligible for CMB experiments!

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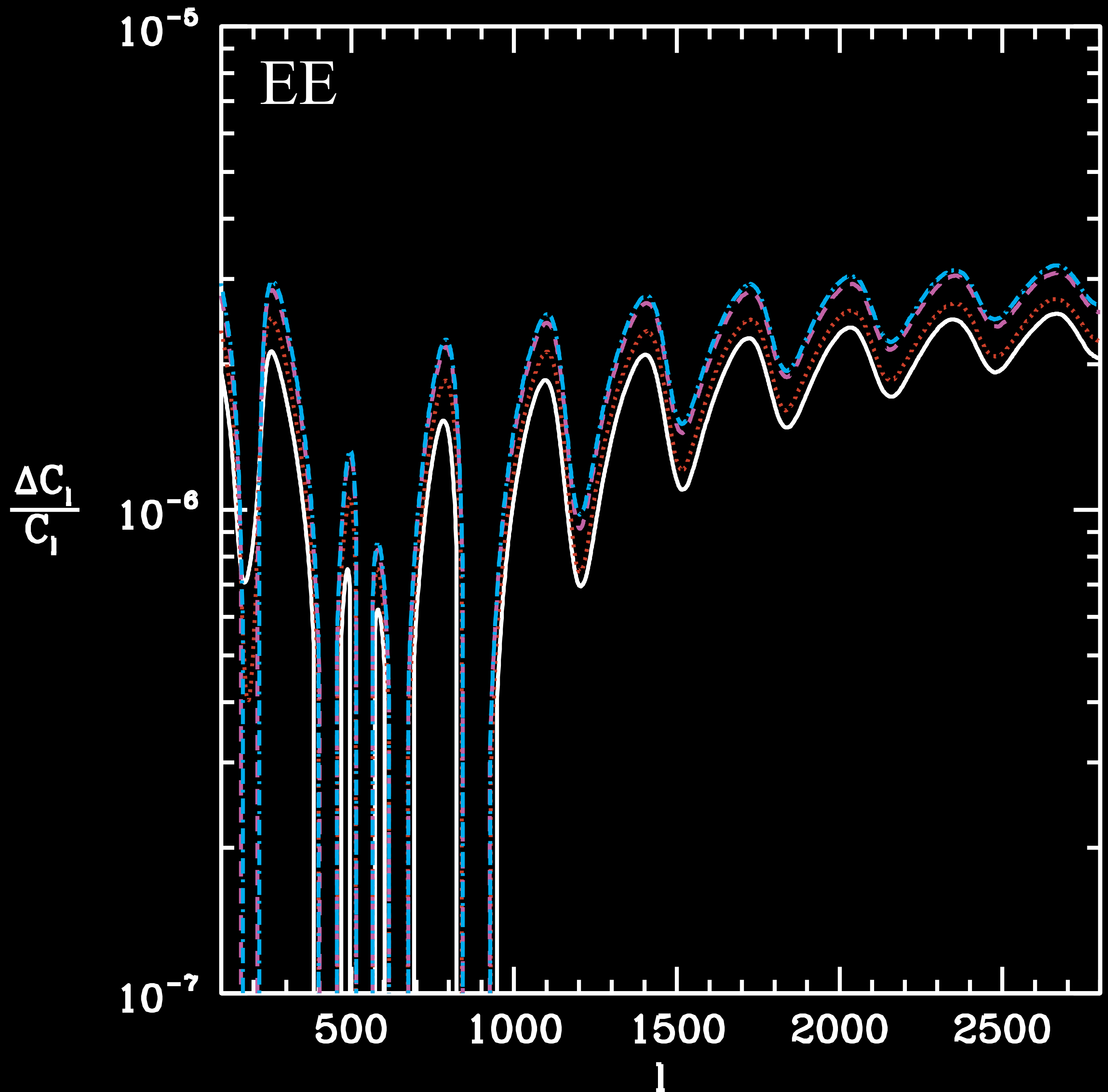
RESULTS: POLARIZATION (EE) C_ls WITH HYDROGEN QUADRUPOLES



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

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

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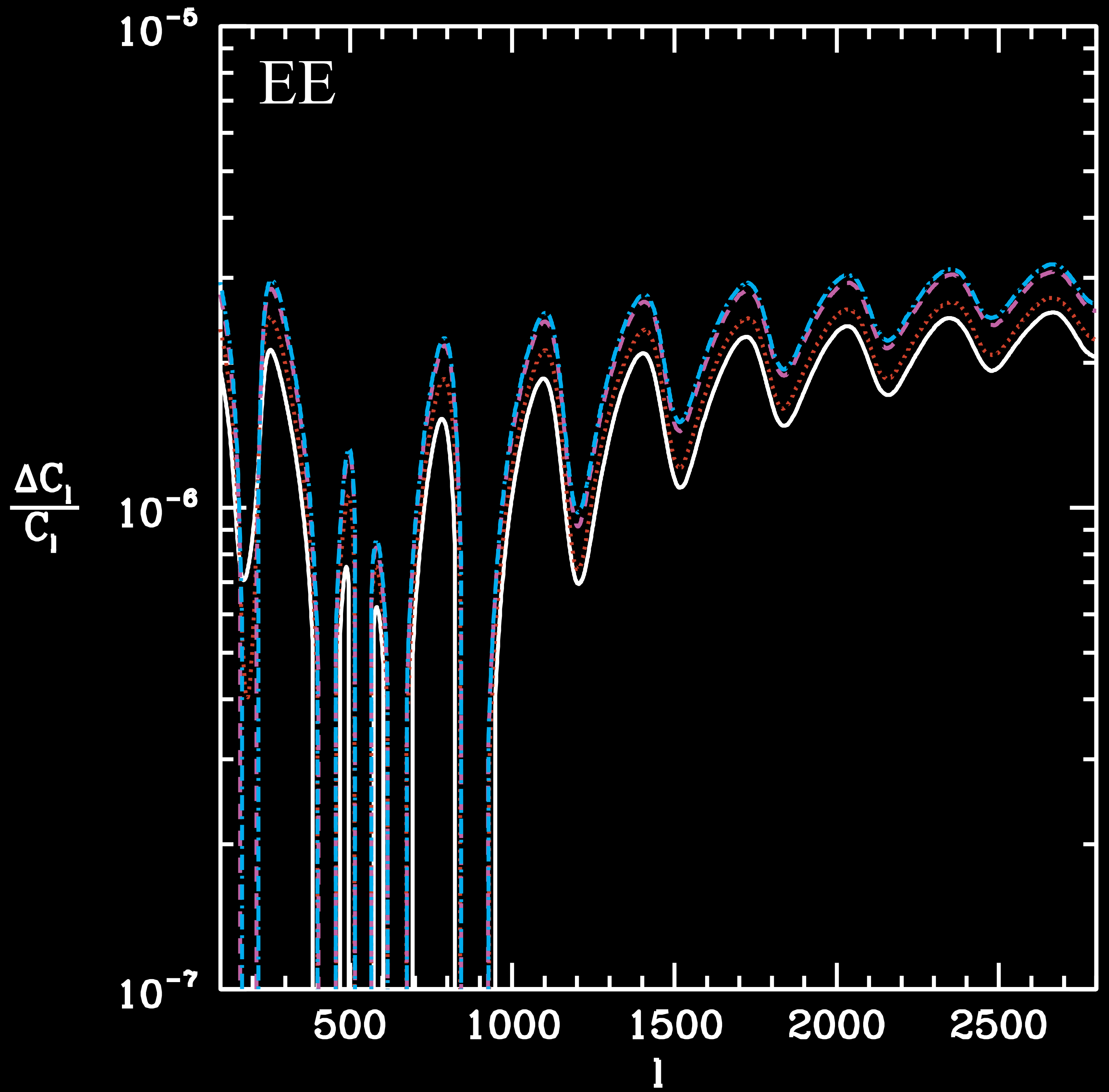
RESULTS: POLARIZATION (EE) C_ls WITH HYDROGEN QUADRUPOLES



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

Overall effect is negligible for upcoming CMB experiments!

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

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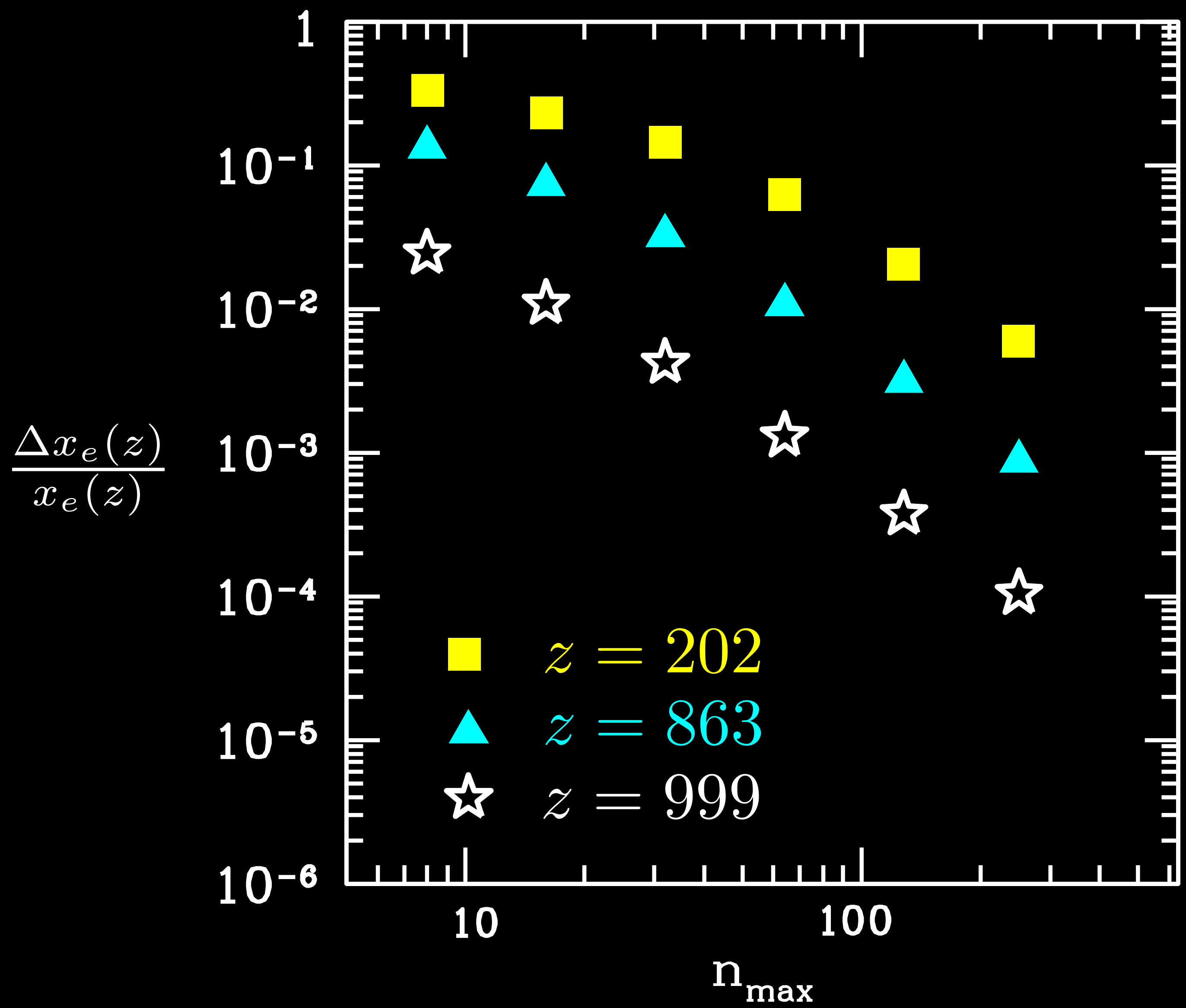
CONVERGENCE



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

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

- Can extrapolate to absolute error

THE UPSHOT FOR COSMOLOGY

- Can explore effect on overall Planck likelihood analysis

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

$$Z = 1.8 \text{ if } n_{\max} = 64,$$
$$Z = 0.50 \text{ if } n_{\max} = 128,$$
$$Z = 0.14 \text{ if } n_{\max} = 250.$$

- Parameter biases can be estimated in Fisher formalism

$$\Delta\alpha^i = \mathcal{F}_{ij}^{-1} B_j$$
$$B_j = \sum_{l,l',X,Y} \frac{\partial C_l^X}{d\alpha^j} F_{ll'} \Delta C_{l'}^Y$$

WRAPPING UP

- RecSparse: a new tool for MLA recombination calculations (watch arXiv in coming weeks for a paper on these results)
  - Highly excited levels (n~64 and higher) are relevant for CMB data analysis
  - E2 transitions in H are not relevant for 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 (homogeneous and perturbed)

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

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

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

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

Fourier transform of classical orbit! Application of correspondence principle!

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

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

$$s = n - n'$$

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

Quadrupole rates: basic formalism

$$A^{\text{quad}}_{n_a,l_a\to n_b,l_b} = \frac{\alpha}{15}\frac{1}{2l_a+1}\frac{\omega^5_{ab}}{c^4}\left\langle l_a||C^{(2)}||l_b\right\rangle^2 \left({}^2R^{n_al_a}_{n_bl_b}\right)^2$$

- 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

$${}^2R^{n_al_a}_{n_bl_b} \equiv \int_0^\infty r^4 R_{n_al_a}(r)R_{n_bl_b}(r)dr$$

Quadrapole rates: Operator algebra

- Radial Schrödinger equation can be factored to yield:

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

$$^{-}\Omega_{nl} R_{nl}(r) = R_{n\ l-1}(r)$$
$$^{+}\Omega_{n\ l-1} R_{nl}(r) = R_{nl}(r)$$

$$A_{nl} = \frac{\sqrt{n^2 - l^2}}{nl}$$

- This algebra can be applied to radial matrix elements:

Quadrapole rates: Operator algebra

- Radial Schrödinger equation can be factored to yield:

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

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

- This algebra can be applied to radial matrix elements:

$$ {}^{2}R^{n\ l-1}_{n'\ l-1} = \frac{1}{A_{nl}} \left\{ A_{n'l}\, {}^{2}R^{nl}_{n'l} + 2^{(1)} R^{nl}_{n'\ l-1} \right\} \qquad {}^{(2)}R^{n\ n'-1}_{n'\ n'-1} = \frac{2nn'}{\sqrt{n^2 - n'^2}} {}^{(1)}R^{nn'}_{n\ n'-1} $$

Diagonal!

Quadrapole rates: Operator algebra

- Radial Schrödinger equation can be factored to yield:

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

$$ {}^{-}\Omega_{nl} R_{nl}(r) = R_{n\ l-1}(r) $$
$$ {}^{+}\Omega_{n\ l-1} R_{nl}(r) = R_{nl}(r) $$

$$ A_{nl} = \frac{\sqrt{n^2 - l^2}}{nl} $$

- This algebra can be applied to radial matrix elements:

$$ l(2l+3)A_{n'l}\,{}^{(2)}R^{n\ l+1}_{n'\ l-1} = (2l+1)(l+2)A_{n\ l+2}\,{}^{(2)}R^{n\ l+2}_{n'l} + 2(l+1)A_{n'\ l+1}\,{}^{(2)}R^{n\ l+1}_{n'\ l+1} + 2(2l+1)(3l+5)\,{}^{(1)}R^{n\ l+1}_{n'l} \quad (1 \le l \le\ n'-1) $$

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

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

Off-diagonal!