



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
CITA Seminar
11/19/09

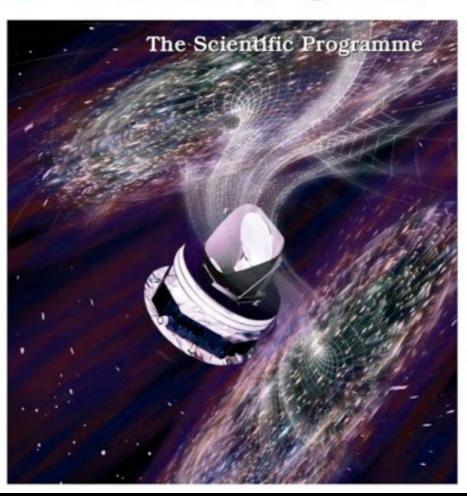
OUTLINE

- * 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

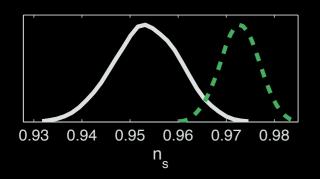


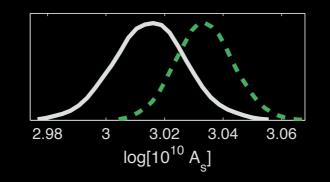
- * Planck (launched May 2009) will make cosmic-variance limited CMB anisotropy measurements up to 1~2500 (T), and 1~1500 (E)
- * Wong 2007 and Lewis 2006 show that $x_e(z)$ needs to be predicted to several parts in 10^4 accuracy for Planck data analysis

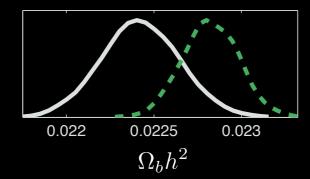
RECOMBINATION, INFLATION, AND REIONIZATION

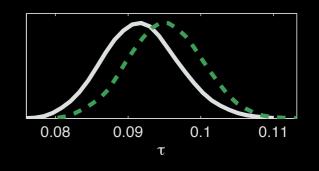
$$P(k) = A_s \left(k\eta_0\right)^{n_s}$$

* 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

$$n_s = 1 - 4\epsilon + 2\eta$$

$$\epsilon = rac{m_{
m pl}^2}{16\pi} \left[rac{V'(\phi)}{V(\phi)}
ight]^2$$

$$\epsilon = \frac{m_{\rm pl}^2}{16\pi} \left[\frac{V'(\phi)}{V(\phi)} \right]^2 \qquad A_s^2 = \left. \frac{32}{75} \frac{V}{m_{\rm pl}^4 \epsilon} \right|_{k_{\rm pivot} = aH}$$

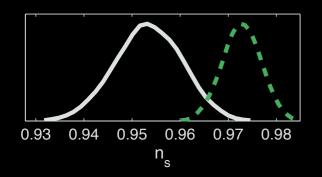
CAVEAT EMPTOR: $3 \lesssim ? \lesssim 16$

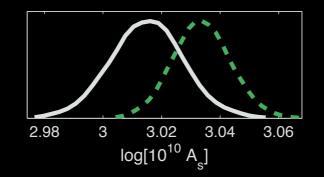
$$3 \lesssim ? \lesssim 16$$

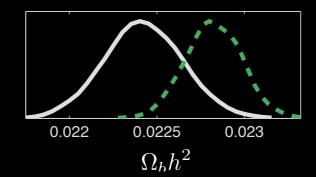
Need to do eV physics right to infer anything about 10? GeV physics! 4

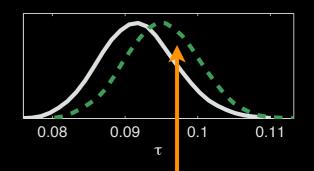
RECOMBINATION, INFLATION, AND REIONIZATION

* 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

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

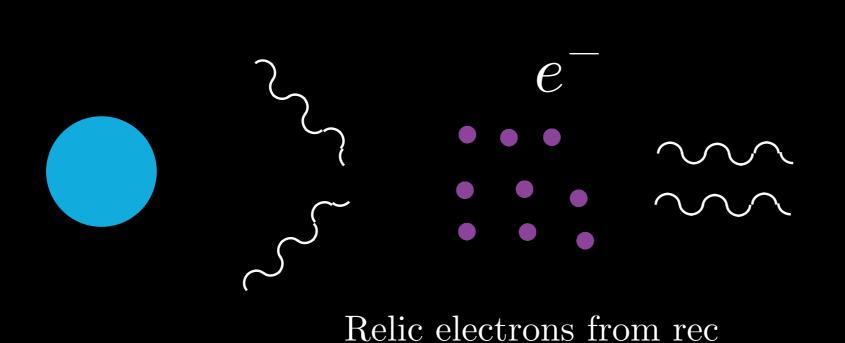
* $z_{\rm dec} \simeq 1100$: Decoupling occurs during recombination

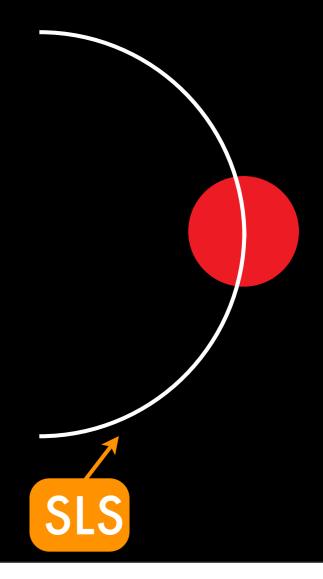
$$C_l \to C_l e^{-2\tau(z)}$$
 if $l > \eta_{\rm dec}/\eta(z)$

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

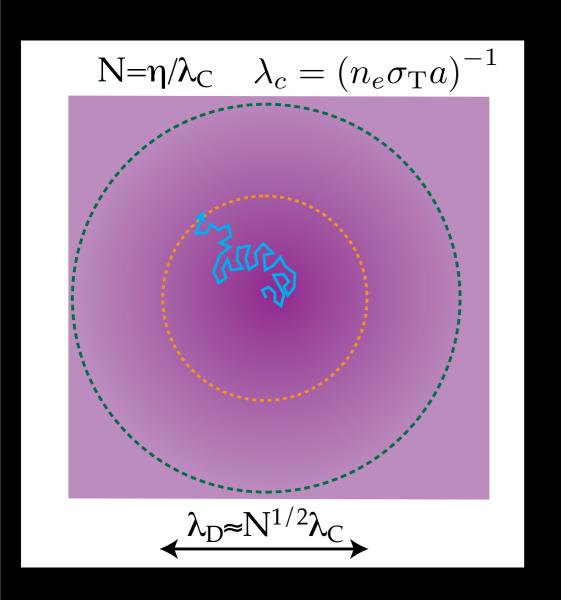
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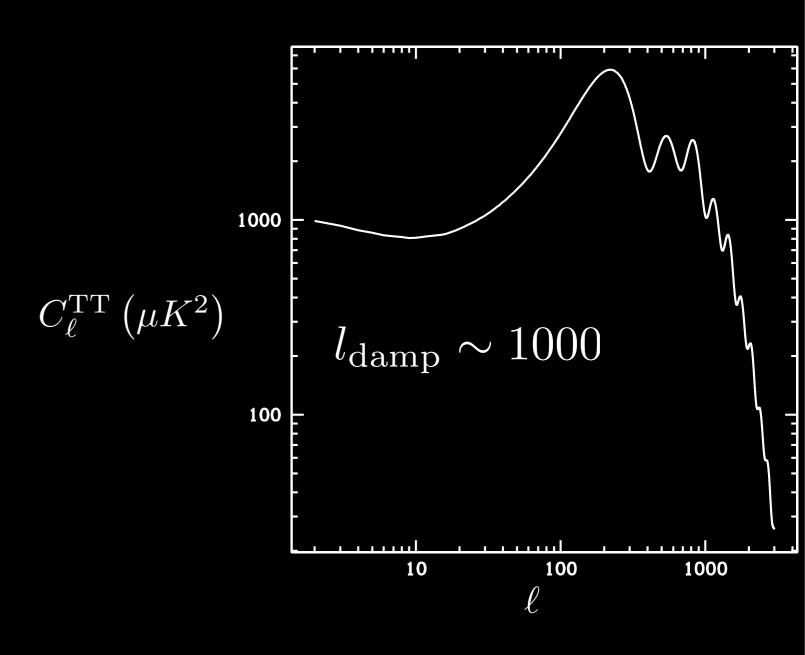
$$\gamma + e^- \Leftrightarrow \gamma + e^-$$





PHYSICAL RELEVANCE FOR CMB: THE SILK DAMPING TAIL





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

PHYSICAL RELEVANCE FOR CMB: POLARIZATION

Isotropic radiation

Quadrupole moment

No polarization

Polarization

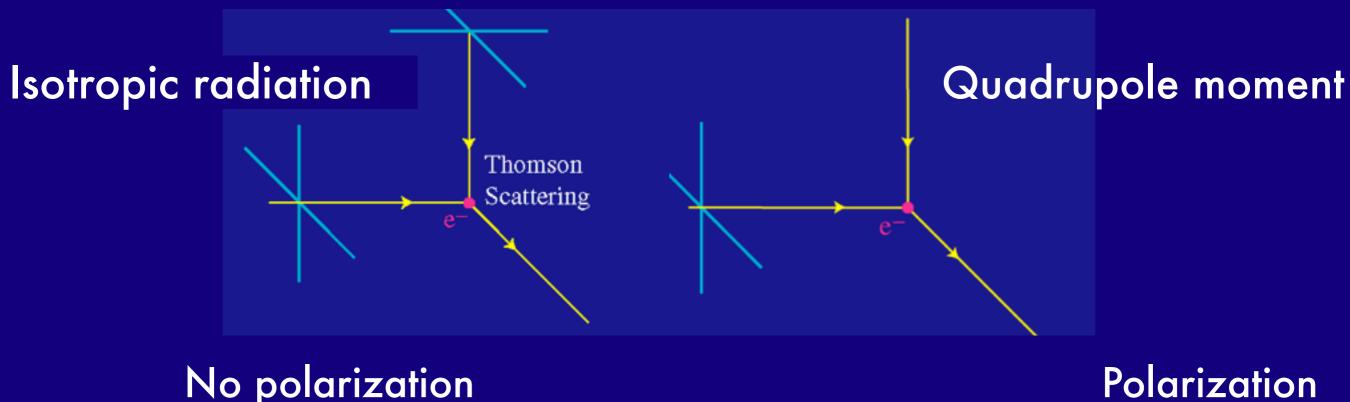
From Wayne Hu's website

* Need time to develop a quadrapole

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

* Need to scatter quadrapole to polarize CMB

PHYSICAL RELEVANCE FOR CMB: POLARIZATION



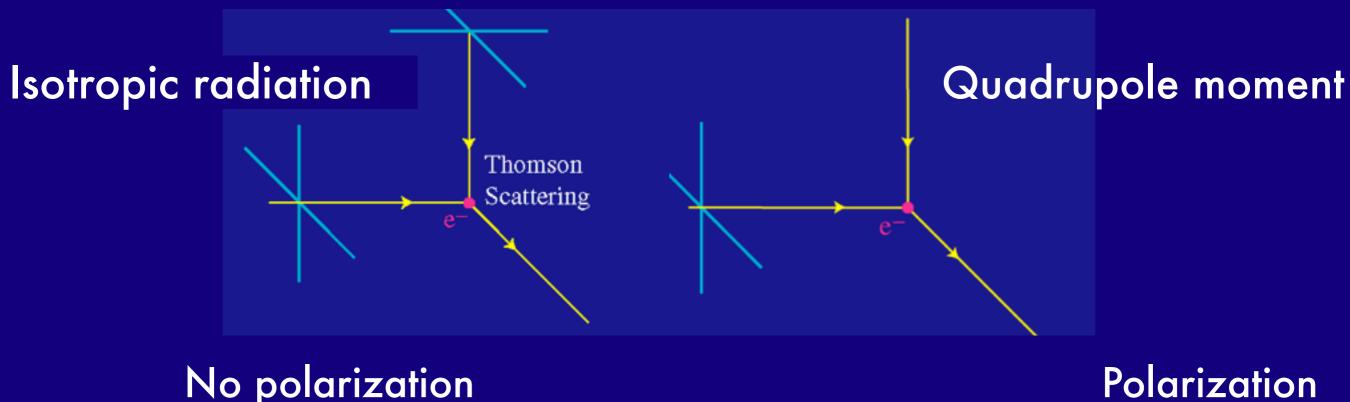
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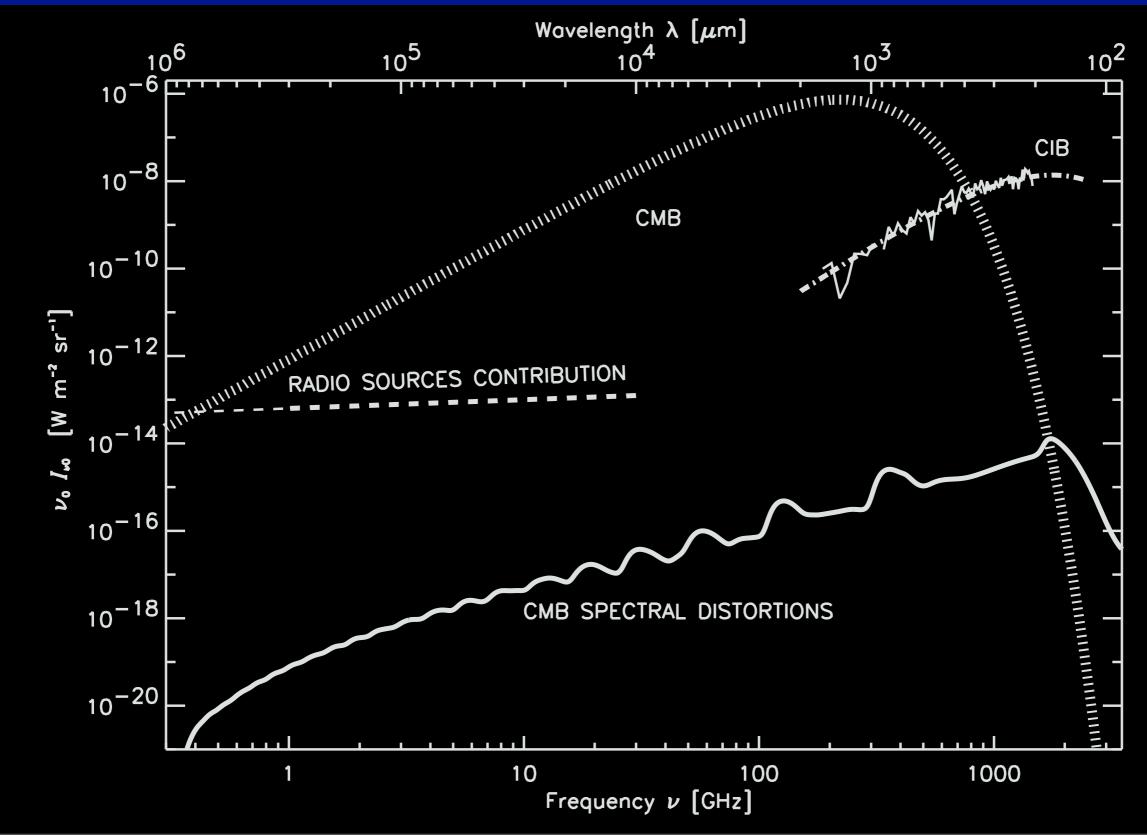
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PHYSICAL RELEVANCE FOR CMB: SPECTRAL DISTORTIONS FROM RECOMBINATION



SAHA EQUILIBRIUM IS INADEQUATE

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

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

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

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

$$z_{\rm rec} \simeq 1300$$

*Further evolution falls prey to reaction freeze-out

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

BOTTLENECKS/ESCAPE ROUTES

BOTTLENECKS

* Ground state recombinations are ineffective

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

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

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

ESCAPE ROUTES (e.g. n=2)

* Two-photon processes

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

* Redshifting off resonance

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

* Only n=2 bottlenecks are treated

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

* Only n=2 bottlenecks are treated

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

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

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

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

*Net Rate is suppressed by bottleneck vs. escape factor

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 Rec

Redshifting term

$$S = \frac{\frac{8\pi}{\lambda_{\alpha}^{3} n_{1s}} H + \Lambda_{2s \to 1s}}{\frac{8\pi}{\lambda_{\alpha}^{3} n_{1s}} H + (\Lambda_{2s \to 1s} + \beta_{c})}$$
 2 γ term

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 Ionization Term

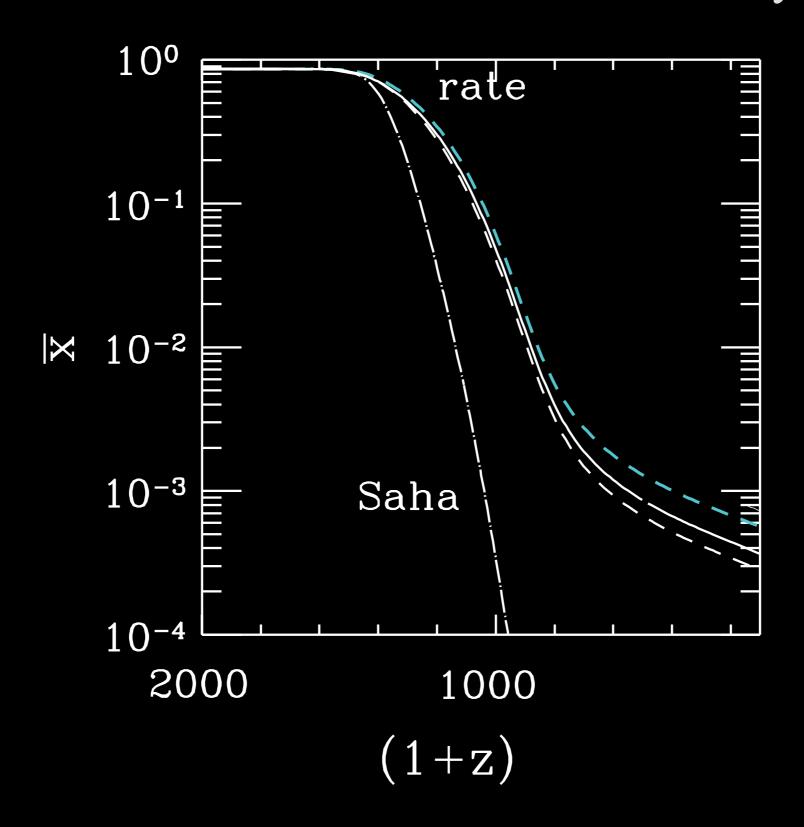
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 Ionization Term

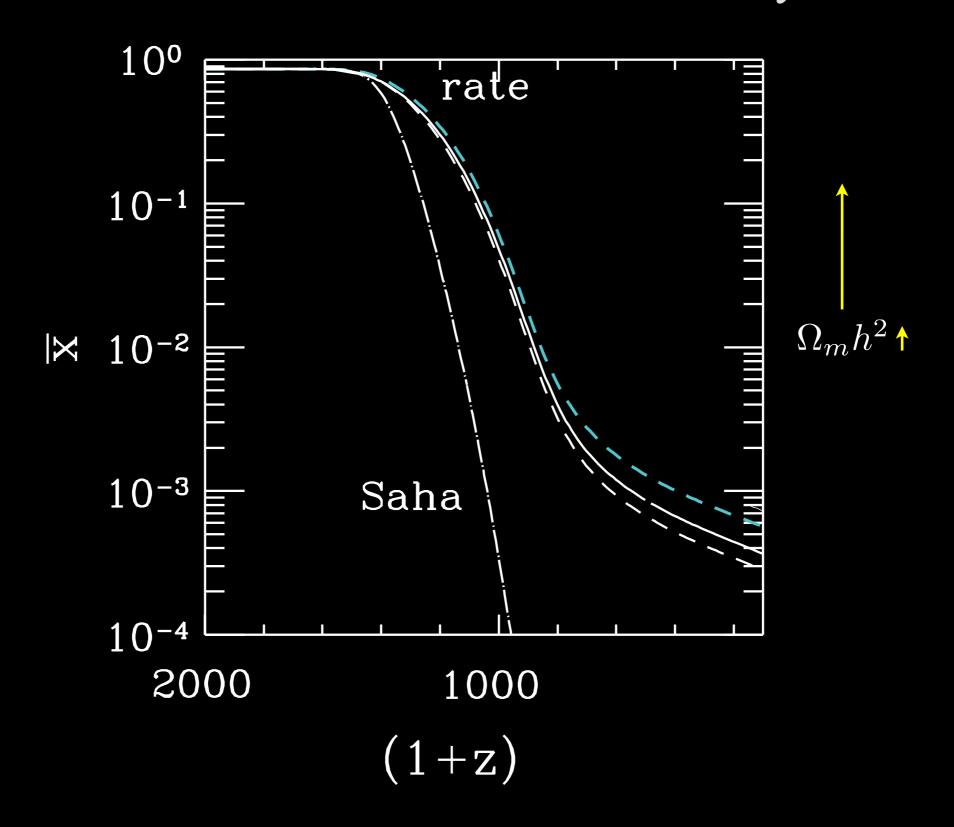
$$\frac{\text{redshift term}}{2\gamma \text{ term}} \simeq 0.02 \frac{\Omega_{m}^{1/2}}{(1 - x_{e}[z]) \left(\frac{1+z}{1100}\right)^{3/2}}$$

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

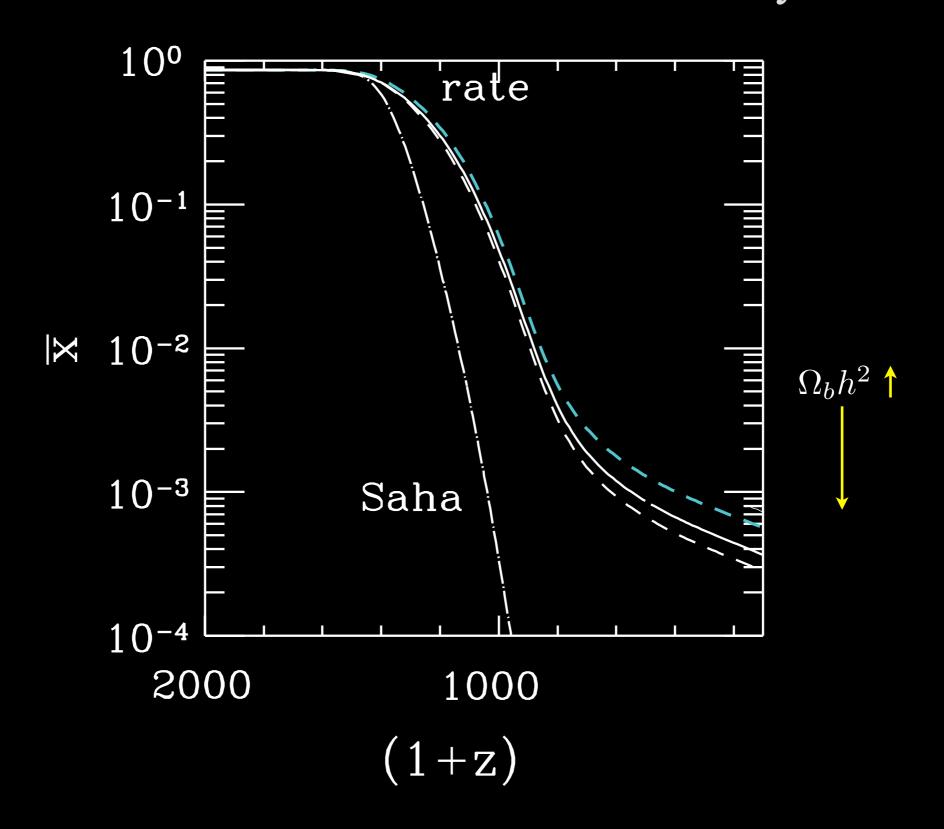
* Peebles 1967: State of the Art for 30 years!



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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

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

EQUILIBRIUM ASSUMPTIONS

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

Seager/Scott/Sasselov 2000/RECFAST!

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

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 $n_{\rm max}=100$
- * 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_{max} is hard!

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

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

THESE ARE REAL STATES

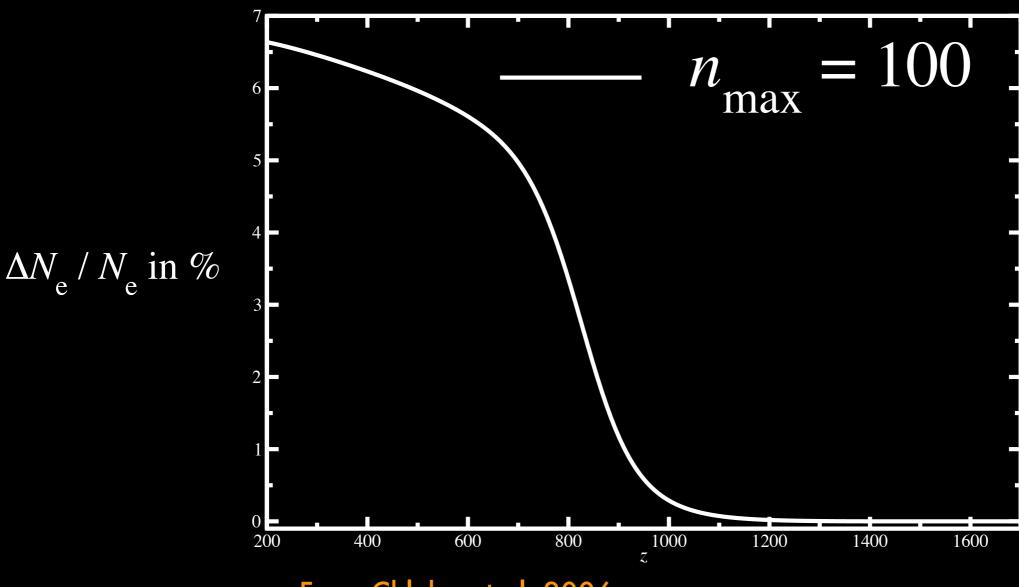
- * Still inside plasma shielding length for n<100000
- * $r \sim a_0 n^2$ is as large as $2\mu \text{m}$ for $n_{\text{max}} = 200$

$$\frac{*}{E} \frac{\Delta E|_{\text{thermal}}}{E} < \frac{2}{n^3}$$

* Similarly high n are seen in emission line nebulae

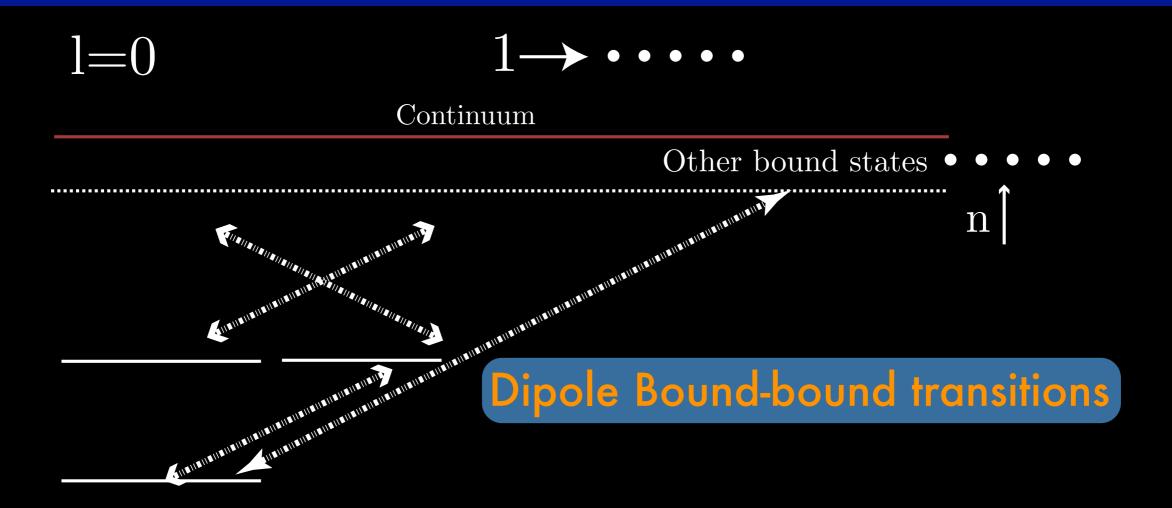
THE EFFECT OF RESOLVING 1- SUBSTATES

Resolved I vs unresolved I

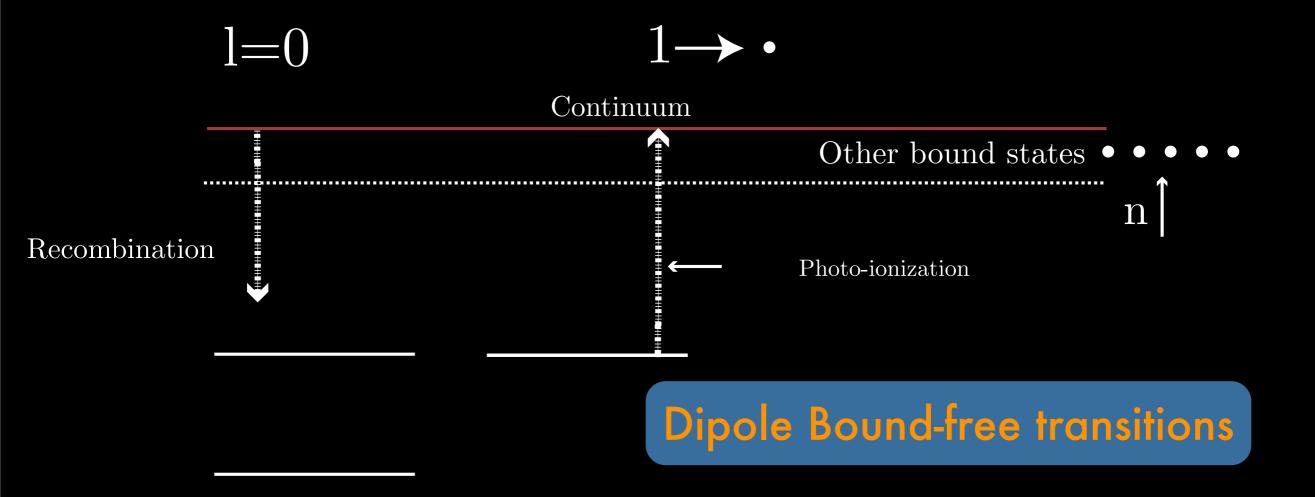


From Chluba et al. 2006

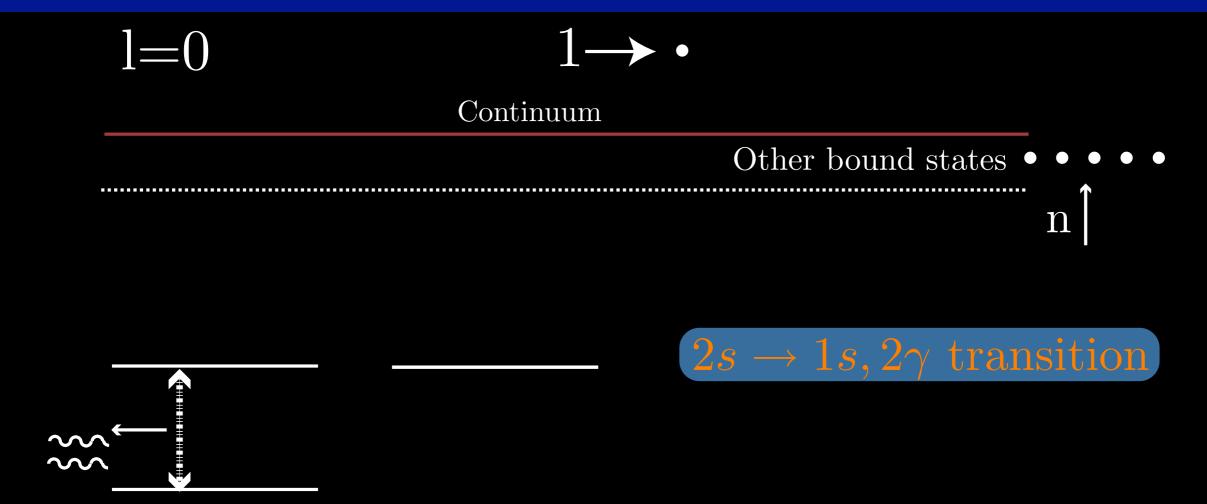
* 'Bottlenecked' l-substates decay slowly to 1s: Recombination is slower; Chluba al. 2006



- * 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



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*Free electron fraction evolved according to

$$\dot{x}_e = -\dot{x}_{1s}
= -\Lambda_{2s \to 1s} \left(x_{2s} - x_{1s} e^{-E_{2s \to 1s}/T_{\gamma}} \right) + \sum_{n,l>1s} A_{n1}^{l \ 0} P_{n1}^{l0} \left\{ g(T,n,l) \right\}$$

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 2s-1s decay rate

RECSPARSE AND THE MULTI-LEVEL ATOM

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Einstein coeff.

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Escape probability

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Lyman series current to ground state

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

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

$$au_s \propto rac{n_{
m H} x_n^l A_{nn'}^{ll'}}{H\left(z
ight)} \quad n' > n_s$$

- * 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

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Resonant absorber density

$$au_s \propto rac{n_{
m H} x_n^l A_{nn'}^{ll'}}{H\left(z
ight)} \quad n' > n$$

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Einstein coefficient
$$\tau_s \propto \frac{n_{\rm H} x_n^l A_{nn'}^{ll'}}{H\left(z\right)} \quad n' > n$$

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Cosmological expansion

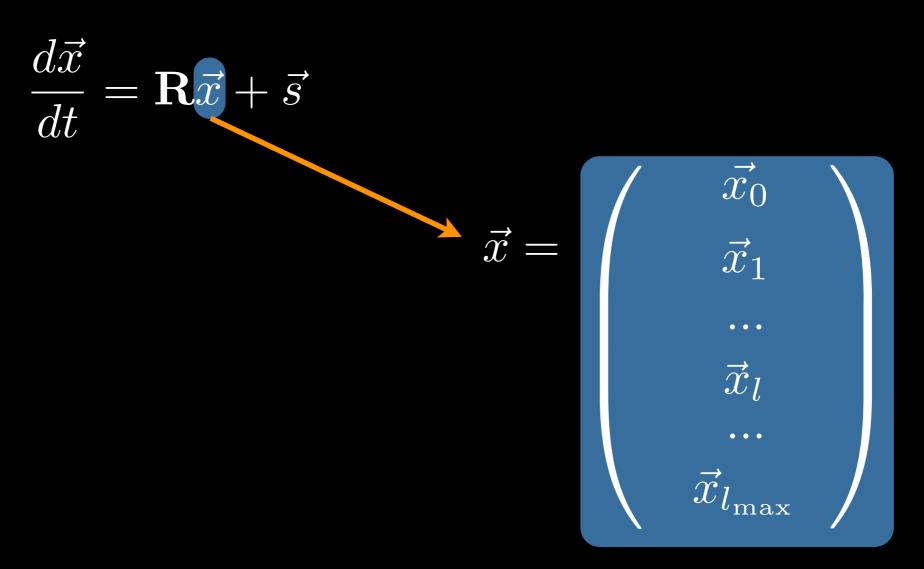
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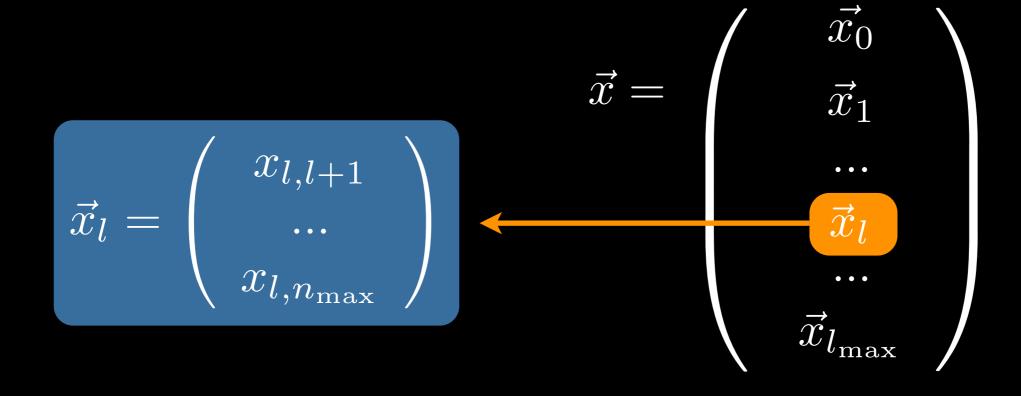
OTHER CORRECTIONS TO RECOMBINATION

- * Deviations from steady-state approx (Chluba/Sunyaev 2008)
- * Coherent scattering
- * 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)

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



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



* Evolution equations may be re-written in matrix form



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

* Evolution equations may be re-written in matrix form



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

* Evolution equations may be re-written in matrix form

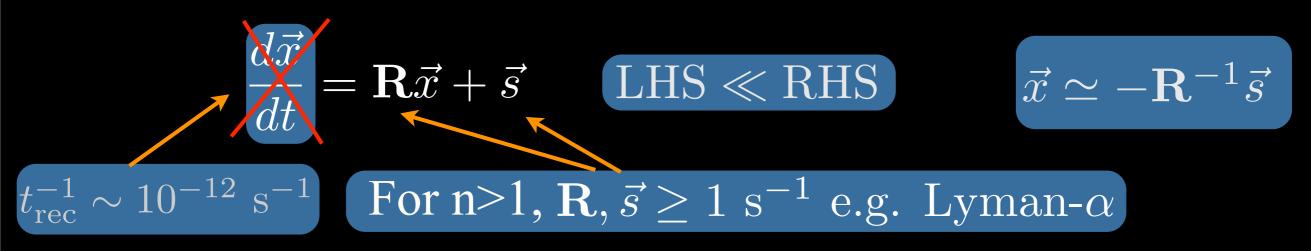
$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$

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

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$
 For n>1, $\mathbf{R}, \vec{s} \ge 1 \text{ s}^{-1} \text{ e.g. Lyman-}\alpha$

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

$$t_{\rm rec}^{-1} \sim 10^{-12} \text{ s}^{-1}$$
 For n>1, $\mathbf{R}, \vec{s} \ge 1 \text{ s}^{-1}$ 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 $An_{max}^6 \sim 10^5 \text{ s for } n_{max} = 200$ for a single time step
- * Dipole selection rules: $\Delta l = \pm 1$

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

$$\mathbf{M}_{l,l-1}\vec{x}_{l-1} + \mathbf{M}_{l,l}\vec{x}_l + \mathbf{M}_{l,l+1}\vec{x}_{l+1} = \vec{s}_l \quad \left(\begin{array}{c} \mathbf{N} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{N} & \mathbf{N} \\ \mathbf{N} & \mathbf{N}$$

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

RAPID MATRIX INVERSION: SPARSITY TO THE RESCUE

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

$$P_{n,n'}^{l,l'} = \frac{1 - e^{-\tau_s}}{\tau_s}$$
 $R \propto AP \propto A/\tau \text{ if } \tau \gg 1$
 $\tau \propto A \to R \to A/A \to \text{const}$

* Coupling to ground state will overwhelmingly dominate:

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

QUADRUPOLE TRANSITIONS AND RECOMBINATION

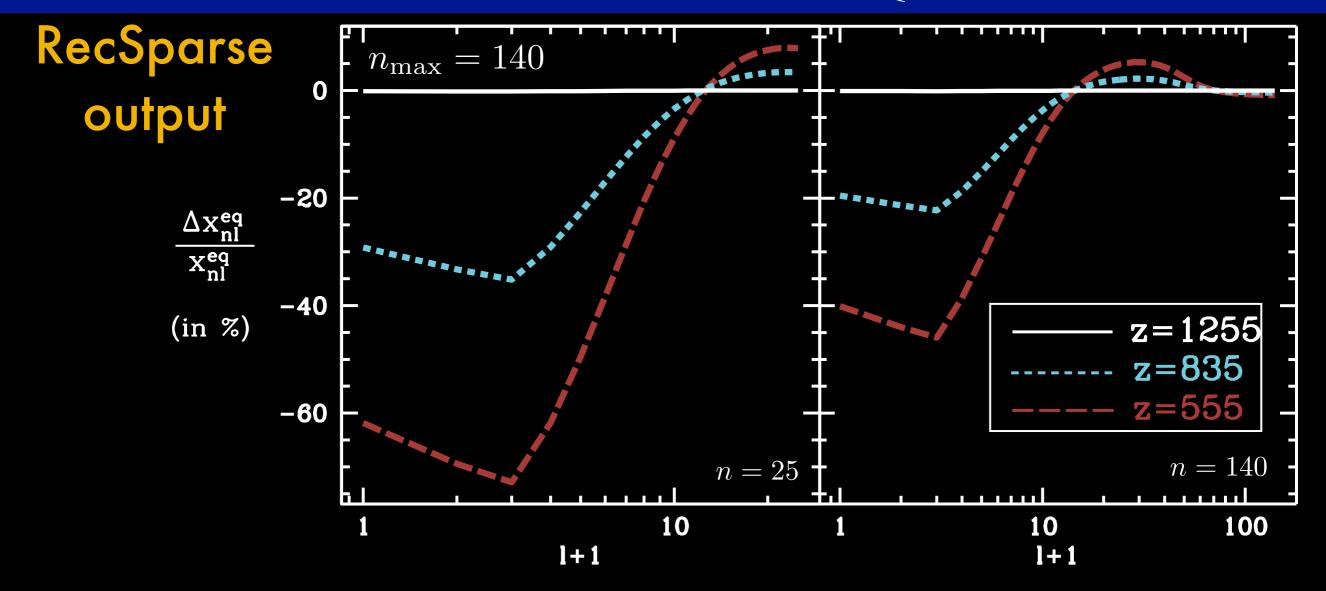
* Lyman lines are optically thick, so $nd \to 1s$ immediately followed by $1s \to np$, so this can be treated as an effective $d \to p$ process with rate $A_{nd \to 1s} x_{nd}$.

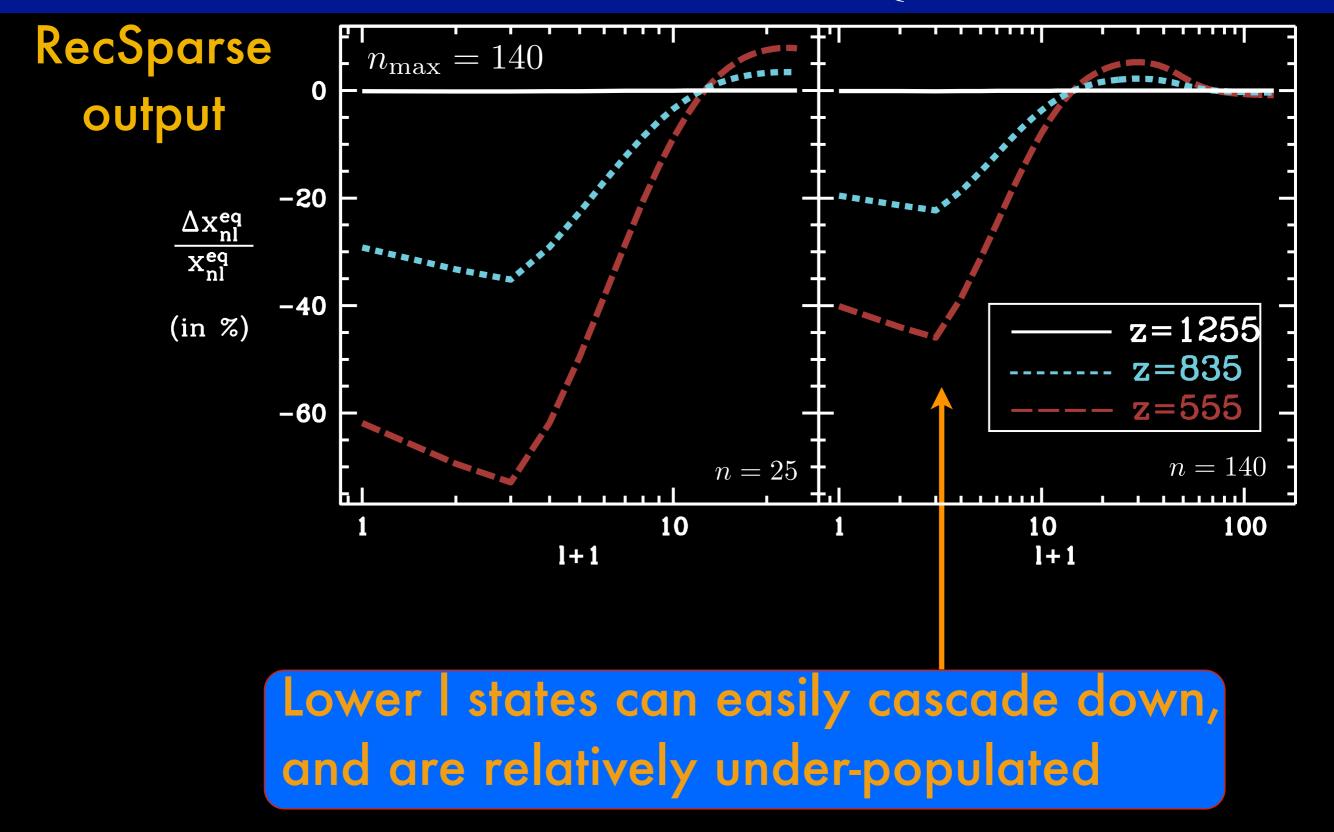
* Same sparsity pattern of rate matrix, similar to 1-changing collisions

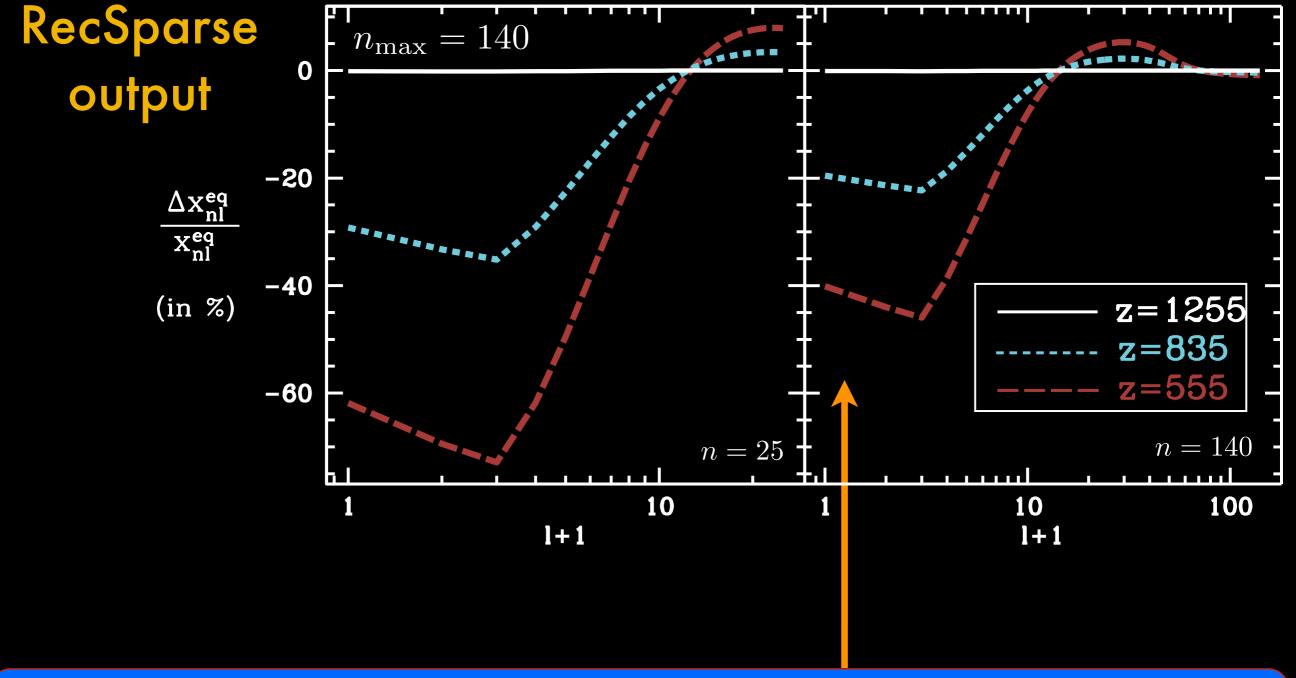
* Detailed balance yields net rate

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

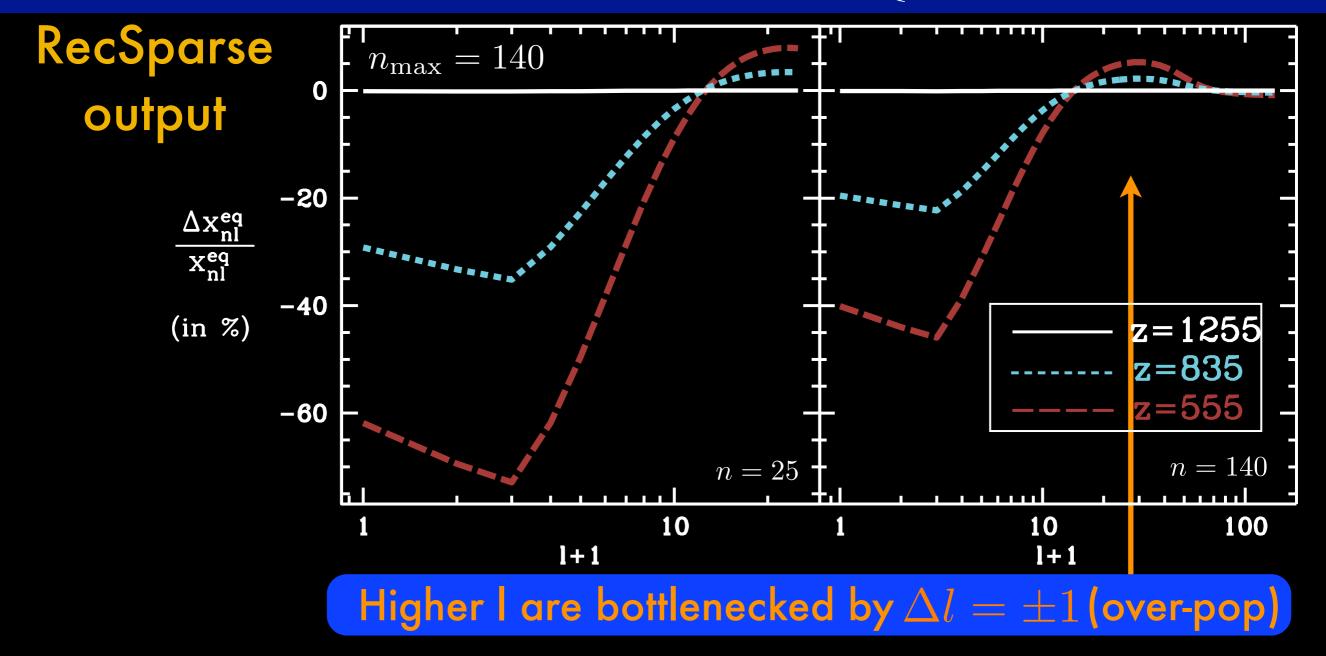
RESULTS: STATE OF THE GAS

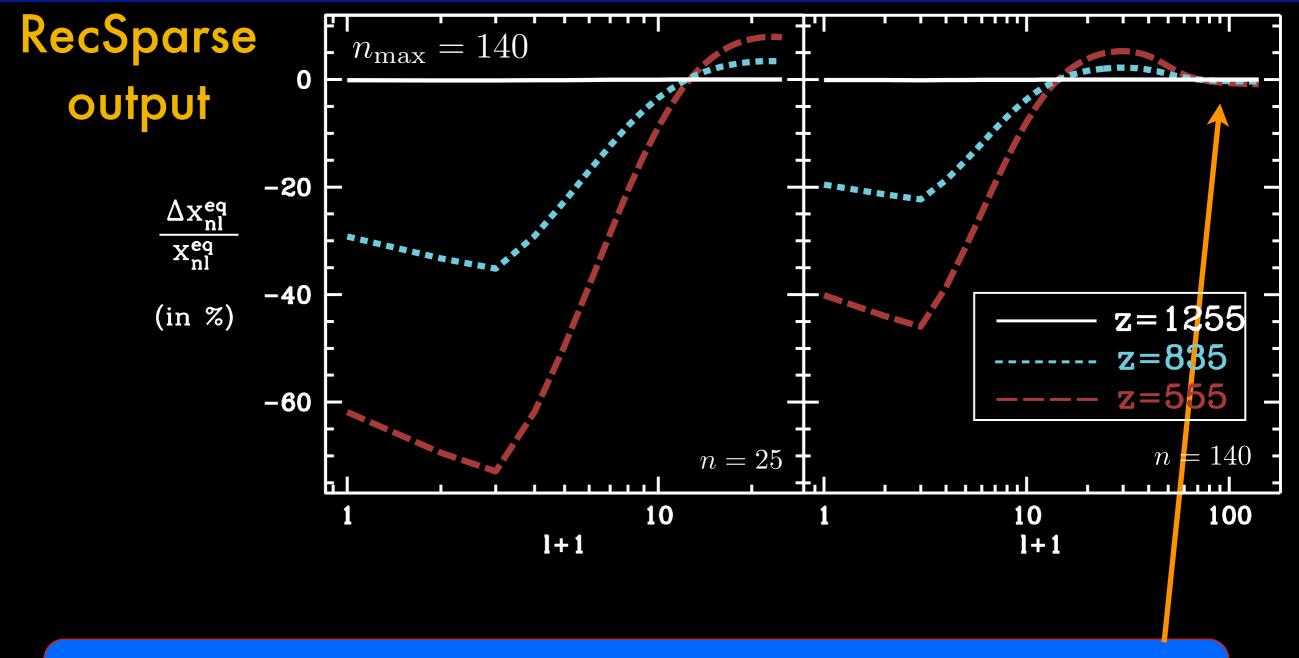




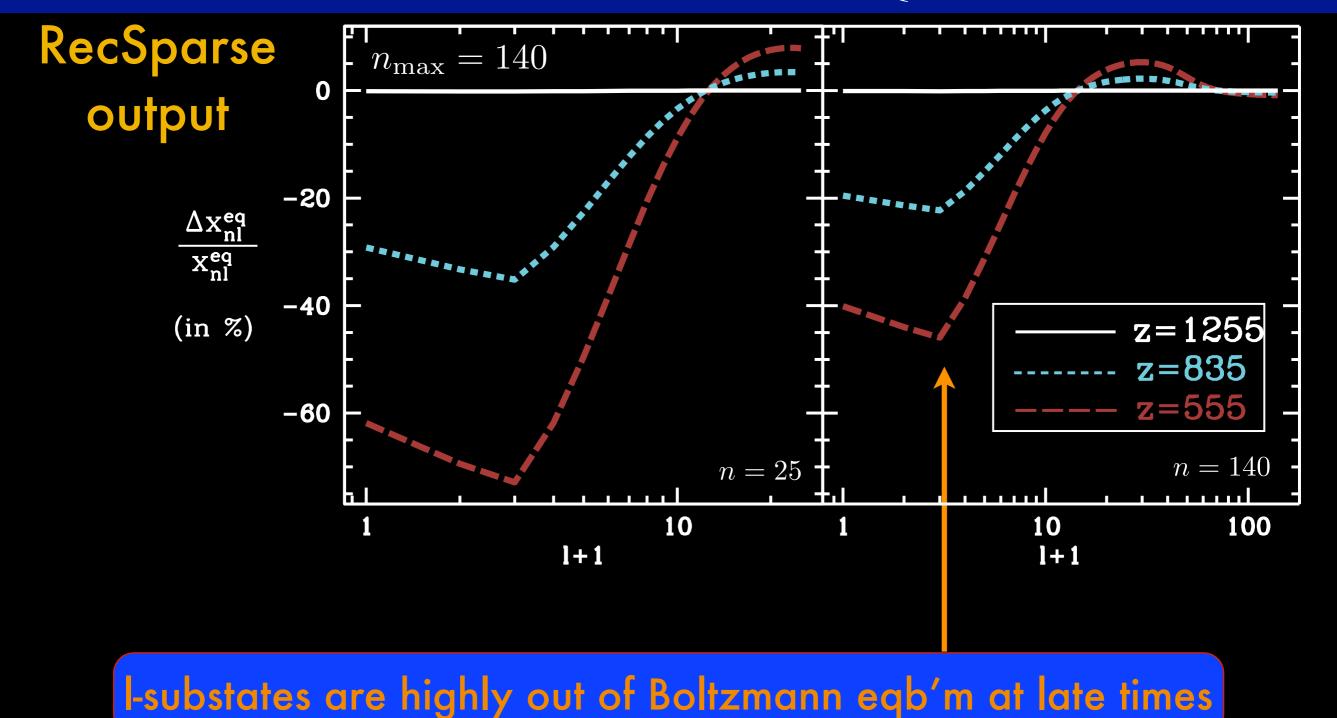


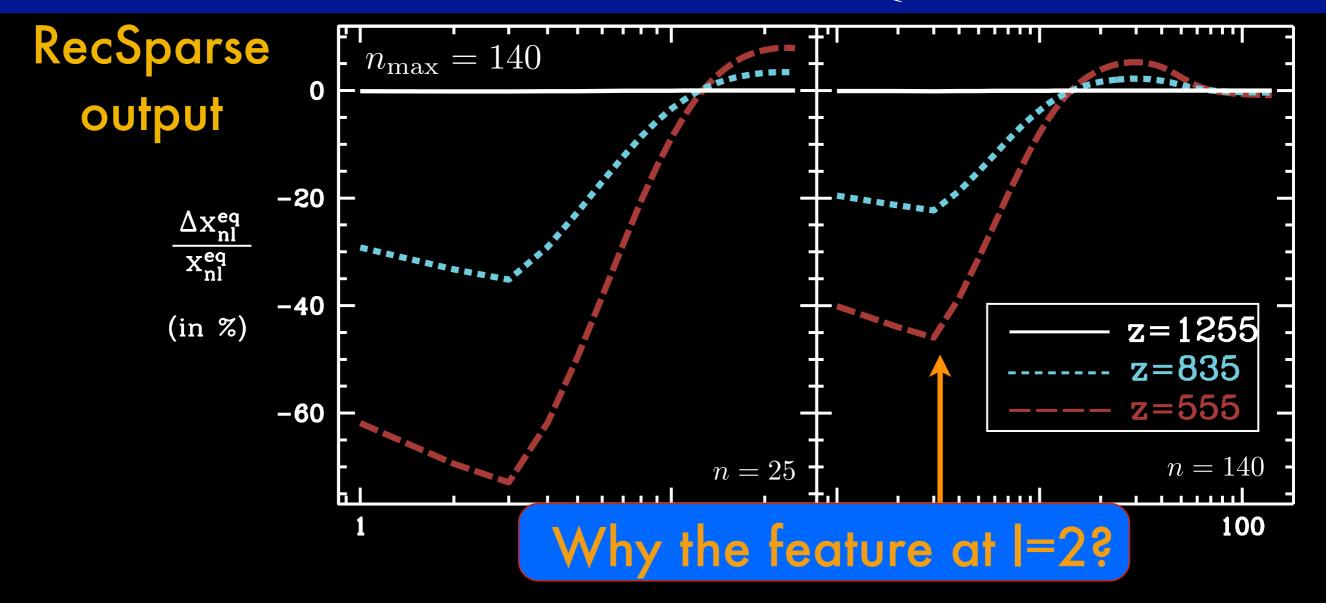
I=0 can't cascade down, so s states are not as under-populated





Highest I states recombine inefficiently, and are under-populated



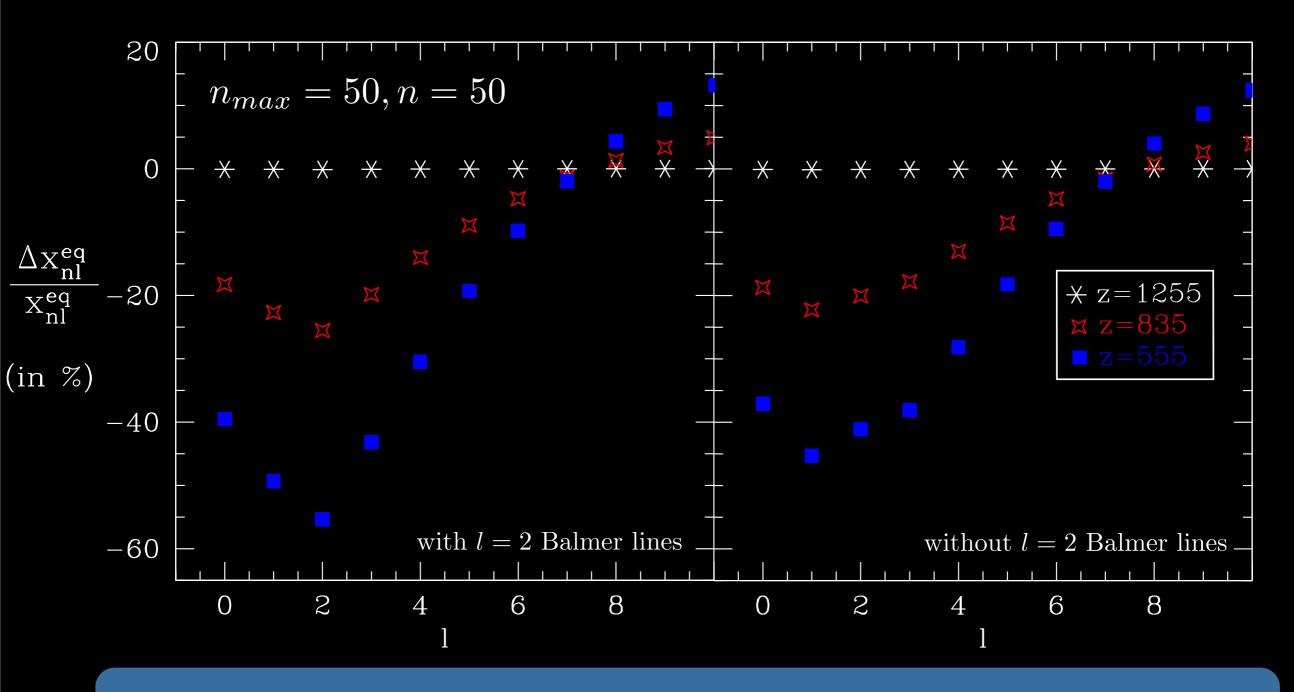


WHAT IS THE ORIGIN OF THE *l*=2 DIP?

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

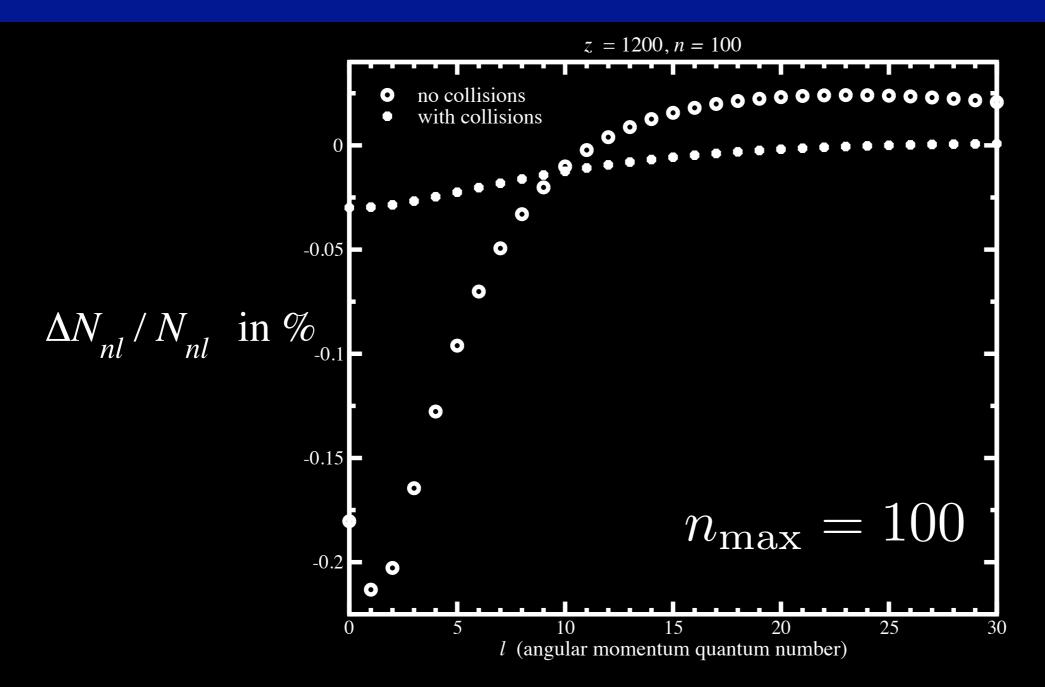
- * l=2 depopulates more rapidly than l=1 for higher (n>2) excited states
- * We can test if this explains the dip at l=2 by running the code with these Balmer transitions the blip should move to l=1

L-SUBSTATE POPULATIONS, BALMER LINES OFF



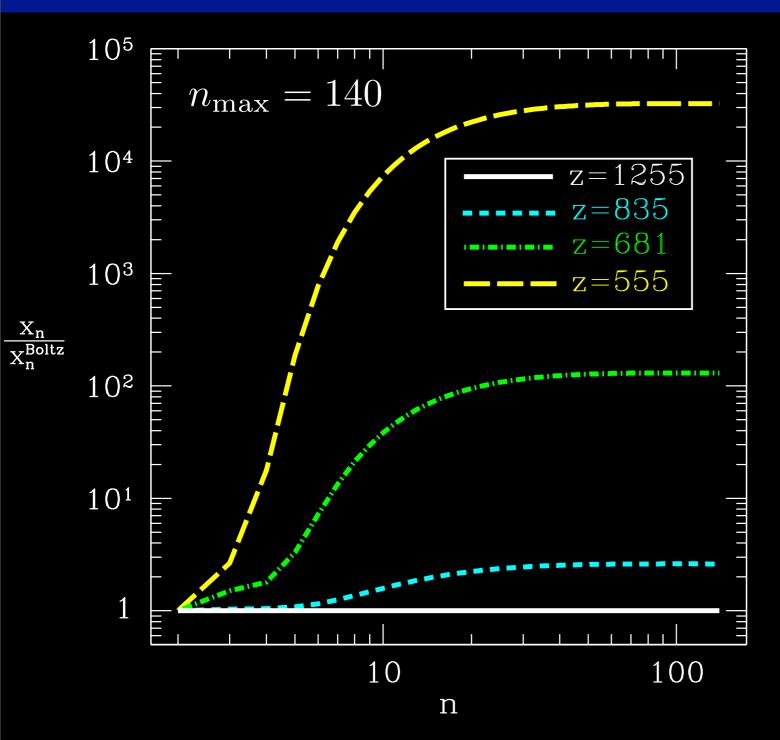
Dip moves as expected when Balmer lines are off!

ATOMIC COLLISIONS



- * 1-changing collisions bring 1-substates closer to statistical equilibrium (SE) (Chluba, Rubino Martin, Sunyaev 2006)
- * Theoretical collision rates unknown to factors of 2!

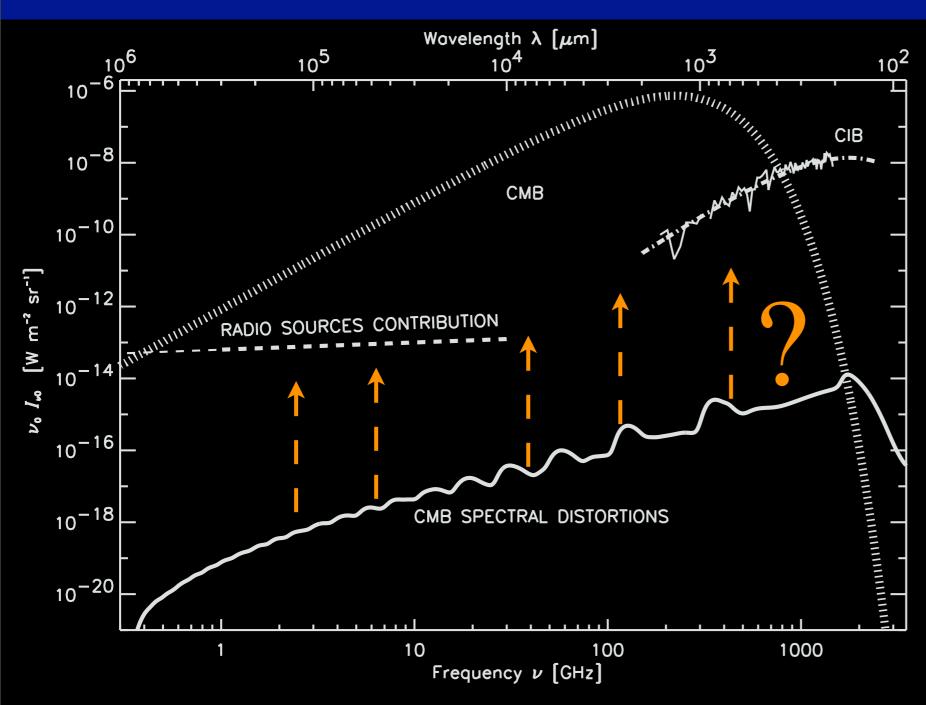
DEVIATIONS FROM BOLTZMANN EQUILIBRIUM: DIFFERENT n-SHELLS



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

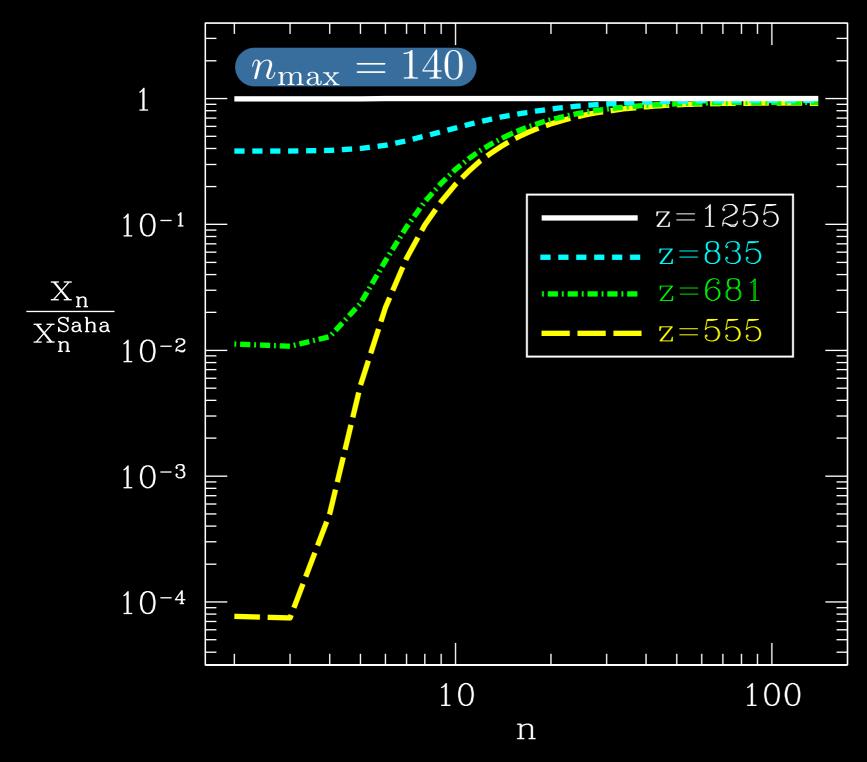
- * No inversion relative to n=2 (just over-population)
- * Population inversion seen between some excited states: Does radiation stay coherent? Does recombination mase?

DEVIATIONS FROM BOLTZMANN EQUILIBRIUM: DIFFERENT *n*-SHELLS



Masing could make spectral distortions detectable!

DEVIATIONS FROM SAHA EQUILIBRIUM

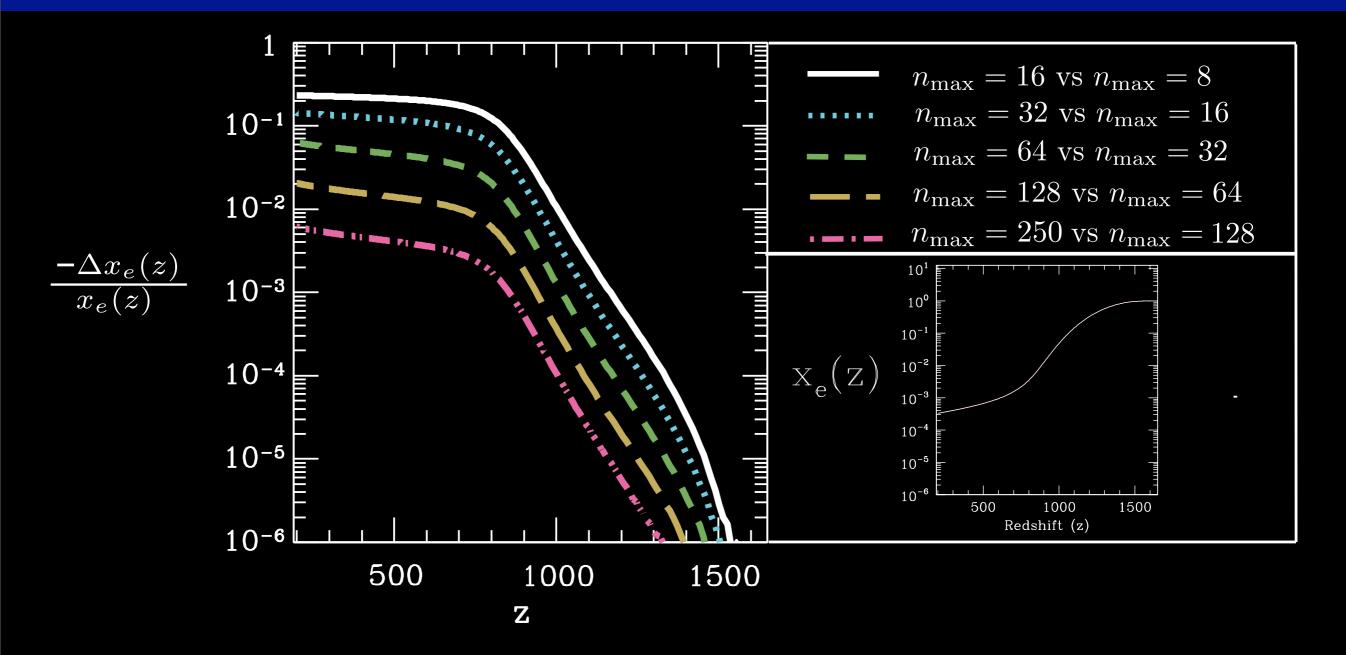


HUGE DEVIATIONS FROM SAHA EQ!

- * 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}~1000 needed, unless collisions included

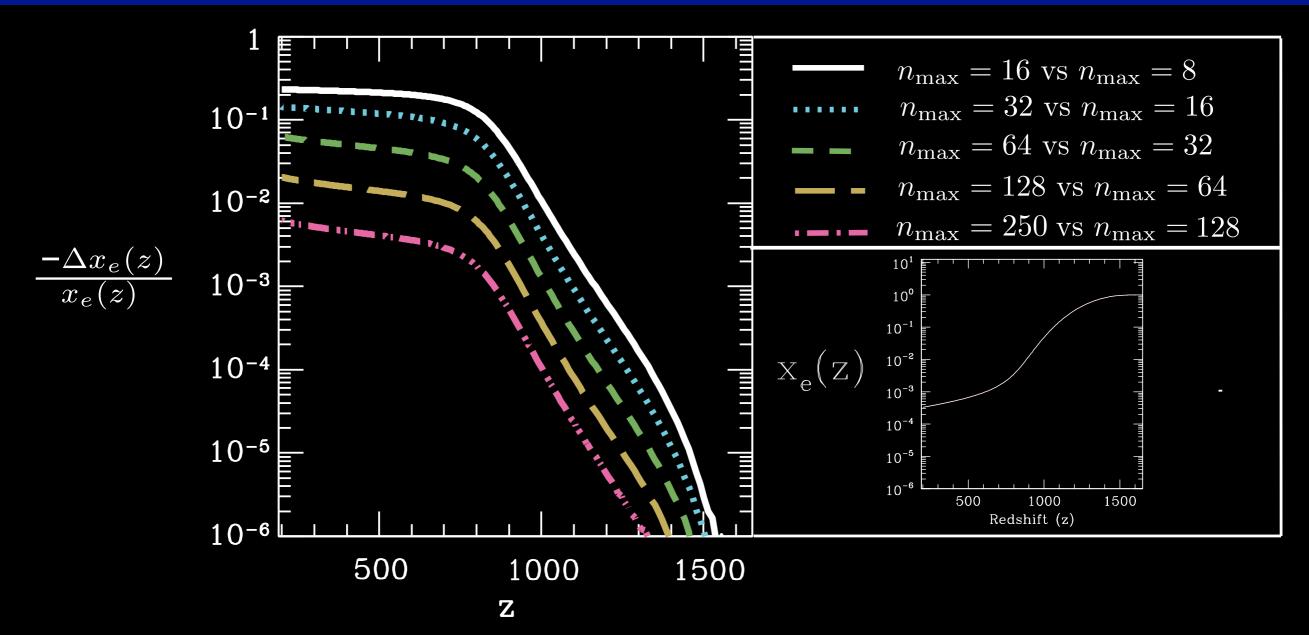


RESULTS: RECOMBINATION HISTORIES INCLUDING HIGH-n

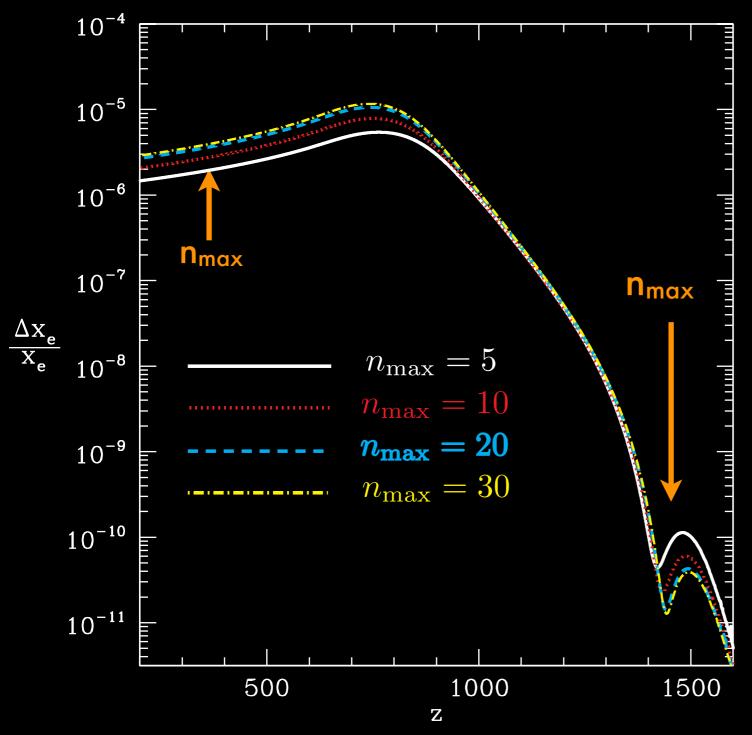


- * $x_e(z)$ falls with increasing $n_{\text{max}} = 10 \rightarrow 250$, as expected.
- * Rec Rate>downward BB Rate> Ionization, upward BB rate
- * For $n_{max} = 100$, code computes in only 2 hours

RESULTS: RECOMBINATION HISTORIES INCLUDING HIGH-n

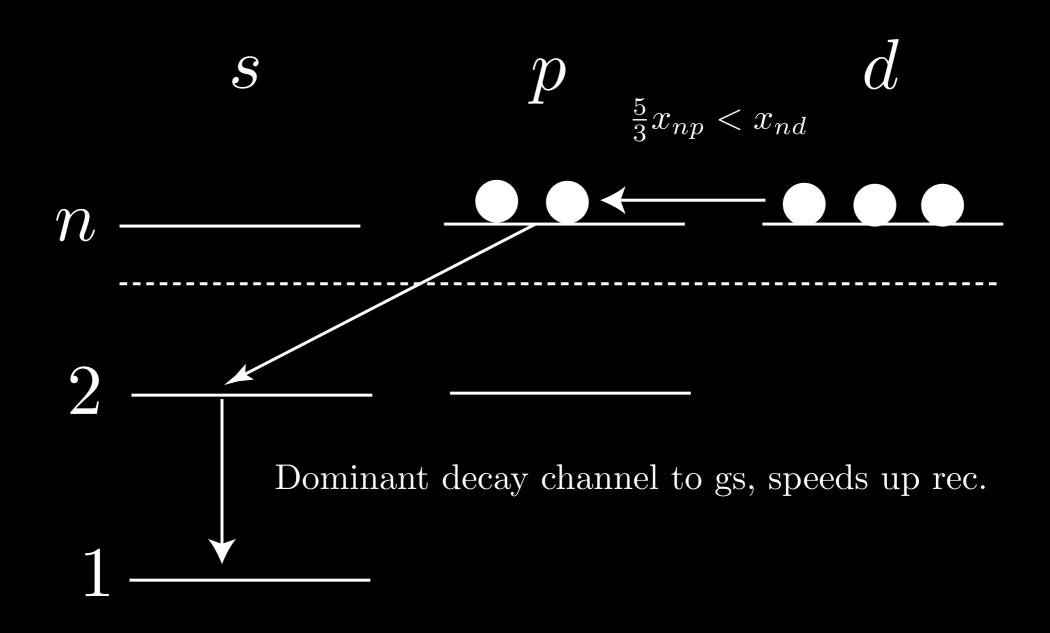


- * Relative convergence is not the same thing as absolute convergence: Want to see Saha asymptote and impose well-motivated cutoff! Collisions could help
- * These are lower limits to the actual error
- * n_{max}=300 under way to further test convergence (more time consuming)



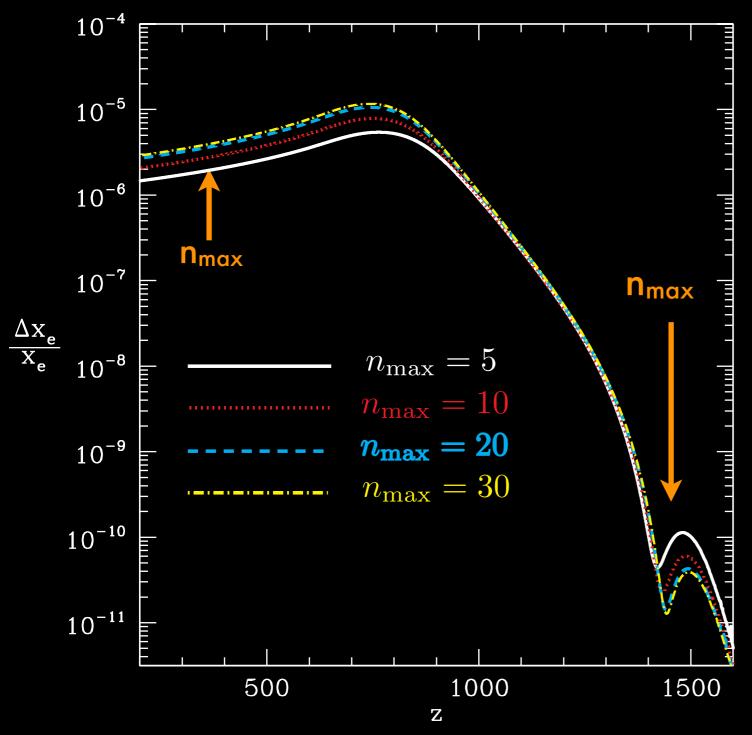
$$\Delta x_e \equiv x_e|_{\text{no }E2 \text{ transitions}} - x_e|_{\text{with }E2 \text{ transitions}}$$

Negligible for Planck!



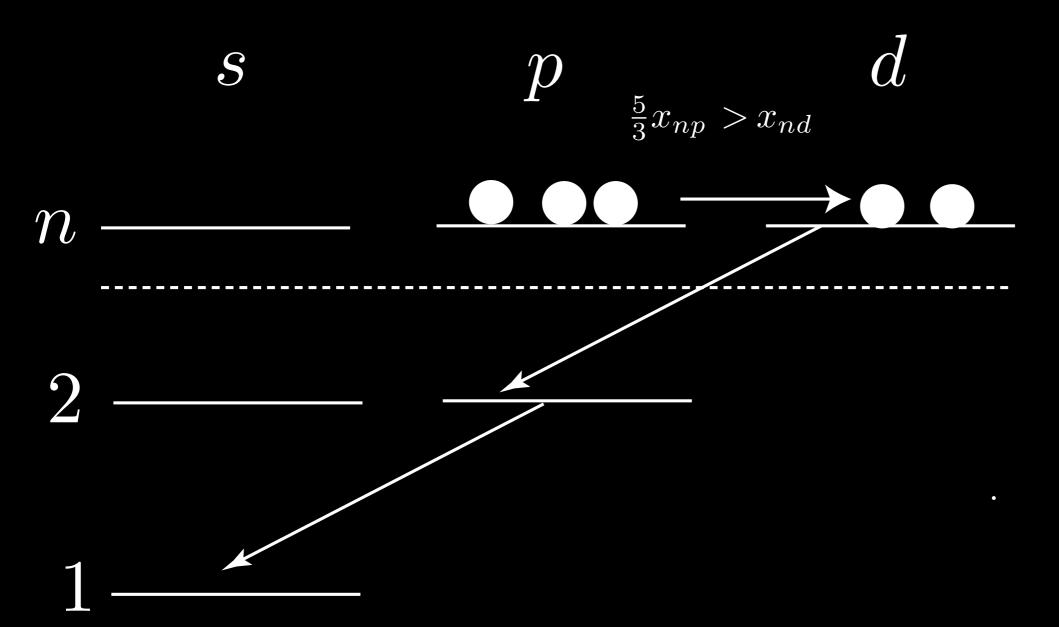
$$R_{nd \to np}^{\text{quad}} = A_{nd \to 1s} \left(x_{nd} - \frac{5}{3} x_{np} \right)$$

n < 5, early times



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

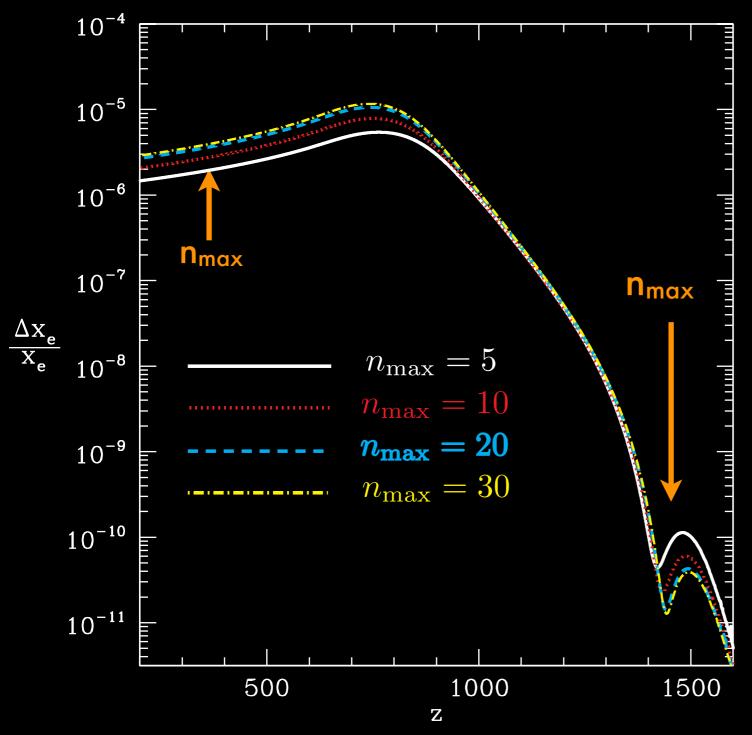
Negligible for Planck!



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

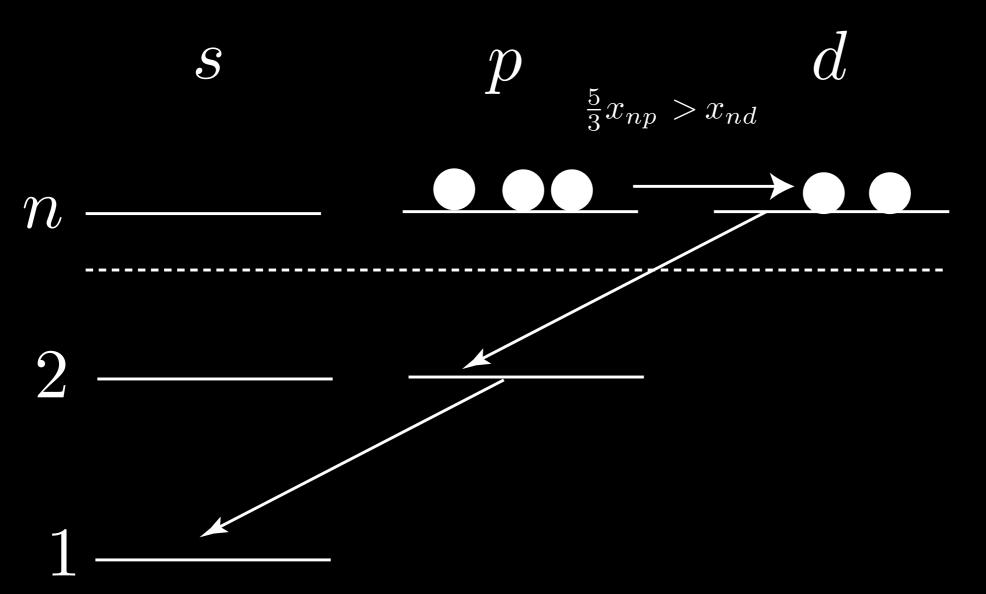
$$R_{nd \to np}^{\text{quad}} = A_{nd \to 1s} \left(x_{nd} - \frac{5}{3} x_{np} \right)$$

 $n \ge 5$, early times



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

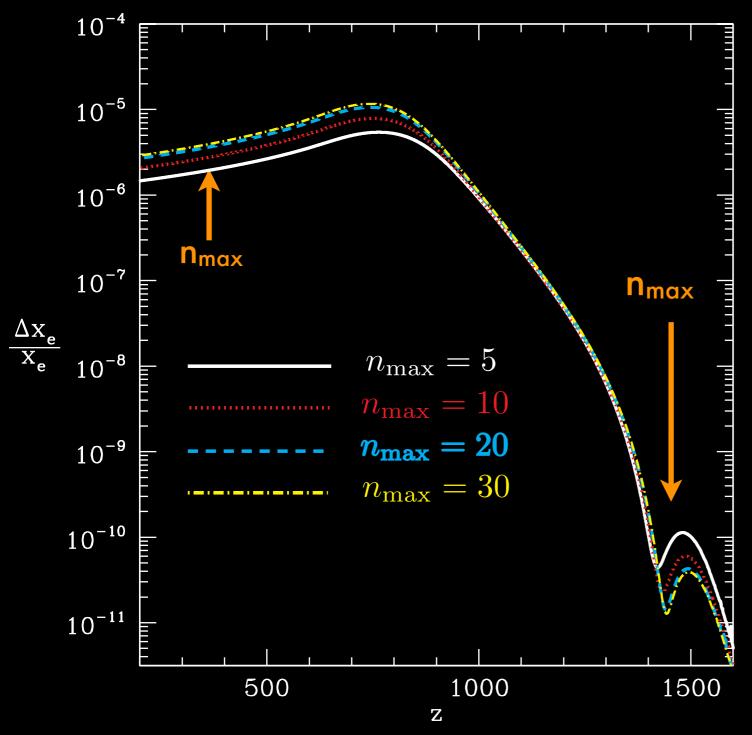
Negligible for Planck!



Dominant decay channel to gs, speeds up rec

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

All n, late times

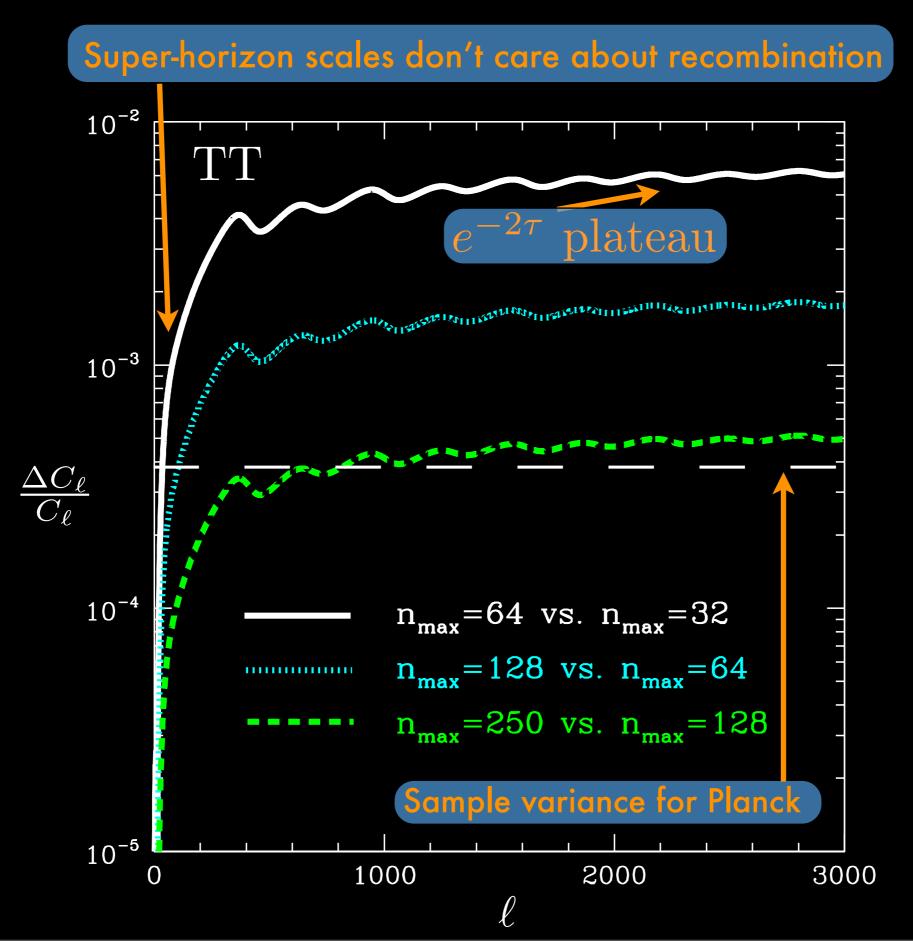


$$\Delta x_e \equiv x_e|_{\text{no }E2 \text{ transitions}} - x_e|_{\text{with }E2 \text{ transitions}}$$

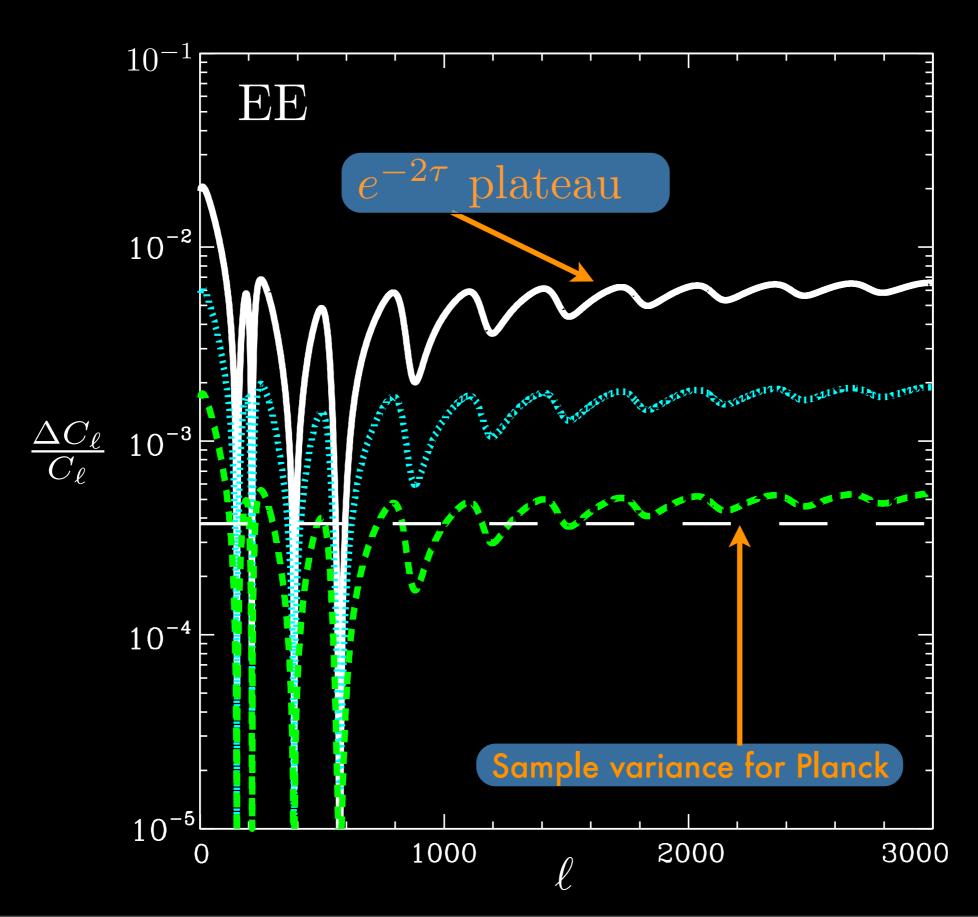
Negligible for Planck!

RESULTS: CMB ANISOTROPIES

RESULTS: TT C_ls WITH HIGH-N STATES

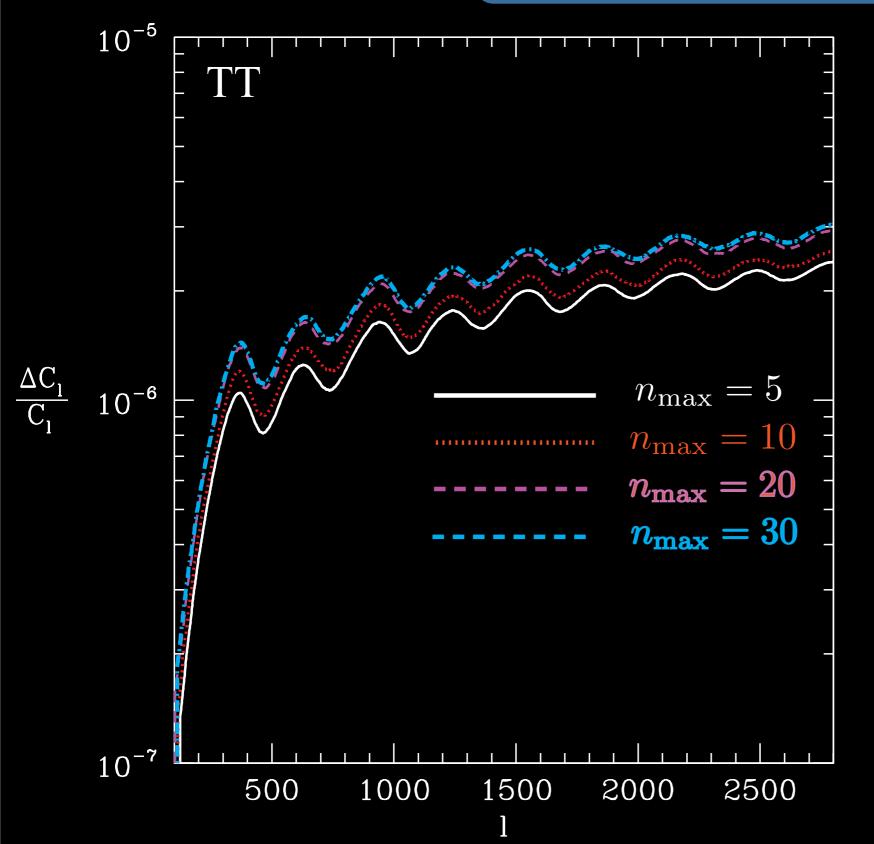


RESULTS: EE C_ls WITH HIGH-N STATES



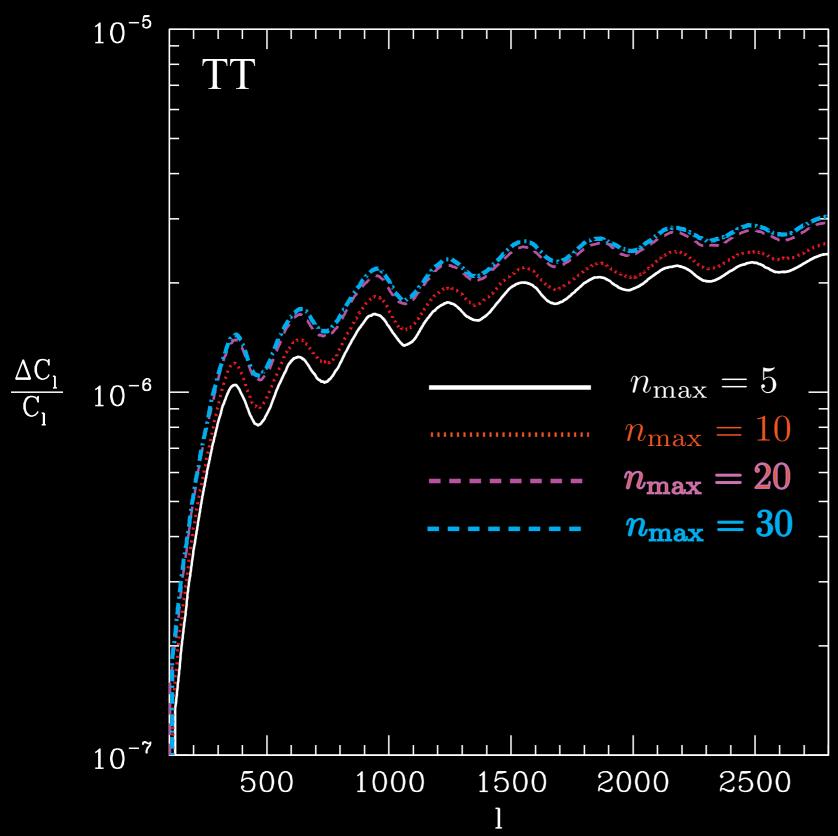
RESULTS: TEMPERATURE (TT) C_ls WITH HYDROGEN QUADRUPOLES,

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



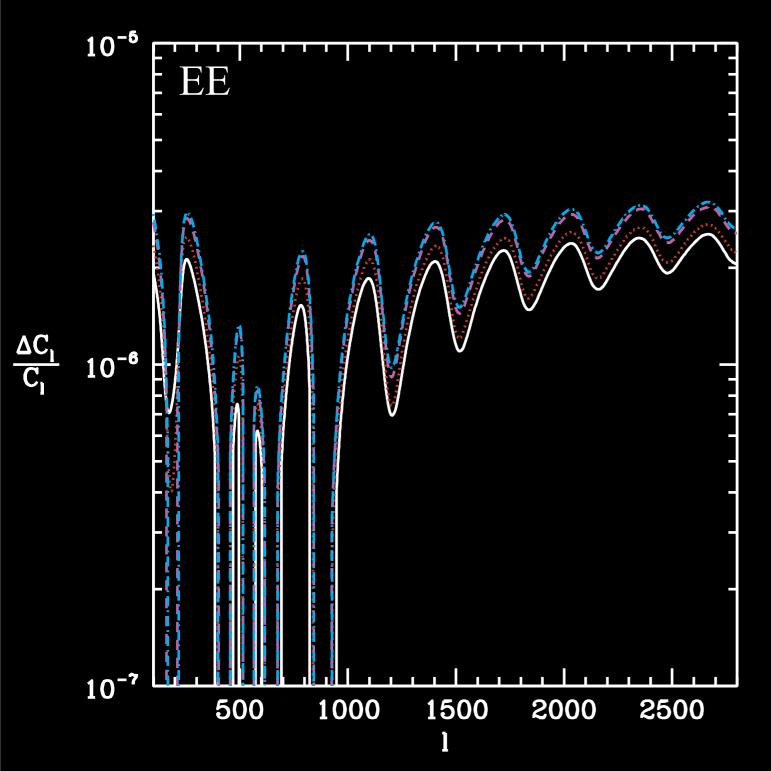
RESULTS: TEMPERATURE (TT) $C_l s$ WITH HYDROGEN QUADRUPOLES,

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



Overall effect is negligible for CMB experiments!

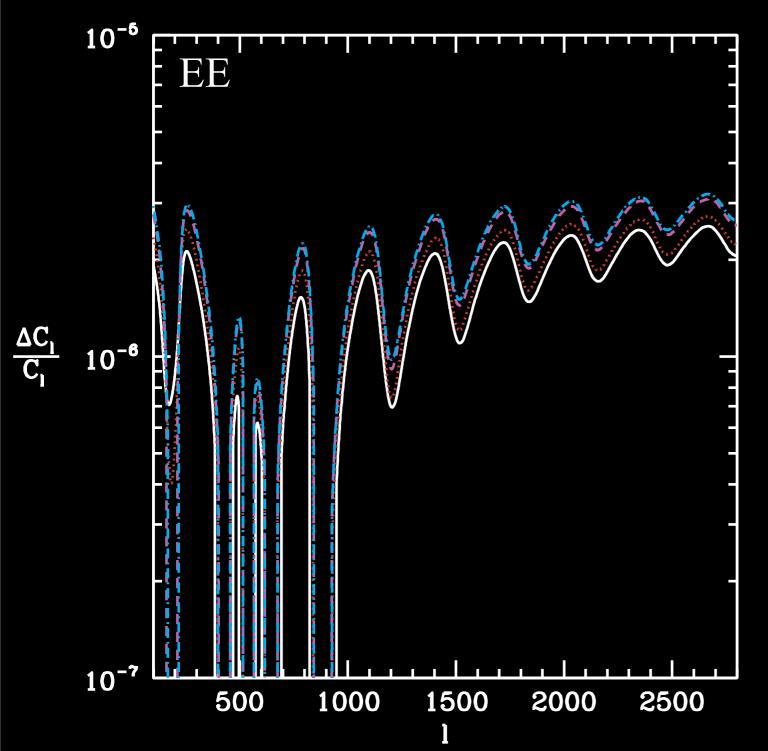
RESULTS: POLARIZATION (EE) $C_l s$ WITH HYDROGEN QUADRUPOLES



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

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

RESULTS: POLARIZATION (EE) C_ls WITH HYDROGEN QUADRUPOLES

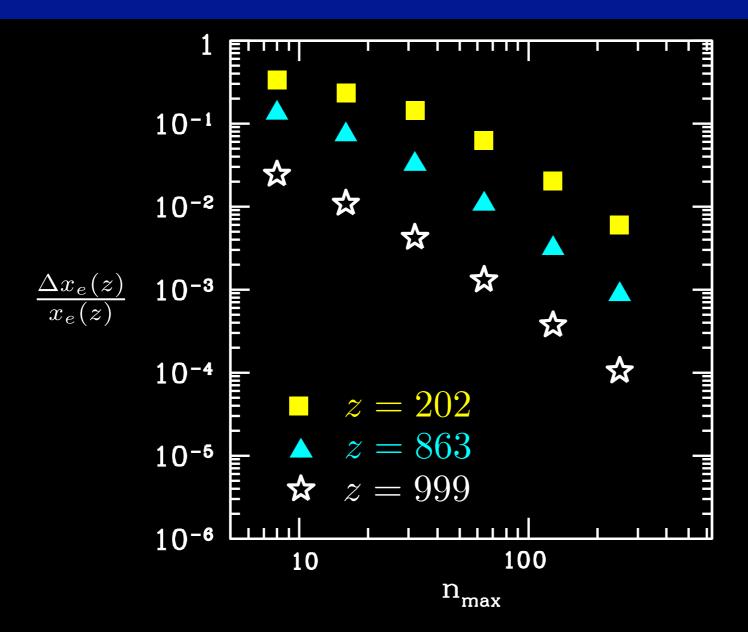


$$\Delta C_l \equiv \left. C_l \right|_{\text{with } E2 \text{ transitions}} - \left. x_e \right|_{\text{no } E2 \text{ transitions}}.$$

Overall effect is negligible for upcoming CMB experiments!

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

CONVERGENCE



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

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

* 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~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

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!

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

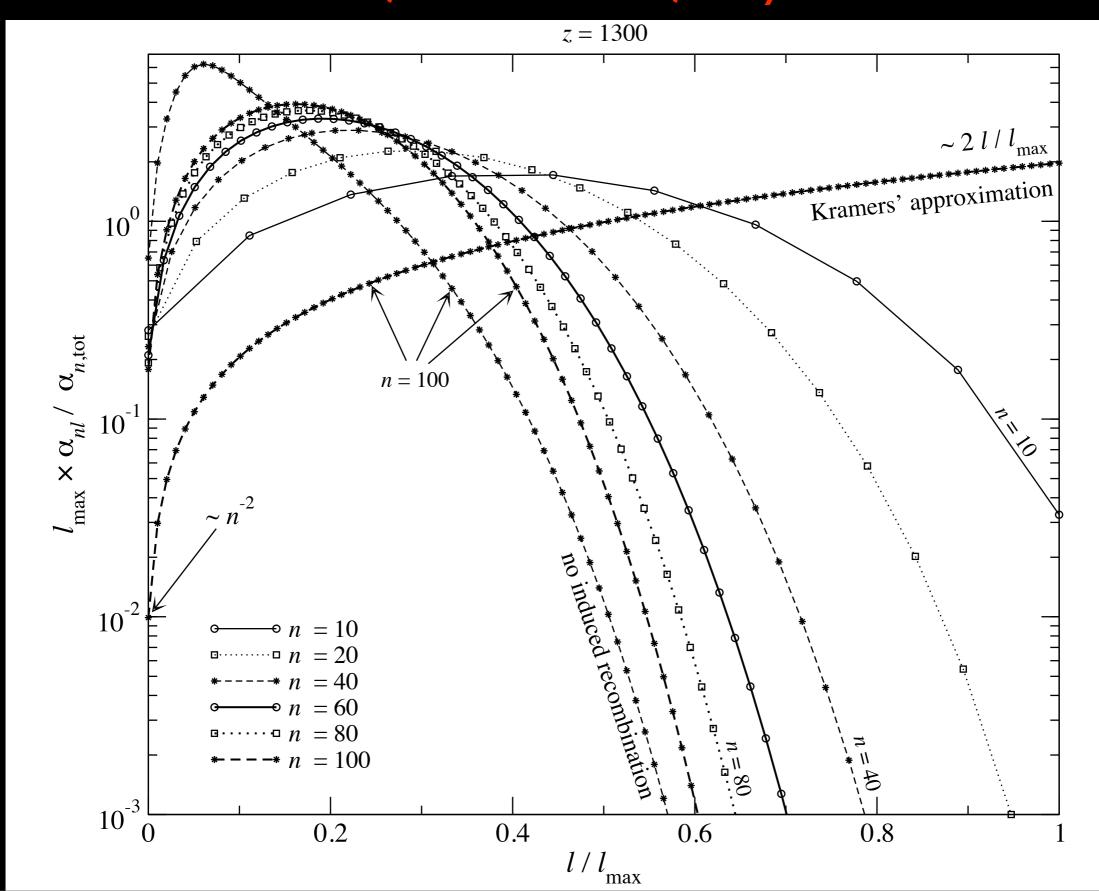
$$\epsilon = \left(1 - \frac{l(l+1)}{n^2} \right)^{1/2}$$

$$s = n - n'$$

• 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

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

Reduced matrix element evaluated using Wigner 3J symbols:

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

Radial matrix element evaluated using operator methods

$${}^{2}R_{n_{b}l_{b}}^{n_{a}l_{a}} \equiv \int_{0}^{\infty} r^{4}R_{n_{a}l_{a}}(r)R_{n_{b}l_{b}}(r)dr$$

Quadrapole rates: Operator algebra

* Radial Schrödinger equation can be factored to yield:

$$-\Omega_{nl} = \frac{1}{lA_{nl}} \left[1 - l \left(\frac{d}{dr} + \frac{l+1}{r} \right) \right] + \Omega_{nl} = \frac{1}{lA_{nl}} \left[1 + l \left(\frac{d}{dr} - \frac{l-1}{r} \right) \right] \\
-\Omega_{nl} R_{nl}(r) = R_{n-l-1}(r) \\
+\Omega_{n-l-1} R_{nl}(r) = R_{nl}(r) + A_{nl} = \frac{\sqrt{n^2 - l^2}}{nl}$$

• This algebra can be applied to radial matrix elements:

Quadrapole rates: Operator algebra

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

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

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

This algebra can be applied to radial matrix elements:

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

$${}^{(2)}R_{n'}^{n}{}^{n'-1}_{n'-1} = \frac{2nn'}{\sqrt{n^{2} - n'^{2}}} {}^{(1)}R_{n}^{nn'}{}_{n'-1}$$

Diagonal!

Quadrapole rates: Operator algebra

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

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

This algebra can be applied to radial matrix elements:

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

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

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