COSMOLOGICAL HYDROGEN RECOMBINATION: THE EFFECT OF HIGH-N STATES

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Recombination in a nutshell

Breaking the Peebles mold: past work on high-n states

Motivation from CMB anisotropies and recombination spectra

RecSparse: a new-tool for including high-n states

Forbidden transitions

Results

Ongoing/future work
SAHA EQUILIBRIUM IS INADEQUATE

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

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

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

\[ x_e = 0.5 \text{ when } T = T_{\text{rec}} \simeq 0.3 \text{ eV} \quad z_{\text{rec}} \simeq 1300 \]

- Further evolution falls prey to reaction freeze-out

\[
\Gamma = 6 \times 10^{-22} \text{ eV} \quad x_e(T) \left( \frac{13.6}{T_{eV}} \right)^{-5/2} \ln \left( \frac{13.6}{T_{eV}} \right)
\]

\[ H = 1.1 \times 10^{-26} \text{ eV} \quad T_{eV}^{3/2} \]

\[ \Gamma < H \text{ when } T < T_F \simeq 0.25 \text{ eV} \]
Bottlenecks and Escape Routes

Bottlenecks

- Ground state recombinations are ineffective
  \[ \tau_{c\rightarrow 1s}^{-1} = 10^{-1} \text{ s}^{-1} \gg H \simeq 10^{-12} \text{ s}^{-1} \]

- Resonance photons are re-captured, e.g. Lyman \( \alpha \)
  \[ \tau_{2p\rightarrow 1s}^{-1} = 10^{-2} \text{ s}^{-1} \gg H \simeq 10^{-12} \text{ s}^{-1} \]

Escape Routes (e.g. \( n=2 \))

- Two-photon processes
  \[ H^{2s} \rightarrow H^{1s} + \gamma + \gamma \]
  \[ \Lambda_{2s\rightarrow 1s} = 8.22 \text{ s}^{-1} \]

- Redshifting off resonance
  \[ R \sim \left( n_H \lambda_\alpha^3 \right)^{-1} \left( \frac{\dot{a}}{a} \right) \]
EQUILIBRIUM ASSUMPTIONS

- Radiative eq. between different n-states

\[ \mathcal{N}_n = \mathcal{N}_2 e^{-(E_n - E_2)/T} \]

- Radiative/collisional eq. between different \( l \)

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

- Matter in eq. with radiation due to Thompson scattering

\[ T_m = T_\gamma \text{ since } \frac{\sigma_T a T_\gamma^4 c}{m_e c^2} < H(T) \]
THE PEEBLES PUNCHLINE

- Only $n=2$ bottlenecks are treated

$$\Gamma_{\text{net},H} = \Lambda_{2s \to 1s} \left[ n_{2s} - n_{1s} e^{-(B_1-B_2)/kT} \right] + \frac{8\pi \dot{a}}{\lambda_\alpha^3 a} \times \left( f_\alpha - e^{-\hbar \nu_\alpha/kT} \right)$$

- Net Rate is suppressed by bottleneck vs. escape factor

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

$$\mathcal{C} = \frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + \frac{\Lambda_{2s \to 1s}}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + \left( \Lambda_{2s \to 1s} + \beta_C \right)$$
THE PEEBLES PUNCHLINE

- Net Rate is suppressed by bottleneck vs. escape factor

\[ C = \frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + \Lambda_{2s \rightarrow 1s} \]

\[ \frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + (\Lambda_{2s \rightarrow 1s} + \beta_c) \]
THE PEEBLES PUNCHLINE

- Net Rate is suppressed by bottleneck vs. escape factor

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\]
The Peebles Punchline

- Net Rate is suppressed by bottleneck vs. escape factor

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THE PEEBLES PUNCHLINE

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\]

Ionization Term
THE PEEBLES PUNCHLINE

- Net Rate is suppressed by bottleneck vs. escape factor

\[ C = \frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + \Lambda_{2s \rightarrow 1s} \]

\[ \frac{8\pi}{\lambda_\alpha^3 n_{1s}} \frac{\dot{a}}{a} + (\Lambda_{2s \rightarrow 1s} + \beta_c) \]

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

\[ 2\gamma \text{ process dominates until late times } (z \lesssim 850) \]
State of the Art for 30 years!
**Breaking the Naive Model**

- Radiation field is cool: Boltzmann eq. of higher $n$

  Seager/Sasselov/Scott (2000) $n_{\text{max}} = 300$ RecFAST!!

- Equilibrium between $l$ states

- Treated by Chluba et al. (2005) for $n_{\text{max}} = 100$

- Radiation and matter field fall out of eq.

\[
\dot{T}_M + 2HT_m = \frac{8x_e \sigma_T a T_\gamma^4}{3m_e c (1 + f_{\text{He}} + x_e)} (T_M - T_\gamma)
\]
BREAKING THE NAIVE MODEL

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- Equilibrium between $l$ states

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- Beyond this, testing convergence with $n_{\text{max}}$ is hard!

\[ t_{\text{compute}} \sim \mathcal{O} (\text{weeks}) \]

How to proceed if we want 0.1% accuracy in $x_e(z)$?
THE EFFECT OF RESOLVING 1- SUBSTATES

Putting free-electrons in ‘bottlenecked’ l-substates slows down the decay to 1s: Recombination is slower; Chluba, Rubino-Martin, Sunyaev 2006
**AND SO?**

- 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 0.1% accuracy for Planck data analysis
Planck uncertainty forecasts using MCMC

\[ P(k) = A_s \left( k \eta_0 \right)^{n_s - 1} \]

- Cosmological parameter inferences will be off if recombination is improperly modeled.
- Leverage on new physics comes from high l. This is where the details of recombination matter!
- Inferences about inflation will be wrong if recombination is improperly modeled.
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\[ n_s = 1 - 4\epsilon + 2\eta \quad \epsilon = \frac{m_{\text{pl}}^2}{16\pi} \left[ \frac{V'(\phi)}{V(\phi)} \right]^2 \quad \eta = \frac{m_{\text{pl}}^2}{16\pi} \left[ 2V'' - \epsilon \right] \]
**Recombination and Inflation**

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\begin{align*}
    n_s &= 1 - 4\epsilon + 2\eta \\
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    \eta &= \frac{m_{pl}^2}{16\pi} \left[ 2V'' - \epsilon \right]
\end{align*}
\]

CMB `observable' \quad Curvature/slope of inflationary potential
**Recombination and Inflation**

- Planck uncertainty forecasts using MCMC
  
  - Cosmological parameter inferences will be off if recombination is improperly modeled.
  
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  - Inferences about inflation will be wrong if recombination is improperly modeled.

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P(k) = A_s \left( k \eta_0 \right)^{n_s - 1}
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Cosmological parameter inferences will be off if recombination is improperly modeled.

Leverage on new physics comes from high $l$. This is where the details of recombination matter!

Inferences about inflation will be wrong if recombination is improperly modeled.

You have to get eV-scale physics right to get $10^{15}$ GeV physics right!
WMAP TE measurement constrains reionization: Newly free electrons re-scatter quadrupole due to large-scale modes: low-l feature implies

\[ z_r = 11.0 \pm 1.4, \quad \tau = 0.087 \pm 0.017 \]

Planck EE measurement at will constrain \( \tau \) and \( z_r \) AND distinguish different reion. histories with same \( \tau \) (6 EE peaks vs 2 with WMAP5).

Planck constraints on reion. will also come from small angular scales (TT, TE, EE)

Will yield constraints to first astrophysical ionizing sources (QSOs, galaxies, Pop III stars?)
I. SMEARING AND MOVING THE SURFACE OF LAST SCATTERING (SLSS)

- Photons kin. decouple when Thompson scattering freezes out
  \[ \gamma + e^- \Leftrightarrow \gamma + e^- \]
  \[ \Gamma = n_e \sigma_T c = 2.2 \times 10^{-19} \text{ s}^{-1} \frac{x_e \Omega_b h^2}{a^3} = \]
  \[ H = H_0 \Omega_m^{1/2} a^{-3/2} \left[ 1 + \frac{a_{eq}}{a} \right]^{1/2} \]

- \( z_{\text{dec}} \approx 1100 \): Decoupling occurs during recombination

\[ C_l \rightarrow C_l e^{-2\tau} \quad \text{if} \ l > \frac{\eta_0}{\eta_{\text{rec}}} \]

\[ \tau = \int_0^{\eta_{\text{dec}}} d\eta n_e [\eta] \sigma_T a (\eta) \]
WHO CARES?

II. THE SILK DAMPING TAIL

From Wayne Hu’s website

\[ N = \frac{\eta}{\lambda_c} \quad \lambda_c = (n_e \sigma_T a)^{-1} \]

\[ \lambda_D = \frac{N^{1/2}}{\lambda_c} \]

\[ l_{\text{damp}} \sim 1000 \]

Inhomogeneities are damped for \( \lambda < \lambda_D \)

\[ k_D^{-2} (\eta) \approx \int_0^\eta \frac{d\eta'}{6(1+R)n_e[\eta'][\sigma_T a[\eta']]} \left[ \frac{R^2}{1+R} + \frac{8}{9} \right] \]

\[ R = \frac{3\rho_b^0}{4\rho^\gamma} \]

\[ |\Theta_l(\eta_0)| \approx \int_0^{\eta_0} d\eta ~ \tau e^{-\tau(\eta)} e^{ikf \int d\eta c_s} e^{-k^2 / k_D^2 (\eta)} \tilde{\delta}(k) j_l(k(\eta - \eta_0)) dk \]
Inhomogeneities are damped for $\lambda < \lambda_D$

$$k_D^{-2}(\eta) \approx \int_0^\eta \frac{d\eta'}{6(1+R)n_e[\eta'][\sigma_T a[\eta']]} \left[ \frac{R^2}{1+R} + \frac{8}{9} \right]$$

$$R = \frac{3\rho_b^0}{4\rho^\gamma}$$

$$|\Theta_l(\eta_0)| \approx \int_0^{\eta_0} d\eta \, \tilde{e}^{-(\tau)}(\eta) e^{ik} \int d\eta c_s e^{-k^2/k_D^2(\eta)} \tilde{\delta}(k) j_l(k(\eta - \eta_0)) dk$$
III. Finite thickness of the SLSS

Additional damping of form

$$|\Theta_l (\eta_0, k)| \rightarrow |\Theta_l (\eta_0, k)| e^{-\sigma^2 \eta_{rec}^2 k^2}$$
WHO CARES?
IV. CMB POLARIZATION

- Need to scatter quadrupole to polarize CMB
  \[ \Theta^P_l (k) = \int d\eta \dot{\tau} e^{-\tau(\eta)} \Theta_{T,2} (k, \eta) \frac{l^2}{(k\eta)^2} j_l (k\eta) \]
- Need time to develop a quadrupole
  \[ \Theta_l (k\eta) \sim \frac{k\eta}{2\tau} \Theta_l (k\eta) \ll \Theta_l (\eta) \text{ if } l \geq 2, \text{ in tight coupling regime} \]
WHO CARES?

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\[ \Theta_l (k\eta) \sim \frac{k\eta}{2\tau} \Theta_l (k\eta) \ll \Theta_l (\eta) \text{ if } l \geq 2, \text{ in tight coupling regime} \]
Even CMB is an imperfect blackbody, and someday we might detect deviations from pre-recombination spectral lines.
**BREAKING THE NAIVE MODEL**

- Radiation field is cool: Boltzmann eq. of higher $n$

- Treated by Seager et al. (2000) $n_{\text{max}} = 300$

- Eq. between $l$ states: dipole selection bottleneck: $\Delta l = \pm 1$

- Treated by Chluba et al. (2005) for $n_{\text{max}} = 100$

- Beyond this, testing convergence with $n_{\text{max}}$ is hard!
  
  $t_{\text{compute}} \sim \mathcal{O} (\text{weeks})$
The multi-level atom (MLA)

**Bound-free rate equation**

\[
\dot{x}_{nl}^{bf} = \int dE_e P_M(T_m, E_e) n_H x_e x_p [1 + f(E_e - E_n)] \alpha_{nl}(E_e)
\]

\[
- \int dE_e \, g(E_E - E_n) \, x_{nl} \, f(E_e - E_{nl}) \alpha_{nl}(E_E)/g_{nl}
\]

**Bound-bound rate equation**

\[
\dot{x}_{nl}^{bb} = \sum_{n',l'=l\pm 1} (A_{nn'}^{ll'} (1 + f_{nn'}) \, x_{n',l'} - \frac{g_{n'l'}}{g_{nl}} f_{nn'} x_{nl}) \, P_{nn'}^{ll'}
\]
THE MULTI-LEVEL ATOM (MLA)

- Bound-free rate equation
\[ \dot{x}_{nl}^{bf} = \int dE_e P_M(T_m, E_e)n_H x_e x_p [1 + f(E_e - E_n)] \alpha_{nl}(E_e) \]
\[ \quad - \int dE_e g(E_E - E_n) x_{nl} f(E_e - E_{nl}) \alpha_{nl}(E_E)/g_{nl} \]

- Bound-bound rate equation
\[ \dot{x}_{nl}^{bb} = \sum_{n',l'=l\pm 1}(A_{nn'}^{ll'}(1 + f_{nn'})x_{n',l'} - \frac{g_{n'l'}}{g_{nl}} f_{nn'} x_{nl}) P_{nn'}^{ll'} \]
**The Multi-level Atom (MLA)**

- **Bound-free rate equation**
  \[
  \dot{x}_{nl}^{bf} = \int dE_e P_M(T_m, E_e)n_H x_e x_p [1 + f(E_e - E_n)] \alpha_{nl}(E_e) \\
  - \int dE_e g(E_E - E_n) x_{nl} f(E_e - E_{nl}) \alpha_{nl}(E_E) / g_{nl}
  \]

- **Bound-bound rate equation**
  \[
  \dot{x}_{nl}^{bb} = \sum_{n',l'} = l \pm 1 (A_{nn'}^{ll'} (1 + f_{nn'}) x_{n',l'} - \frac{g_{n'l'}}{g_{nl}} f_{nn'} x_{nl}) P_{nn'}^{ll'}
  \]

- Phase-space density blueward of line
- Escape probability of $\gamma$ in line
**THE MULTI-LEVEL ATOM (MLA)**

Stimulated emission/absorption

- **Bound-free rate equation**

\[ \dot{x}_{nl}^{bf} = \int dE_e P_M(T_m, E_e)n_H x_e x_p \left[ 1 + f(E_e - E_n) \right] \alpha_{nl}(E_e) \]

\[ - \int dE_e g(E_E - E_n) x_{nl} f(E_e - E_{nl}) \alpha_{nl}(E_E)/g_{nl} \]

- **Bound-bound rate equation**

\[ \dot{x}_{nl}^{bb} = \sum_{n',l'} (A_{nn'}^{ll'} (1 + f_{nn'}) x_{n',l'} - g_{n'l'}/g_{nl} f_{nn'} x_{nl}) P_{nn'}^{ll'} \]
**The Multi-level Atom (MLA)**

**Spontaneous Emission**

- **Bound-free rate equation**
  \[
  \dot{x}_{nl}^{bf} = \int dE_e P_M(T_m, E_e) n_H x_e x_p \left[ 1 + f(E_e - E_n) \right] \alpha_{nl}(E_e) \\
  - \int dE_e g(E_E - E_n) x_{nl} f(E_e - E_{nl}) \alpha_{nl}(E_E) / g_{nl}
  \]

- **Bound-bound rate equation**
  \[
  \dot{x}_{nl}^{bb} = \sum_{n', l'} = l \pm 1 \left( A_{nn'}^{ll'} (1 + f_{nn'}) x_{n', l'} - \frac{g_{n' l'}}{g_{nl}} f_{nn'} x_{nl} \right) P_{nn'}^{ll'}
  \]
Two photon transitions between $n=1$ and $n=2$ are included:

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

Net recombination rate:

$$
x_e \simeq 1 - x_{1s} \rightarrow \dot{x}_e \simeq -\dot{x}_{1s} = -\dot{x}_{1s \rightarrow 2s}
+ \sum_{n,l>1s} A_{n1}^l P_{n1}^l \left\{ \frac{g_{nl}}{2} f_{n1}^+ x_{1s} - (1 + f_{n1}^+) x_{nl} \right\}
$$
Bound-bound rates given by Fermi’s golden rule and matrix element

\[ \rho(n'l', nl) = \int_{0}^{\infty} u_{n'l'}(r)u_{nl}(r)r^3 dr = C \times \left[ F_{2,1} \left( -n + l + 1, -n' + l, 2l, \frac{-4nn'}{(n-n')^2} \right) \right. \]

\[ - \left( \frac{n-n'}{n+n'} \right)^2 F_{2,1} \left( -n + l - 1, -n' + l, 2l, \frac{-4nn'}{(n-n')^2} \right)^2 \]

Power-series destabilizes at high-\( n \), recursion relation used

Rates are calculated, tabulated, and stored
BB RATE COEFFICIENTS: VERIFICATION

- WKB estimate of matrix elements
  \[ \rho(n'l', nl) = a_0 n'^2 \int_{-\pi}^{\pi} d\tau e^{i\Omega \tau} (1 + \cos \eta) \]
  \[ \Omega = \omega_n - \omega_{n'} \]
  \[ r = r_{\max} (1 + \cos \eta) / 2 \]
  \[ \tau = \eta + \sin \eta \]

Fourier transform of classical orbit!
Application of correspondence principle!

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

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

- Radial matrix elements checked against WKB (10%), published rates of Brocklehurst (1971), Green, Rush, and Chandler (1967) (agreement to their published 4 digits)
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.
**Radiation Field: Black Body**

- Escape probability treated in Sobolev approx.

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

\[ \tau_s = \frac{c^3 n_H}{8\pi H \nu_{nn'}^3} A_{nn'}^{ll'} \left[ \frac{g_{n'}^{l'}}{g_n^l} x_n^l - x_{n'}^{l'} \right] \]

\[ R(\nu, \nu') = \phi(\nu)\phi(\nu') \]

\[ \frac{v_{th}}{H(z)} \ll \lambda \]

- Excess line photons injected into radiation field

\[ \left( \frac{8\pi \nu_{nn'}^3}{c^3 n_H} \right) \left( f_{nn'}^+ - f_{nn'}^- \right) = A_{nn'}^{ll'} P_{nn'}^{ll'} \left[ x_n^l (1 + f_{nn'}^+) - \frac{g_n^l}{g_n'} x_{n'}^{l'} f_{nn'}^+ \right] \]

- Photons are conserved outside of line regions

\[ f_{n1}^{+10} = f_{n+1,1}^{-10} \left[ \frac{1 - (n + 1)^{-2}}{1 - n^{-2}} (1 + z) - 1 \right] \]
Radiation Field: Black Body+

- Escape probability treated in Sobolev approx.

\[ P_{n,n'}^{l,l'} = 1 - e^{-\tau_s} \]

\[ \tau_s = \frac{c^3 n_H}{8\pi H \nu_{nn'}^3} A_{nn'}^{l,l'} \left[ \frac{g_n^{l'}}{g_l^n} x_n^l - x_n^{l'} \right] \]

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

- Ongoing work by collabs and others uses FP eqn. to obtain evolution of \( f(\nu) \) more generally, including atomic recoil/diffusion, \( 2\gamma \) decay and full time-dependence of problem, coherent and incoherent scattering, overlap of higher-order Lyman lines
Evolution equations may be re-written in matrix form:

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$
Evolution equations may be re-written in matrix form

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

$$\vec{x} = \begin{pmatrix} \vec{x}_0 \\ \vec{x}_1 \\ \vdots \\ \vec{x}_{n_{\text{max}}-1} \end{pmatrix}$$
Evolution equations may be re-written in matrix form:

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

For state \( l \), includes BB transitions out of \( l \) to all other \( l' \), photo-ionization, \( 2\gamma \) transitions to ground state.
Evolution equations may be re-written in matrix form

\[ \frac{dx}{dt} = R \vec{x} + \vec{s} \]

For state \( l \), includes BB transitions into \( l \) from all other \( l' \)

For state \( l \), includes BB transitions into \( l \) from all other \( l' \)
Includes recombination to $l$, $1$, and $2\gamma$ transitions from ground state.

Evolution equations may be re-written in matrix form:

$$\frac{d\vec{x}}{dt} = \mathbf{R}\vec{x} + \vec{s}$$
Evolution equations may be re-written in matrix form:

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

- For \( n > 1 \), \( t_{\text{rec}}^{-1} \sim 10^{-12} \text{s}^{-1} \ll \mathbf{R} \), \( \vec{s} \rightarrow -\vec{x} \sim \mathbf{R}^{-1} \vec{s} \)

\[ \mathbf{R} \lesssim 1 \text{ s}^{-1} \text{ (e.g. Lyman-}\alpha) \]
Rapid matrix inversion: Sparsity to the rescue

- Matrix is \( \approx n_{\text{max}}^2 \times n_{\text{max}}^2 \)

- Brute force would require \( n_{\text{max}}^6 \approx 1000 \text{ s} \) for \( n_{\text{max}} = 200 \) for a single time step

- Sparsity to the rescue \( \Delta l = \pm 1 \)

\[
\begin{pmatrix}
M_{l,l-1}\vec{x}_{l-1} + M_{l,l}\vec{x}_l + M_{l,l+1}\vec{x}_{l+1} = \vec{s}_l \\
\end{pmatrix}
\]

\[
\vec{v}_l = \chi_l \left[ \vec{s}_l - M_{1,l+1}\vec{v}_l + \sum_{l'=l-1}^0 \sigma_{l,l'}\vec{s}_{l'}(-1)^{l'-l} \right]
\]

\[
\chi_l = \begin{cases}
    M_{00}\quad & \text{if } l = 0 \\
    (M_{l+1,l+1} - M_{l+1,l}\chi_l M_{l,l+1})^{-1} & \text{if } l > 0
\end{cases}
\]

\[
\sigma_{l,l-1} = M_{l,l-1}\chi_{l-1} \\
\sigma_{l,i} = \sigma_{l,i+1} M_{i+1,i}\chi_i
\]
Some computational notes

- Ingredients incorporated into user-friendly code (RecSparse) which outputs $x(z)$ for all times and atomic populations at several chosen slices.
- Collisions neglected for time being
- LAPACK libraries used for inversion of submatrices
- Simple rk4 ode solver used
- Checked on MLA code of Hirata et al. with higher level two-photon transitions turned off and dense time grid (19548 steps in dlna going from $z=1606$ to $z=700$), agreement to several parts in $10^5$, with and without feedback
Higher-n $2\gamma$ transitions in H important at 7-$\sigma$ 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.

Unfinished business: Are other forbidden transitions in hydrogen important, particularly for Planck data analysis?
Electric quadrupole (E2) transitions are suppressed but conceivably not irrelevant at the desired level of accuracy:

\[ \frac{A_{quad}^{m,l \pm 2 \rightarrow n,l}}{A_{dipole}^{m,l \pm 1 \rightarrow n,l}} \sim \alpha^2 \approx 5 \times 10^{-5} \]

Coupling to ground state will overwhelmingly dominate:

\[ \frac{A_{quad}^{n,2 \rightarrow 1,0}}{A_{quad}^{n,2 \rightarrow m,0}} \propto \frac{\omega_{n1}^5}{\omega_{nm}^5} = \left( \frac{1 - \frac{1}{n^2}}{\frac{1}{m^2} - \frac{1}{n^2}} \right)^5 \geq 1024 \text{ if } m \geq 2 \]

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 RATES: BASIC FORMALISM

- Reduced matrix element evaluated using Wigner 3J symbols:
  \[
  \langle l_a \parallel C^{(2)} \parallel l_b \rangle = (-1)^{l_a} \sqrt{(2l_a + 1)(2l_b + 1)} \begin{pmatrix} l_a & 2 & l_b \\ 0 & 0 & 0 \end{pmatrix}
  \]

- Radial matrix element evaluated using operator methods
  \[
  2 R_{n_a l_a}^{n_b l_b} \equiv \int_0^\infty r^4 R_{n_a l_a} (r) R_{n_b l_b} (r) dr
  \]
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 $A_{nd\rightarrow 1s} x_{nd}$. 
QUADRUPLE 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

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

- For $n < 5$ at early times, $x_{nd} > \frac{5}{3} x_{np}$: net effect is $nd \rightarrow np$, np decays to 2s. Dominant rec. channel is $2s \rightarrow 1s$ accelerates rec.

- For $n > 5$ at early times, $x_{nd} < \frac{5}{3} x_{np}$: net effect is $np \rightarrow nd$, nd decays to 2p. Dominant rec. channel is $2s \rightarrow 1s$ so higher quadrupoles decelerate rec.

- For all $n$ at late times, $x_{nd} < \frac{5}{3} x_{np}$: net effect is $np \rightarrow nd$, nd decays to 2p. Dominant rec. channel is $2p \rightarrow 1s$ at late times, so all quadrupoles accelerate rec.
Quadrupole rates: Operator algebra

- Radial Schrödinger equation can be factored to yield:

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

\[- \Omega_{nl} R_{nl}(r) = R_n \ l_{-1}(r) \quad + \Omega_{nl} \ l_{-1} R_{nl}(r) = R_{nl}(r) \]

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

- This algebra can be applied to radial matrix elements:
Radial Schrödinger equation can be factored to yield:

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

\[-\Omega_{nl} R_{nl}(r) = R_{n\,l-1}(r) \]
\[+ \Omega_{n\,l-1} R_{nl}(r) = R_{nl}(r) \]

This algebra can be applied to radial matrix elements:

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

Diagonal!
Quadrapole rates: Operator Algebra

Radial Schrödinger equation can be factored to yield:

\[-\Omega_{nl} = \frac{1}{l A_{nl}} \left[ 1 - l \left( \frac{d}{dr} + \frac{l + 1}{r} \right) \right] \quad \text{and} \quad +\Omega_{nl} = \frac{1}{l A_{nl}} \left[ 1 + l \left( \frac{d}{dr} - \frac{l - 1}{r} \right) \right] \]

\[-\Omega_{nl} R_{nl}(r) = R_{n' l-1}(r) \quad \text{and} \quad +\Omega_{n' l-1} R_{nl}(r) = R_{nl}(r) \]

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

This algebra can be applied to radial matrix elements:

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

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

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

Off-diagonal!
Rates were checked using WKB expressions like dipole rates

Compared to published numerical rates of Jitrik and Bunge: 4-5 digits of agreement (Dirac vs. non-rel wf), but this would be a correction to a small correction
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 ($n=1 \rightarrow n=2$) yield less suppression for $n>1$

Effect larger at late times (low $z$) as rates fall
Deviations from SAHA equilibrium

- $n=1$ suppressed due to freeze-out of $x_e$
- Remaining levels ‘try’ to remain in Boltzmann eq. with $n=2$
- Super-Boltz effects and two-$\gamma$ transitions ($n=1 \rightarrow n=2$) yield less suppression for $n>1$
- Effect larger at late times (low $z$) as rates fall
Deviations from Boltzmann Eq: High-n

\( \alpha n \gtrsim A_{bb,dow} \).

\( n_{max} = 120 \)

\( z = 206 \)

\( z = 474 \)

\( z = 611 \)

\( z = 749 \)

\( z = 1573 \)
DEVIATIONS FROM BOLTZMANN EQ: 1-substates

RecSparse results \( n_{\text{max}} = 30 \)

\( \frac{(N - N_{\text{eq}})}{N_{\text{eq}}} \) (in %)

\( n = 18 \)

\( n = 22 \)

\( n = 10 \)

\( n = 14 \)

\( n = 6 \)

\( x \quad z = 1417 \)

\( x \quad z = 1281 \)
**DEViations FROM BOLTZMANN EQ: l-substates**

**RecSparse results** \( n_{\text{max}} = 30 \)

\[
\frac{(N - N_{eq})}{N_{eq}} \quad (\text{in } \%) 
\]

- \( n = 18 \)
  - Lower \( l \) states can easily cascade down, and are relatively under-populated

- \( n = 22 \)
  - \( x \) \( z = 1417 \)
  - \( x \) \( z = 1281 \)

- \( n = 10 \)
- \( n = 14 \)
- \( n = 6 \)

Lower \( l \) states can easily cascade down, and are relatively under-populated
DEVIATIONS FROM BOLTZMANN EQ: l-substates

RecSparse results \( n_{\text{max}} = 30 \)

Higher l states can’t easily cascade down, and are relatively over-populated

\[
\frac{(N - N_{eq})}{N_{eq}} \quad \text{(in \%)}
\]

\( n = 18 \)

\( n = 22 \)

\( n = 10 \)

\( n = 14 \)

\( n = 6 \)

\( \times \quad z = 1417 \)

\( \times \quad z = 1281 \)

Thursday, September 24, 2009
Deviations from Boltzmann Eq: $l$-substates

RecSparse results $n_{\text{max}} = 30$

Chluba/Rubino-Martin/Sunyaev 2006

Highest $l$ states recombine inefficiently, and are relatively under-populated

$\times \ z = 1417$

$\times \ z = 1281$
Deviations from Boltzmann Eq: $I$-Substates

RecSparse results $n_{\text{max}} = 30$

$\frac{(N - N_{\text{eq}})}{N_{\text{eq}}}$ (in %)

$n = 18$

$n = 22$

$\times z = 1417$

$\times z = 1281$

$n = 10$

$n = 14$

$n = 6$
DEVIATIONS FROM BOLTZMANN EQ: l-substates

RecSparse results \( n_{\text{max}} = 30 \)

\[
\frac{N - N_{\text{eq}}}{N_{\text{eq}}} \quad \text{(in %)}
\]

\( n = 18 \)

\( n = 22 \)

\( n = 10 \)

\( n = 14 \)

\( n = 6 \)

\( \times \ z = 1417 \)

\( \times \ z = 1281 \)

\( l=0 \) can’t cascade down, so s states are not as under-populated
DEVIANATIONS FROM BOLTZMANN EQ: $l$-substates

RecSparse results $n_{\text{max}} = 30$

Why the feature at $l=2$?

$\frac{(N - N_{eq})}{N_{eq}}$ (in %)

$n = 18$

$n = 22$

$\times z = 1417$

$\times z = 1281$

$n = 10$

$n = 14$

$n = 6$

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Deviations from Boltzmann Eq: l-substates

RecSparse results

\[ n_{\text{max}} = 30 \]

\[ \frac{(N - N_{\text{eq}})}{N_{\text{eq}}} \text{ (in %)} \]

- \( n = 18 \)
  - \( z = 1417 \)
- \( n = 22 \)
  - \( z = 1281 \)

- \( n = 10 \)
- \( n = 14 \)
- \( n = 6 \)
DEViations FROM BOLTZMANN EQ: I-substates

Compare with Rubino-Martin, Chluba, and Sunyaev 2006: Similar Features!
DEViations FROM BOLTzmann EQ: l-substates

RecSparse output

\[
\frac{(n_n/n_l)}{(2l+1)/n^2}
\]

\(n_{\text{max}} = 120, \quad n = 61\)

\(z = 1573\)
\(z = 749\)
\(z = 612\)
\(z = 206\)
DEVIATIONS FROM BOLTZMANN EQ: $l$-substates

RecSparse output

Patterns persist for high $n$, $n_{\text{max}}$
DEVIATIONS FROM BOLTZMANN EQ: I-substates

RecSparse output

I-substates are highly out of Boltzmann eqb’m at late times
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 efficiently 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 Balmer transitions from $l=2$ artificially disabled: the blip should move to $l=1$. 
$n_{\text{max}} = 50$

$z = 440$

$z = 320$

$z = 205$
$n_{\text{max}} = 50$

$n = 10$

$n = 18$

$n = 26$

$n = 34$

$n = 42$

$n = 50$

$z = 440$

$z = 320$

$z = 205$
l-substate populations, Balmer lines off

$n_{\text{max}} = 50$

$n = 10$

$n = 18$

$n = 26$

$n = 34$

$n = 42$

$n = 50$

$z = 440$

$z = 320$

$z = 205$

Dip moves as expected when Balmer lines are off!
$l$-substate populations, Balmer lines off

$n_{\text{max}} = 50$

$n = 10$

$n = 18$

$n = 26$

$n = 34$

$n = 42$

$n = 50$

$z = 440$

$z = 320$

$z = 205$
RESULTS: RECOMBINATION HISTORIES
INCLUDING HIGH-N STATES

- $x_e(z)$ falls with increasing $n_{\text{max}} = 10 \rightarrow 200$, as expected.
- Rec Rate $> \text{downward BB Rate} > \text{Ionization, upward BB rate}$
- For $n_{\text{max}} = 100$, code computes in only 2 hours
RESULTS: CMB ANISOTROPIES WITH HIGH-N STATES, TEMPERATURE (TT) $C_l$s

Super-horizon scales don’t care about recombination!

Sample variance for Planck

$n_{\text{max}} = 100 \text{ vs. } n_{\text{max}} = 50$

$n_{\text{max}} = 150 \text{ vs. } n_{\text{max}} = 100$

$n_{\text{max}} = 200 \text{ vs. } n_{\text{max}} = 150$

$e^{-2\tau}$ plateau
RESULTS: CMB ANISOTROPIES WITH HIGH-N STATES, POLARIZATION (EE) $C_{l}$

Lower $\tau$ after LSS, wider LSS $\rightarrow$ more polarization

Sample variance for Planck

$n_{\text{max}} = 100$ vs. $n_{\text{max}} = 50$

$n_{\text{max}} = 150$ vs. $n_{\text{max}} = 100$

$n_{\text{max}} = 200$ vs. $n_{\text{max}} = 150$
RESULTS: RECOMBINATION WITH HYDROGEN QUADRUPOLES

\[ \Delta x_e \equiv x_e \big|_{\text{no } E2 \text{ transitions}} - x_e \big|_{\text{with } E2 \text{ transitions}} \]

Diagram showing the change in \( \Delta x_e \) with \( n_{\text{max}} \):
- \( n_{\text{max}} = 5 \)
- \( n_{\text{max}} = 10 \)
- \( n_{\text{max}} = 20 \)
- \( n_{\text{max}} = 30 \)
RESULTS: CMB ANISOTROPIES WITH HYDROGEN QUADRUPOLES, TEMPERATURE \((TT)\) \(C_l\)s

\[
\Delta C_l = C_l\bigg|_{\text{with } E2 \text{ transitions}} - x_e\bigg|_{\text{no } E2 \text{ transitions}}.
\]

Bulk of integral from late times, higher \(n_{\text{max}}\) → lower \(x_e\) → lower \(\tau\) → higher \(e^{-2\tau}\) → higher \(C_l\)
RESULTS: CMB ANISOTROPIES WITH HYDROGEN QUADRUPOLES, TEMPERATURE ($TT$) $C_l$s

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

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 $C_l$
RESULTS: CMB ANISOTROPIES WITH HYDROGEN QUADRUPOLES, POLARIZATION \((EE) C_l\)s

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

Bulk of integral from late times, higher \(n_{\text{max}}\) → lower \(x_e\) → lower \(\tau\) → higher \(e^{-2\tau}\) → higher \(C_l\)
RESULTS: CMB ANISOTROPIES WITH HYDROGEN QUADRUPOLES, POLARIZATION (EE) $C_l$s

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

Overall effect is negligible for upcoming CMB experiments!

Bulk of integral from late times, higher $n_{\text{max}} \rightarrow$ lower $x_e$ → lower $\tau$ → higher $e^{-2\tau}$ → higher $C_l$
For fixed $n$, $l$-changing collisions bring different-$l$ 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!
- $t_{\text{pass}} < t_{\text{orbit}} \rightarrow$ Impulse approximation breaks down!

Next we’ll include them to see if we need to model rates better
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~150 and higher) are relevant for CMB data analysis
  - E2 transitions in H are not relevant for CMB data analysis
- To do: include collisions and line overlap in RecSparse
- Full incorporation into CosmoMC and analysis of errors/degeneracies with cosmo. parameters