Atomic data for kinetics modeling of light element plasmas

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Outline

- Solving rate equations
- Need structure, collisional, radiative data
- Many methods available
- Consistency
- completeness

Rate equations

Time evolution of populations :

$$\frac{dN_{i,j}}{dt} = \sum_k R^I_{i-1,k\to i,j} N_{i-1,k} - \sum_k R^I_{i,j\to i+1,k} N_{i,j} +$$

$$\sum_k R^R_{i+1,k\to i,j} N_{i+1,k} - \sum_k R^R_{i,j\to i-1,k} N_{i,j}$$

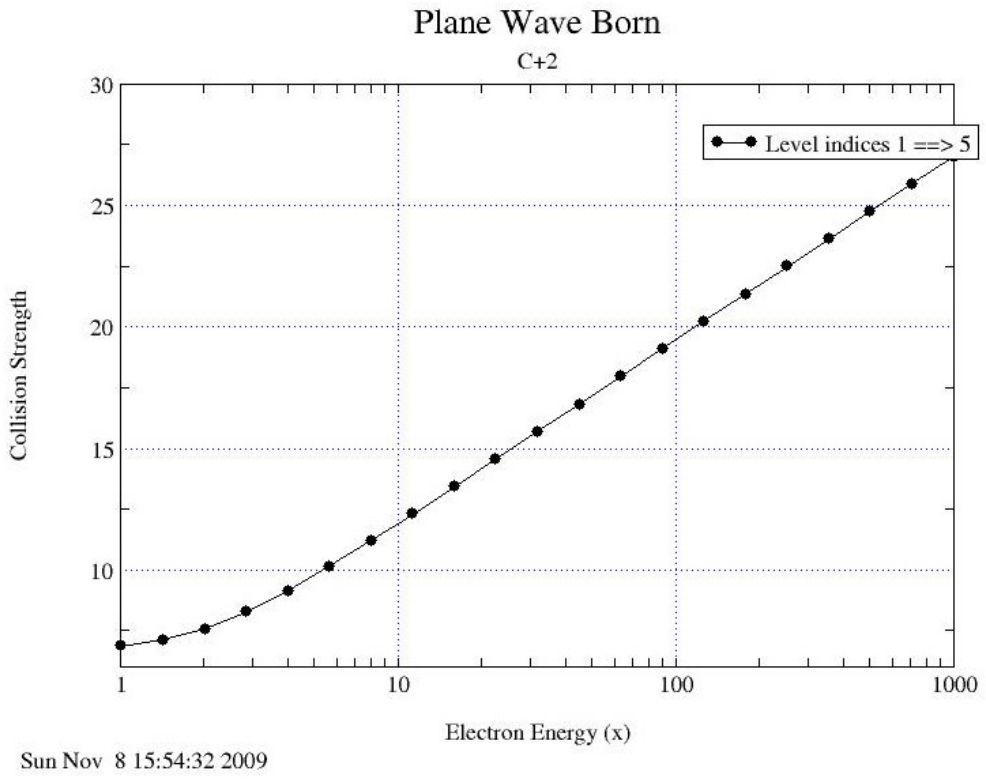
Rate coefficients

- Rate coefficients needed for upward and downward transitions
- Use detailed balance on cross sections, integrate for rate coefficient
- Need to follow all levels unless at very low or high density (coronal or LTE)
- Must connect all levels included in the model
- For full kinetics calculation, need differential cross sections

Excitation methods

- Plane wave Born (PWB) from GOS can be calculated in structure code
- DWA or FOMBT are well known methods
- R-matrix or Close coupling very accurate, but lengthy
- Compare PWB and FOMBT for allowed, forbidden in C II

C II $2s^2 \rightarrow 2s\ 2p\ {}^1P_1$



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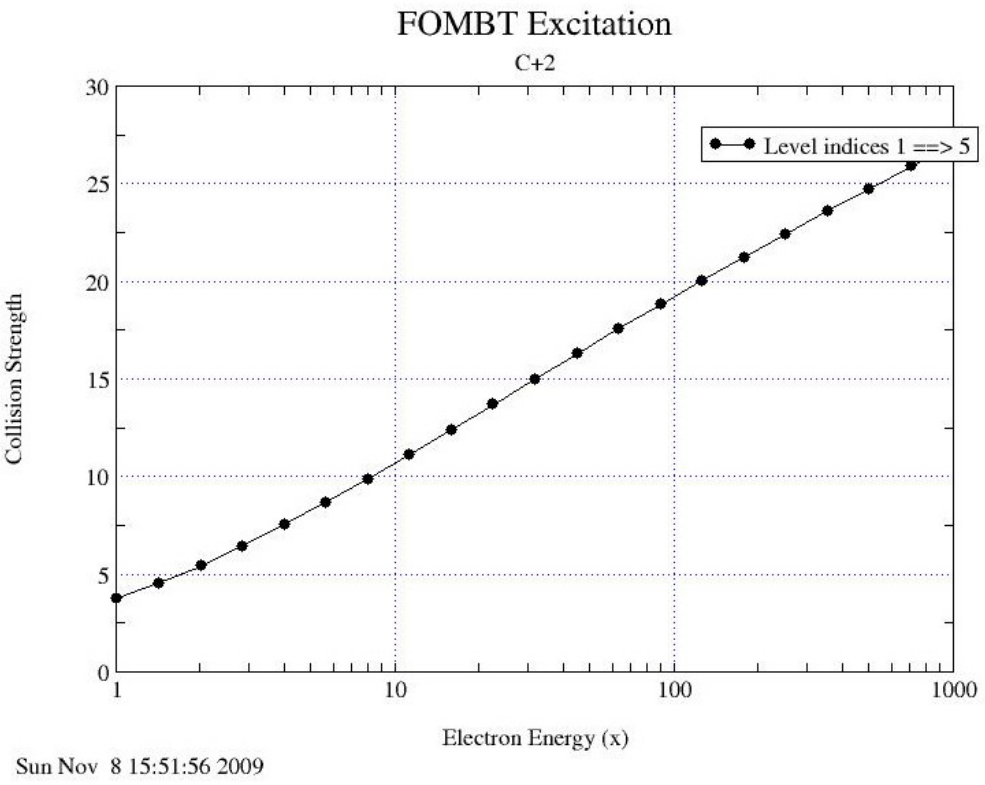
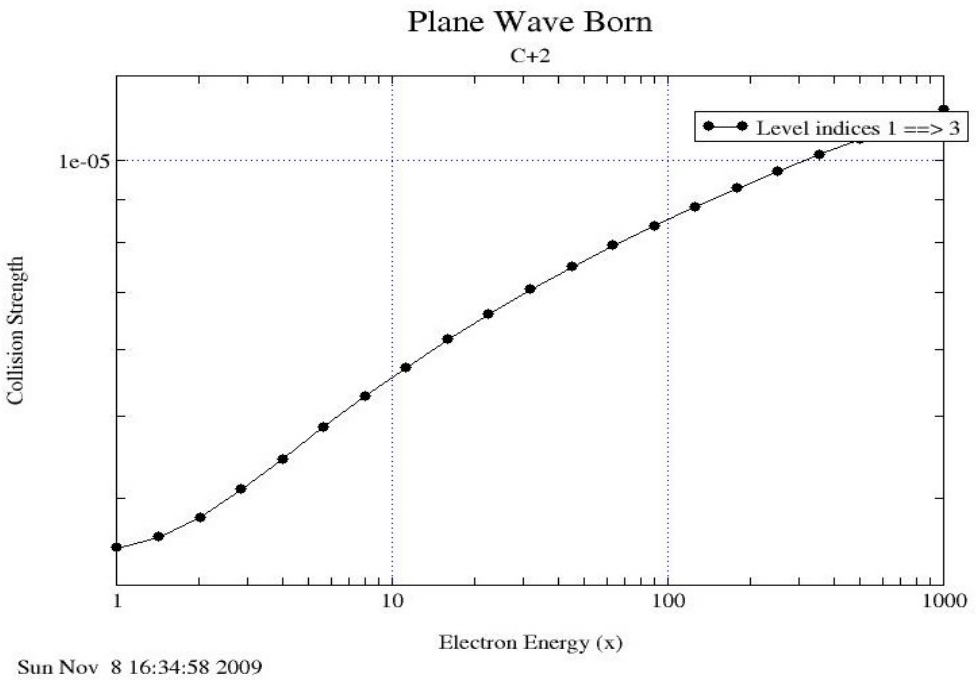


Allowed transitions

- PWB close to FOMBT
- Collision strength is large
- Target state mixing is not a big issue

C II $2s^2 \rightarrow 2s\ 2p\ {}^3P_1$



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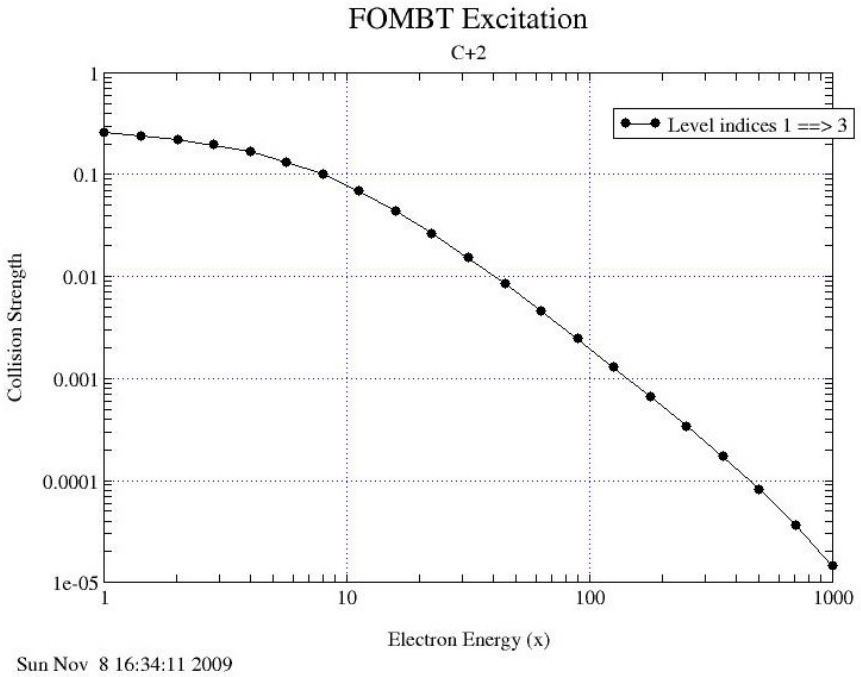


Forbidden states

- PWB is near zero at low energy
- PWB is nonzero due to target mixing
- Spin orbit mixing is very small for carbon
- PWB rises to 10^{-5} at 1000 x
- FOMBT is relatively large at threshold
- Falls to 10^{-5} at 1000x

What to do

- PWB is fine for many transitions
- PWB is very poor for spin change transitions for light elements
- At high enough energy PWB will approach FOMBT
- For excited to excited cross sections transition energy is low, so PWB may not be too bad

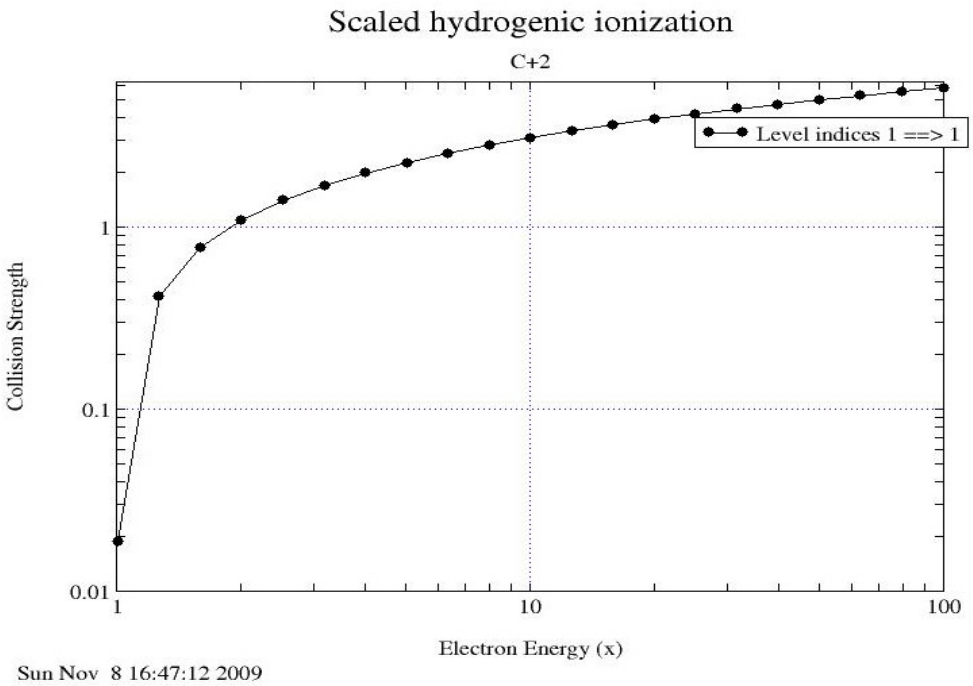
Resonances

- PWB and FOMBT do not include resonances
- R-matrix, close coupling automatically include resonances
- CR model with inclusion of autoionizing levels will give effect of resonances

Collisional ionization

- Work by Sampson et al. calculated scaled hydrogenic cross sections, scaleable to complex ions using screening parameters
- DWA is widely available, but is lengthy
- CCC is best, but very time intensive
- Scaled hydrogenic is not bad for most transitions

C II $2s^2 \rightarrow 2s$



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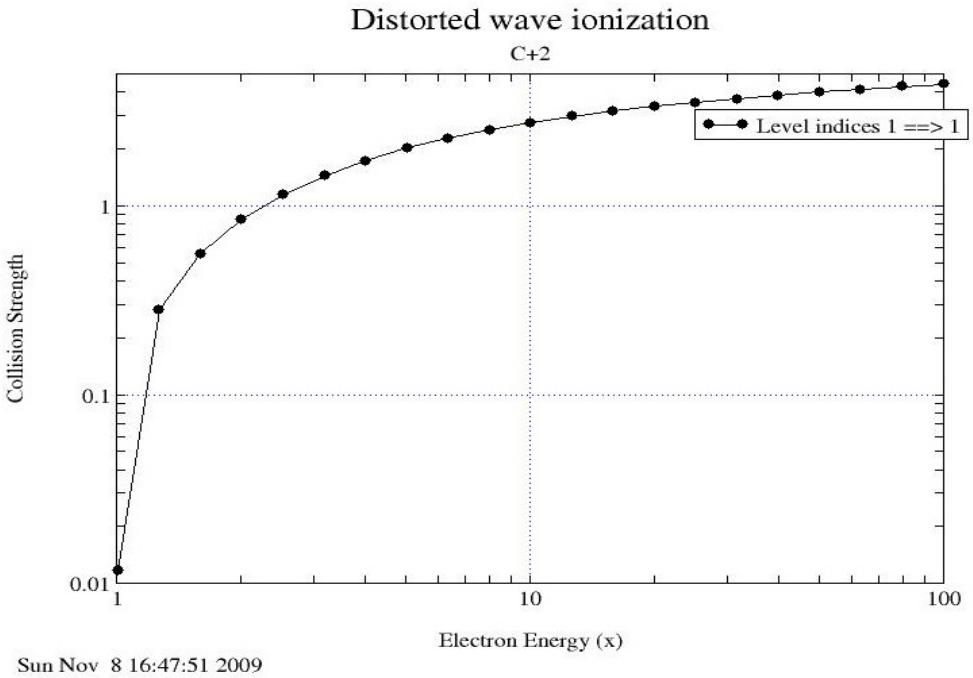

Consistency

- Kinetics calculation requires structure, collision and radiative processes
- Cross sections should use the same wave functions as the energy levels
- If R-matrix or close coupling cross sections are used, care must be taken for consistency with autoionizing states

Resonance considerations

- Assume CR with AI states included
- Using resonances in excitation and/or ionization implicitly includes AI states
- If CR calculation follows AI levels, it can add those effects to excitation/ionizations, giving duplicate contributions

Completeness

- Many levels can contribute to aspects of a plasma
- All levels need to be connected
- Large data sets result
- Recent work at LANL by James Colgan on carbon and Boron include on order of 10^4 levels and 10^8 transitions
- Collisional-radiative calculation is possible but very long

How accurate?

- Do sensitivity studies, DATASENS
- Be model: configuration average, ~100 config/ion, $1s^2$, $1s^1$, $1s^0$ all included → many autoionizations
- Random vs. systematic errors
- Separate scaling for different processes

What is needed in database

- Comprehensive set of energy levels
- Cross sections consistent with those energy levels
- Care must be taken with resonances
- Complete set of transitions among all levels that are followed in kinetics calculation
- Bundling is being explored, but requires an initial complete data set