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Session 5

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Session topics

Atomic models revisited

— Model comparisons

— Closed shell challenges

Radiation transport

— ”Flavors”: continuum, lines, spectral

— Radiation description + transport equation

— Goals: energetics, kinetics / populations / spectra

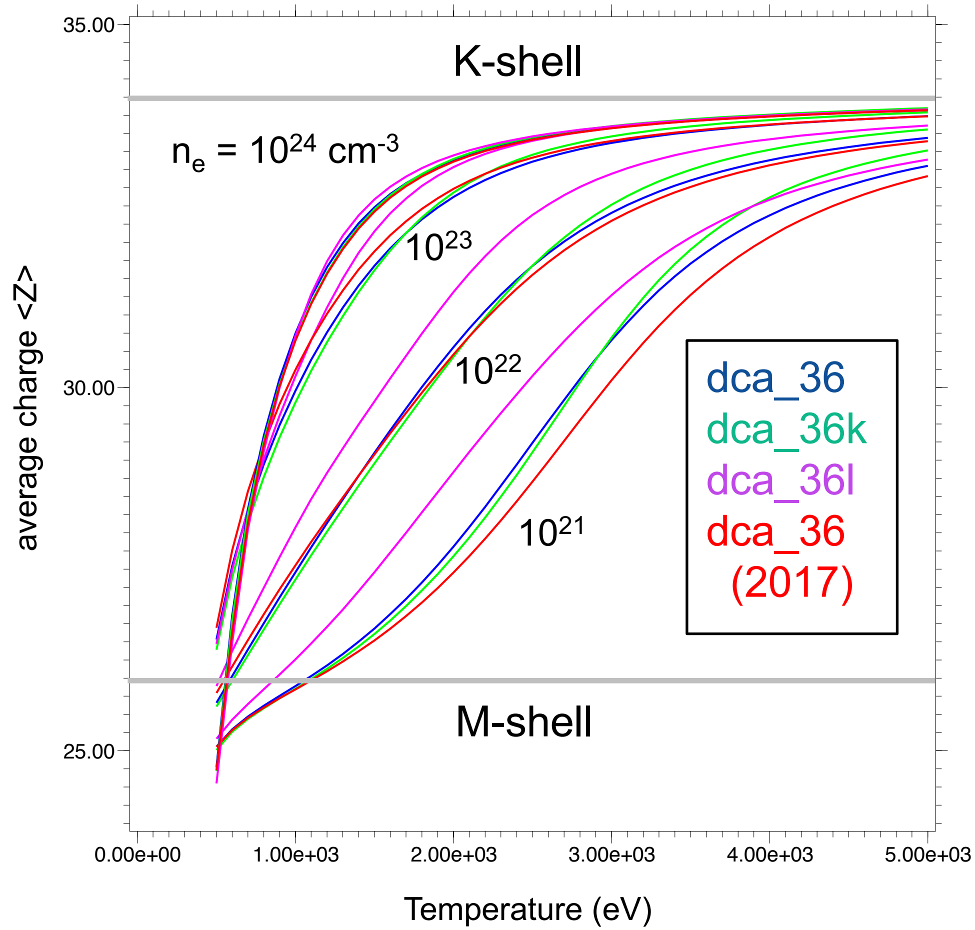
Revisiting atomic models - Kr

Atomic model structure can affect
- Average quantities e.g. <Z>
- Charge state distribution
- Emission / absorption spectra

Effects can vary greatly with density:

Low density is sensitive to
- Detailed structure
- Low-lying levels
- Autoionizing state / transitions

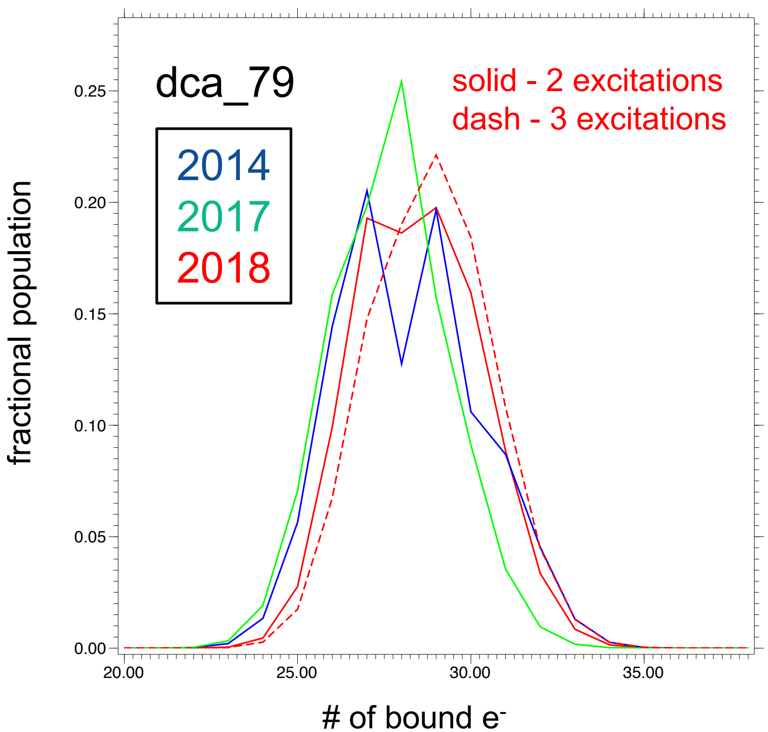
High density is sensitive to
- Extent of excited states (number and multiplicity)



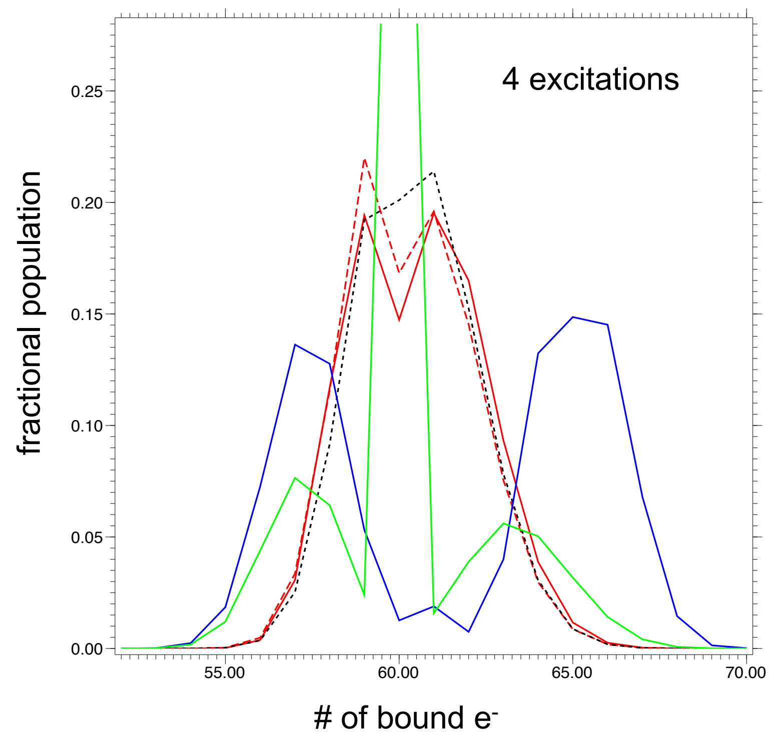
The requirements on an atomic model vary with the application

Closed shells pose a challenge for atomic models

New recommendation for standard models: dca_*xx* (K-shell models will follow soon)
/usr/gdata/dca/Models/2018_05_02



A bug in the 2017 models produced strange behavior at the N-O shell boundary



New (2018) models show improved closed-shell behavior

Radiation transport "flavors"

Continuum, lines and spectra are treated separately for efficiency

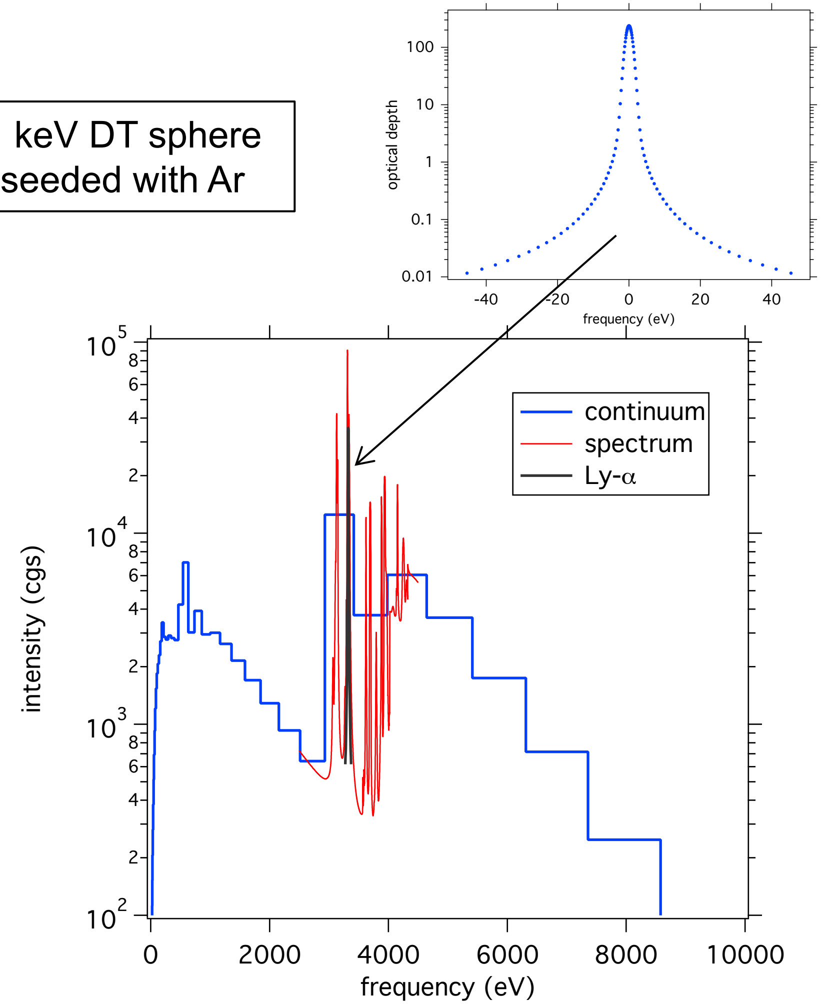
Iterated to consistency with atomic kinetics (and other processes):

- <u>continuum radiation</u> coarsely-binned over full energy range for evaluating photo rates
- <u>line radiation</u> finely-binned for resolving individual line profiles

Evaluated after convergence:

- <u>spectral radiation</u> at arbitrary energies to resolve features of interest

1 keV DT sphere seeded with Ar



Radiation description

- Macroscopic description: specific intensity $\boldsymbol{I_\nu}$
  - energy per (area x solid angle x time) within the frequency range $(\nu + d\nu)$
  - dE = energy crossing area dA within $(d\Omega\, d\nu\, dt)$

$$dE = I_\nu\left(\vec{r},\Omega,t\right)\left(\vec{n}\bullet\vec{\Omega}\right)dA\,d\Omega\,d\nu\,dt$$

- Microscopic description: photon distribution function $\boldsymbol{f_\nu}$

$$dE = \sum_{spins}\left(h\nu\right)f_\nu\left(\vec{r},\vec{p},t\right)\frac{d^3\vec{x}\,d^3\vec{p}}{h^3} \qquad \vec{p} = \frac{h\nu}{c}\vec{\Omega}$$

- Correspondence between descriptions:

$$I_\nu = 2\frac{h\nu^3}{c^2}f_\nu\left(\vec{r},\vec{p},t\right)$$

- Angle-averaged intensity:

$$J_\nu = \frac{1}{4\pi}\int I_\nu\,d\Omega$$

LTE:	Planck function	Bose-Einstein distribution
	$B_\nu = 2\frac{h\nu^3}{c^2}\frac{1}{e^{h\nu/kT_r}-1}$	$f_\nu = \frac{1}{e^{h\nu/kT_r}-1}$

Radiation transport equation

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \vec{\Omega} \bullet \nabla I_\nu = -\alpha_\nu I_\nu + \eta_\nu$$

α_ν = absorption coefficient (fractional energy absorbed per unit length)

η_ν = emissivity (energy emitted per unit time, volume, frequency, solid angle)

Define the source function : $S_\nu = \eta_\nu / \alpha_\nu$ and optical depth τ_ν : $d\tau_\nu = \alpha_\nu dr$

Characteristic form of the transport equation

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \Rightarrow I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S_\nu(\tau'_\nu) d\tau'_\nu$$

Self-consistently determining S_ν and I_ν is the hard part of radiation transport

Radiation transport "goals"

- LTE / energy transport:
  - Solves radiation transport + energy balance equations for J_ν + material temperature
  - Used in rad-hydro codes (with modifications for NLTE)

$$\frac{dE_m}{dt} = 4\pi \int \alpha_\nu (J_\nu - S_\nu) d\nu$$

$$\alpha_\nu = \alpha_\nu(T_e) \; , \; S_\nu = B_\nu(T_e)$$

- NLTE / spectroscopy:
  - Solves radiation transport + rate equations for J_ν + populations

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}\mathbf{y} \; , \; \mathbf{A}_{ij} = \mathbf{A}_{ij}(T_e, J_\nu)$$

$$S_\nu = \tfrac{2h\nu^3}{c^2} S_{ij} \; , \; S_{ij} \approx a + b\bar{J}_{ij}$$

- "Formal" transport:
  - Assumes S_ν is fixed, no self-consistency
  - Used in Cretin for spectral transport

- **Each "goal" uses different methods to achieve self-consistency**
- **Treatment of the radiation transport equation <u>may</u> also change**

Self-consistency and convergence in radiation transport

The combined equations of radiation transport + other physics

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \ , \ S_\nu = S_\nu(T_e, J_\nu) \ , \ J_\nu = \frac{1}{4\pi}\int I_\nu \, d\Omega$$

are non-linear and must be iterated to convergence

Simple iteration (“lambda iteration”) transports the effects of radiation in the combined system $\sim$1 optical depth/iteration

- convergence can require many iterations: $\sim\tau^n, n = 1 - 2$
- false convergence is a problem for $\tau \gg 1$

Controls to set convergence tolerances and maximum iterations depend on the type of transport

Methods to accelerate convergence differ for each type of transport

Major controls on radiation transport

<u>Continuum radiation</u>

- **switch 36** : 0 (off), > 0 (steady-state: c=∞), < 0 (time-dependent)
  1-d options: +/-1 (Feautrier formalism), other (integral formalism)
- Frequencies same as used by kinetics: must cover entire range $[0, > 20\ T_{max}]$
- Convergence by lambda iteration: **switch 44** , **param 56** for charge state populations

<u>Spectral radiation</u>

- Turned on by existence of **spectrum** commands
- Frequencies set by **spectrum** commands: cover only range(s) of interest
- **switch 63** : include Doppler shifts if ≠0

<u>Line radiation</u>

- **switch 37** : 0 (off), other (on)
- Only affects transitions identified with **line** commands
- Frequency mesh for each line set by **lbins** commands
- Convergence by linearization: **switches 40, 41** + **param 57**
- Many options for controlling physics