Atomic data and models: a primer for high resolution X-ray spectroscopy

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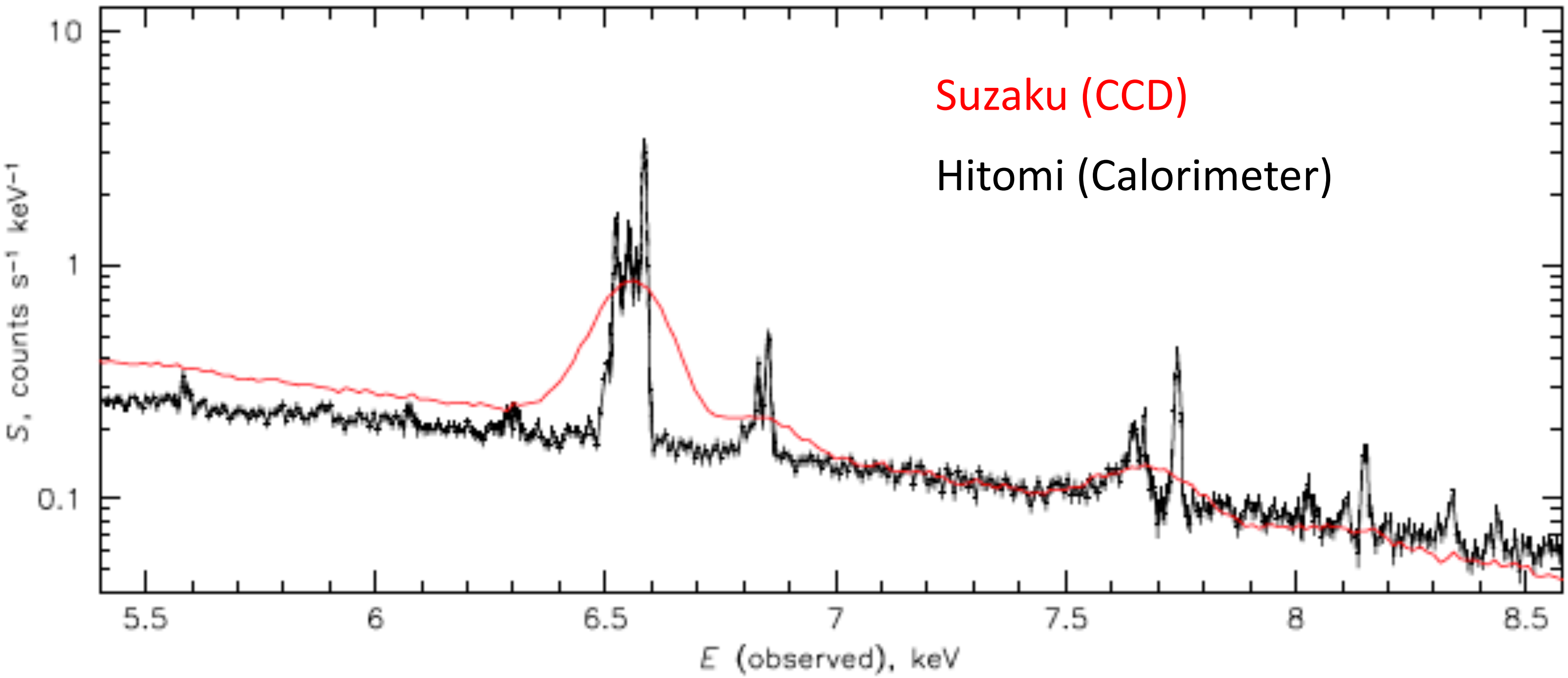
Why care about atomic data?



We see them, and:
there is information in these lines!

Preference for black box?

You can use models (APEC, SPEX, Chianti, XSTAR, ….) as black boxes
It gives you a temperature, an abundance
But what does it mean?
How accurate is it?
Why do I see residuals?
Help!

What can you learn from a spectrum?

1. (Electron) temperature (from continuum or lines present)
2. Ion temperature (from line broadening)
3. Turbulence (from line broadening)
4. Velocity fields (from Doppler shifts)
5. Electron density (from line ratios)
6. Emission measure n^2V (from flux)
7. Abundances (from relative line intensities)
8. Age of the plasma (for transient plasmas)
9. Ionisation process (photons, electrons)
10. Nonthermal electrons
11. Dust
12. Sometimes: magnetic fields
13. Etc.

Steps in understanding a thermal spectrum and how to calculate a model for it

1. Basic physical properties:
    - temperature, density, composition, size, shape, influx, …..
2. Determine ionization balance: how many ions of each species
    - depends on physical conditions
3. Calculate emitted spectrum
4. Calculate absorption by the source:
    can all radiation escape?

Types of plasma

- Type determined by role of collisions of ions with:
  - *Electrons* (always there)
  - *Photons* (relevant for several interesting sources)
  - *Protons* (usually small corrections)
  - *Other ions / atoms* (Charge exchange)
- Always solve balance ionisation ←→ recombination
- Sometimes solve balance heating ← → cooling
- Sometimes consider transient plasmas

Ionisation balance

Plasma type	Ionisation Balances recombination	Heating balances cooling	Time dependent (no balance)	Optical depth
CIE (Collisional Ionisation Equilibrium)	✓	✗	✗	τ=0
PIE (Photo Ionisation Equilibrium)	✓	✓	✗	τ>1
NEI (Non-Equilibrium Ionisation)	✓ With source term	✗	✓	τ=0
Transient PIE	✓ With source term	?	✓	τ>1

Emission components:

not everything is Bremsstrahlung!

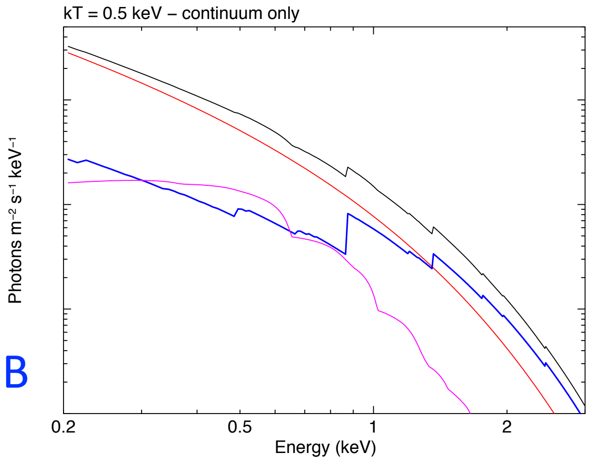
(and not everything is Fe-K….)

- Continuum
  - Bremsstrahlung

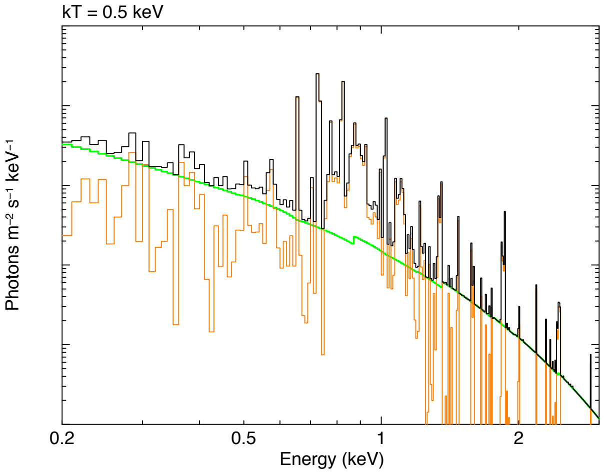
    from all ions, not only hydrogen
  - Radiative Recombination Continuum (RRC)

    narrow, line-like for PIE plasmas
  - Two Photon emission

NB



- Lines
  - Can dominate the flux at lower temperatures



Absorption components

- Continuum ”edges”
  - Easy to find with low-resolution instruments
  - Broad-band
- Absorption lines
  - Much more sensitive to detect low columns of plasma
  - Needs high-resolution
- EXAFS (Extended X-ray Absorption Fine Structure)
  - Tracer for solid state structure (dust)
  - Continuum wiggles near absorption edges

Now where are the atomic data and processes?

Now where are the atomic data and processes?

- *For full plasma model, need many (12+) atomic processes:*
  - Collisional ionisation
  - Collisional excitation
  - Resonant excitation
  - Dielectronic recombination
  - Radiative transition probabilities
  - Auto-ionisation rates
  - Radiative Recombination rates
  - Photoionisation cross sections
  - Escape factors
  - Line energies
  - Charge exchange cross sections
  - Proton excitation
  - Etc.
- *Each process has its own intricacies and (atomic) data*

Plasma codes & models

Code	Applicable	Notes
Raymond-Smith	CIE	Deprecated, use APEC
APEC/ATOMDB	CIE, NEI, CX	
Chianti	CIE	Widely used for Sun
Mekal	CIE, NEI	Deprecated, use SPEX
SPEX	CIE, NEI, PIE, CX	
XSTAR	PIE mainly	Evolved from X-ray band
Cloudy	PIE mainly	Evolved from optical/UV

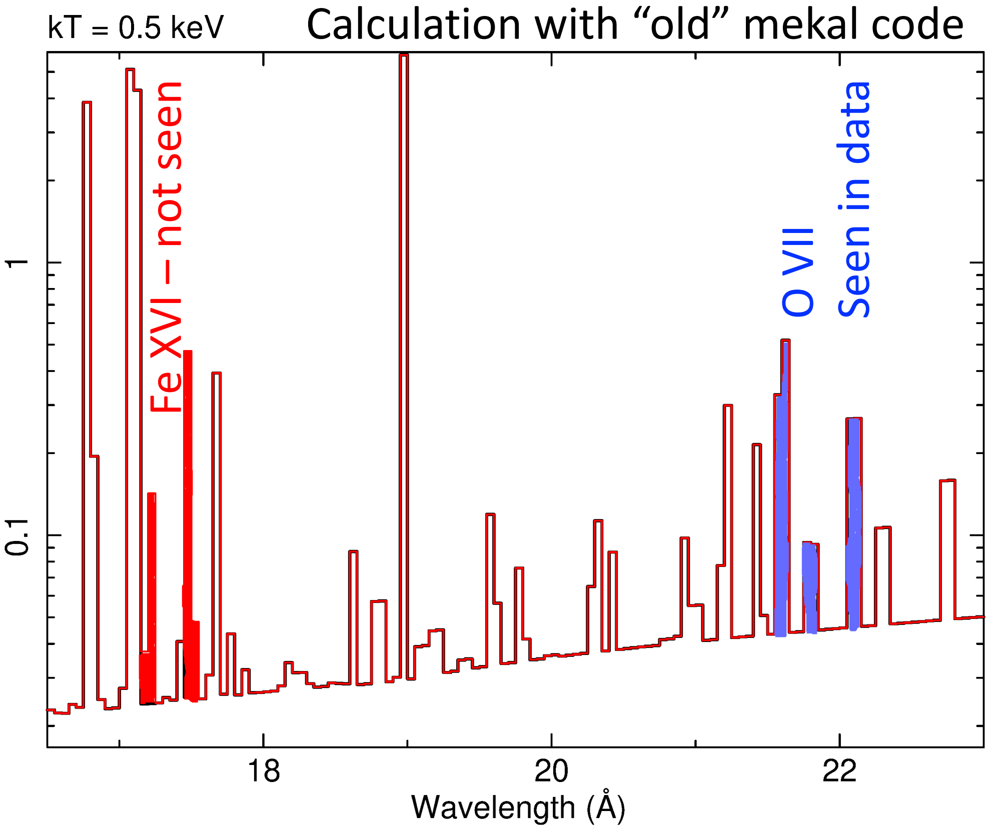
- All codes contain atomic data and algorithms to produce spectra
- Different techniques:
  - on the fly or pre-calculated
  - Original data or approximated data
  - Not always all processes included
- Level of modernity data can differ from code to code and process to process

All things can be important

Real example:

- "old" (pre-2000) mekal code had typo in Fe XVI lines (10x too strong) [not important for CCD but matters for grating]
- For RGS band, Fe XVI "coldest" Fe ion
- Line not seen in spectra, but predicted
- ➔ Make emission measure at low T lower in the model
- O VII formed at same temperatures
- ➔Make O abundance higher
- ➔Strong bias

Most codes had/have similar "glitches"



Analytical versus numerical

- Students learn to solve Schrödinger’s equation $i\hbar\partial\psi/\partial t=H\,\psi$ for Hydrogen analytically
- This is only case you can do this exact
- More than 1 electron → numerical methods
- Relativistic corrections important for e.g. Fe

R-matrix versus distorted wave

- Two methods used frequently to calculate interactions with free electrons in complex ions:
- R-matrix is most accurate, but can deal with fewer levels
- Distorted wave (DW) is less accurate, but can deal with more levels
- Example DW codes: HULLAC (Klapisch et al.), FAC (M.F. Gu et al.)

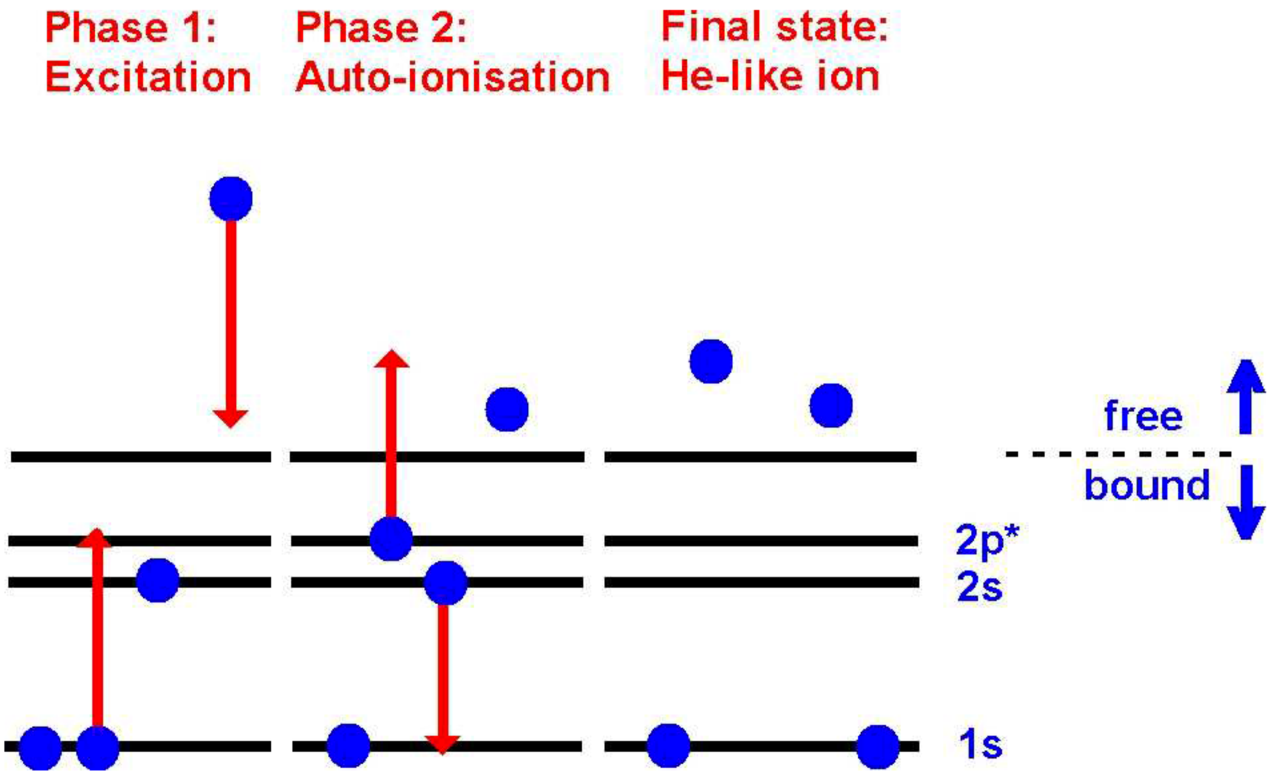
Now are the classical Bohr atom calculation useless?

- *Not at all, can give you useful insights*
- with E_H=13.6 eV, a_0=0.53 Å, α = 1/137
- *Energy* $E_n = -E_H Z^2 / n^2$
  - Higher charge, higher E
- *Size* $r = n^2 a_0 / Z$
  - Higher charge, more compact
- *Orbital velocity* $v/c = \alpha Z/n$
  - For Z=26 (hydrogenic Fe) already significant relativistic effects (~ 20%)
  - Strong interaction if passing particle has this velocity

Worked-out example: collisional ionisation

- Collision of a free electron with an atom can cause ionisation
- Several processes need to be accounted for:
  - Direct ionisation
  - Direct multiple ionisation (for high-E electrons)
  - Excitation autoionisation
- Highest rate if passing electron has similar speed as electron it kicks out

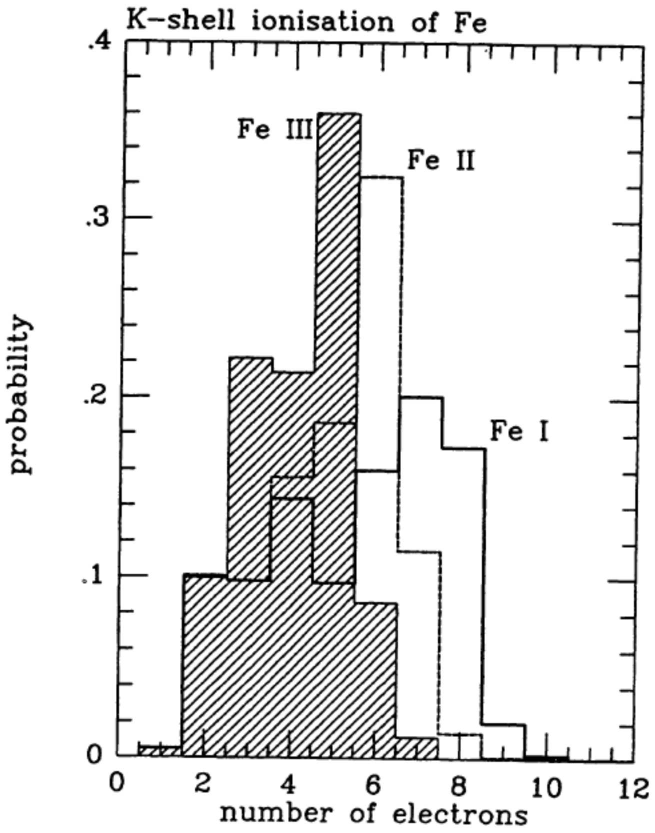
Worked-out example: collisional ionisation



Worked-out example: collisional ionisation

Cascades:

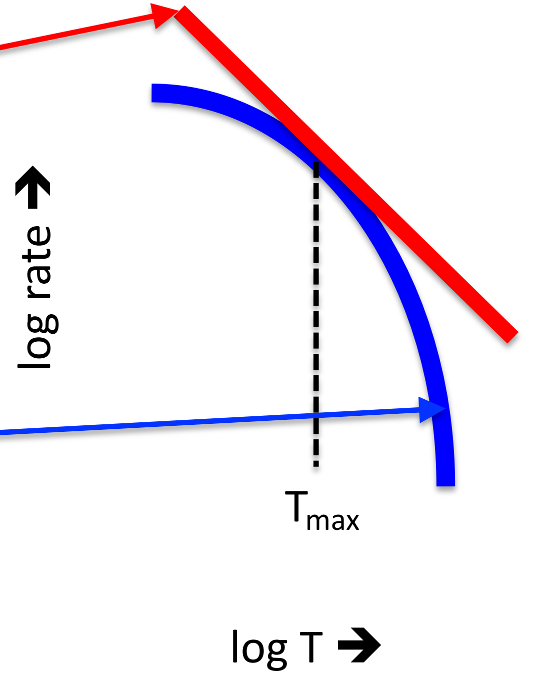
- One primary ionisation can lead to multiple ionisation
- Electrons from higher shells cascade down through fluorescent emission & Auger transitions
- Complex process to calculate because of many combinations



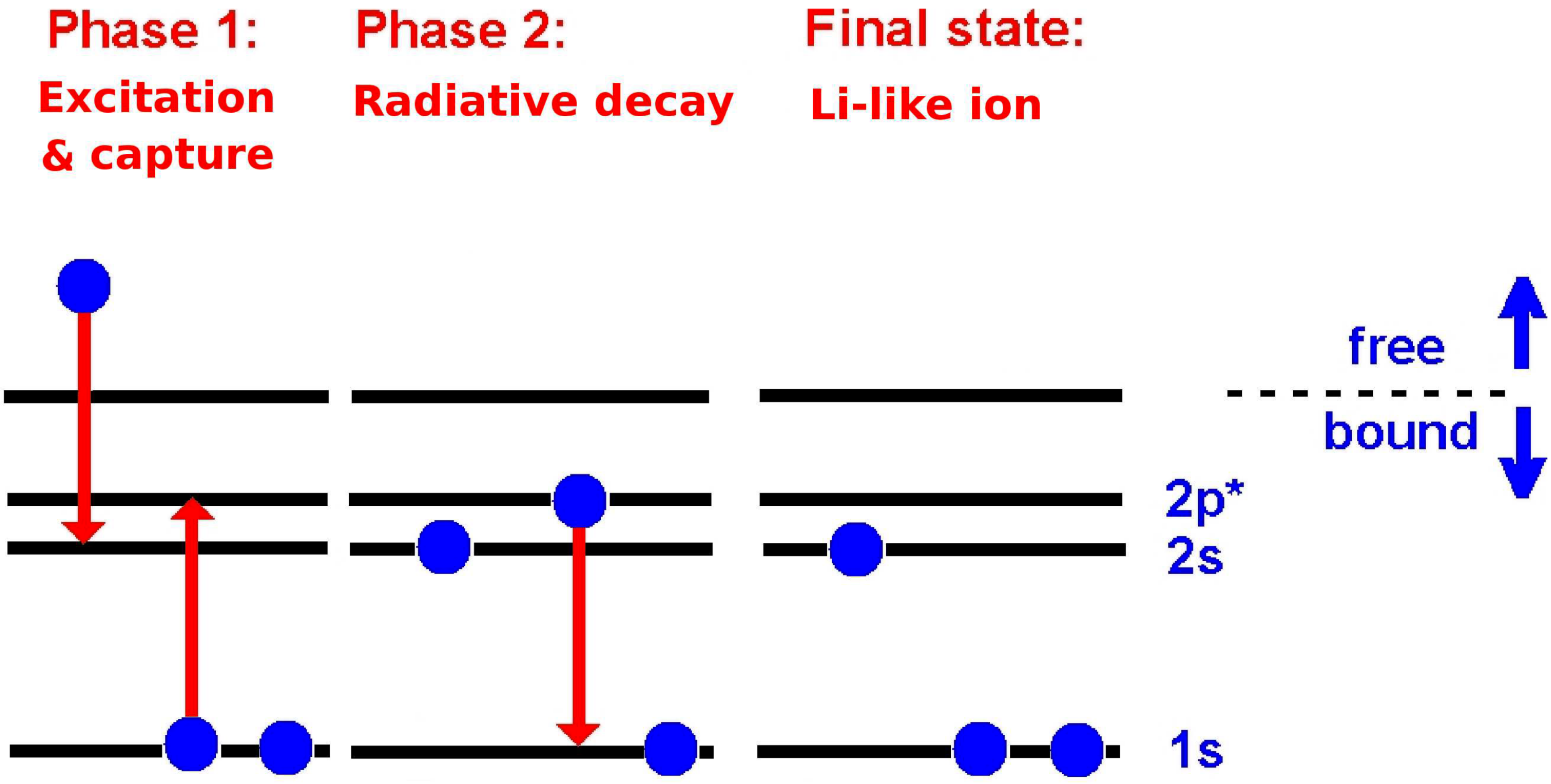
Kaastra & Mewe 1993

Need for updates

- *Example:* Mewe approximated radiative recombination by local *power-law*
- *Okay for CIE* (dominated by collisional excitation) but:
- Large *deviations* for recombining / ionising plasma when true shape is used (Mao et al. 2016)
- Strong consequences for derived O, N abundances in clusters



Dielectronic recombination



Why is dielectronic recombination hard to handle?

- Number of levels (combination of principal quantum number n and angular momentum ℓ) scales $\propto n^2$ (because $0<\ell<n$)
- In the DR process, doubly excited levels involved ➔ scales $\propto n^4$
- For some ions, need to take into account levels up to n = O(10) to get accurate results

Resonant excitation

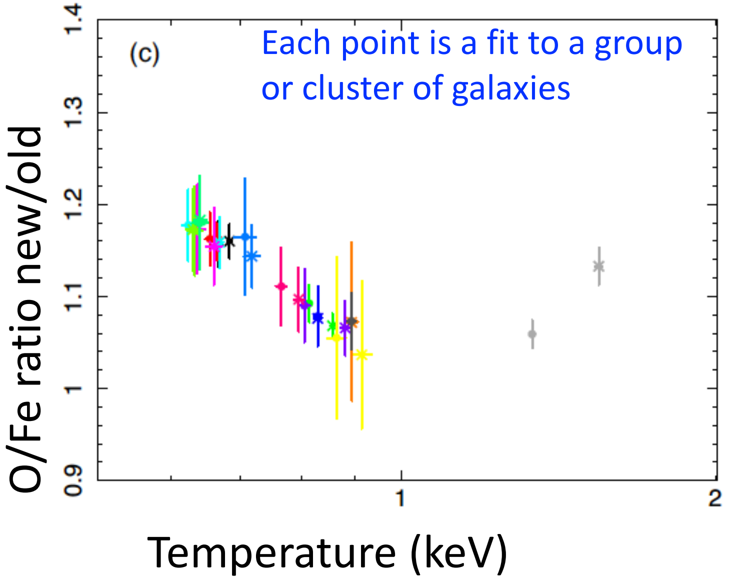
- *First steps equal to dielectronic recombination:*
  - Free electron caught while bound electron excited (with energy conservation, no radiation)
  - This is doubly excited state (2 electrons in excited level)
- *Now the difference with DR:*
  - Auto-ionization, i.e. no radiation but one electron ejected, and other electron to lower level but not to the ground level
  - Ion is left in excited state
- Less energy needed for the initial free electron to start the process
- ➔Excitation (albeit resonant) possible below the threshold energy
- See next talk by Štofanová for one application

Ongoing updates of SPEX:

resonant excitation processes

(Liyi Gu et al. 2019)

- Update Fe L-shell ion spectra
- Focus on Resonant Excitation & Dielectronic Recombination
- Use FAC code with
  - 30.000 energy levels
  - 500.000 radiative transitions
  - 40.000 Auger rates
- Months of computation time
- Important astrophysical implications



Each point is a fit to a group or cluster of galaxies

Final note on accuracies

- Few quantities calculated up to many digits (energies for H-like ions)
- Most quantities uncertain by several %, up to 10-20%
- Sometimes larger deviations (often human errors)
- Need to validate using independent models
- ➔APEC (Smith et al) & SPEX (Kaastra et al.):
  - Will not merge their codes
  - Are not competitors
  - Are friendly colleagues

Conservative

If it's not a power law, it can't be true

Modern times are coming

Conclusions

- Atomic data matter
- Getting accurate atomic data is not trivial
- However, they are needed to avoid biased astrophysical results
- Atomic data intimately linked to the models in which they are applied
- Try to understand the basics of the models to appreciate your astrophysical results