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SCRAM: not a line shape code, but not terrible

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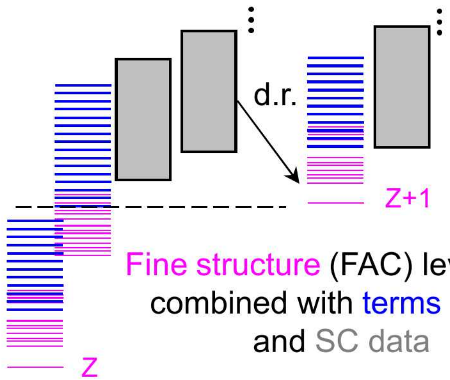
Introduction to SCRAM

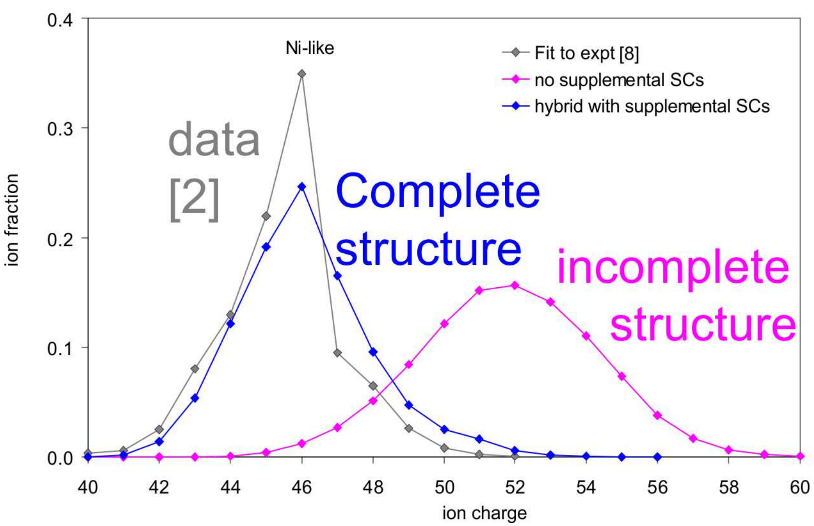
SCRAM is a hybrid-structure atomic kinetics code used primarily for spectroscopic diagnostics. Selected “coronal” states are treated with fine structure with full CI from FAC, some multiply excited states are treated with FAC UTAs, and completeness is ensured by addition of hydrogenic superconfigurations.The NIST database is used to improve accuracy for low-energy transitions.

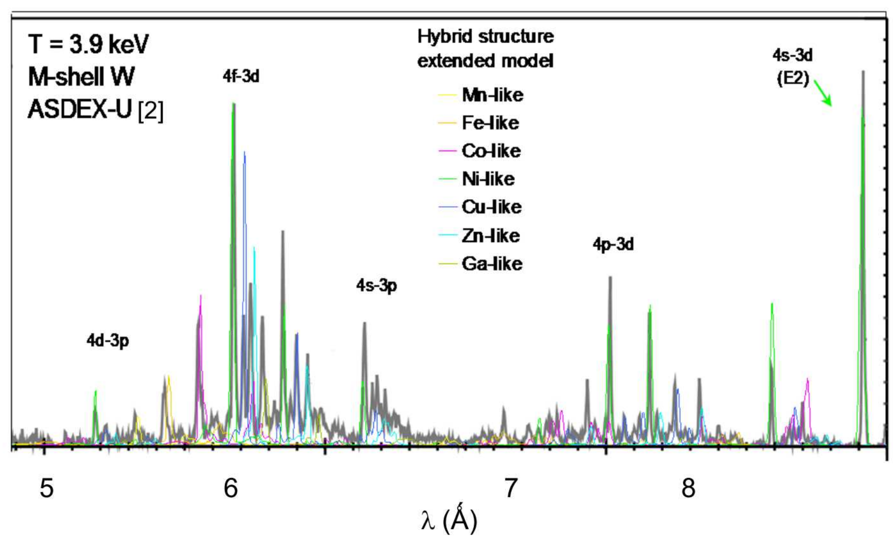
Hybrid level structure [1] ensures statistical completeness in high-*n* states, multiply excited states, and d.r. channels…



Fine structure (FAC) levels are combined with terms (UTA) and SC data

… while retaining spectroscopic accuracy in resonance lines, important satellite features, and emission from metastable states.





1. Hansen, Bauche, Bauche-Arnoult, and Gu, HEDP **3**, 109 (2007); Hansen Can. J. Phys **89**, 633 (2011)
2. Pütterich et al. Plasma Phys. Control. Fusion **50**, 085016 (2008)

Density broadening in SCRAM

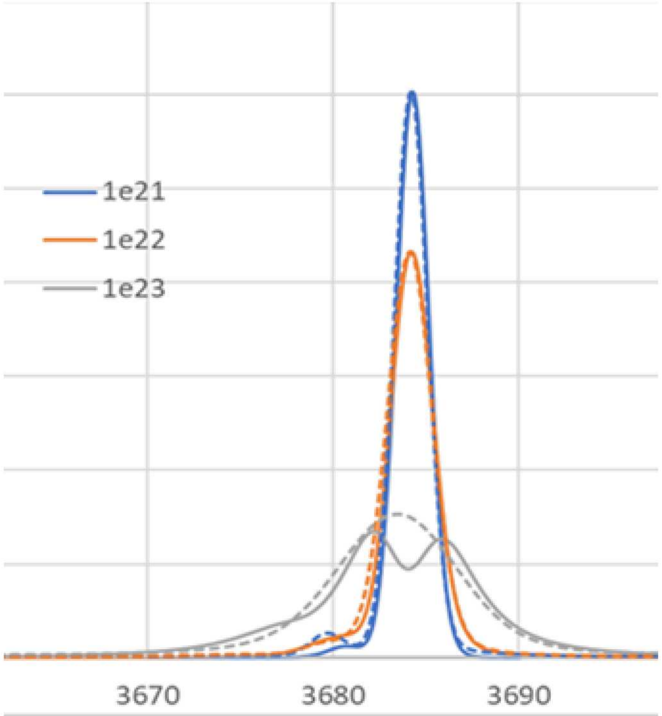
Collisional broadening: impact approximation using total collisional excitation and de-excitation rates out of participating levels. A combination of DW (FAC), Born, and analytical cross sections are used, including E1, E2, M1, M2, and integrated over electron energy distributions that can include suprathermal and degenerate electrons. These rates contribute to the Lorentzian component of Voigt line shapes.

Thanks to Evgeny for helping me find & fix a bug in rates among multiply excited states!

Stark broadening is included based on a very simple scaling adapted from Griem: *fwhm* [eV] ~ $4/Z\,(n_u^2 - n_d^2)\,(n_e/10^{22})^{0.58}$ This contributes to both the Gaussian and Lorentzian widths via the Holtzmark line profile. *May not be generally valid, but SCRAM routinely calculates spectra with millions of lines, so simple and general approximations are essential.*

Thermal, natural, and instrument broadening (if needed) are generally included

Continuum lowering & plasma polarization are introduced via *ad-hoc* models (ion sphere ΔE + Nguyen), with configurations gradually vanishing with valence orbitals; bound-free edges are broadened like the last surviving line



Ar Heβ @ T = 2 keV not terrible.
Thanks, Thomas!

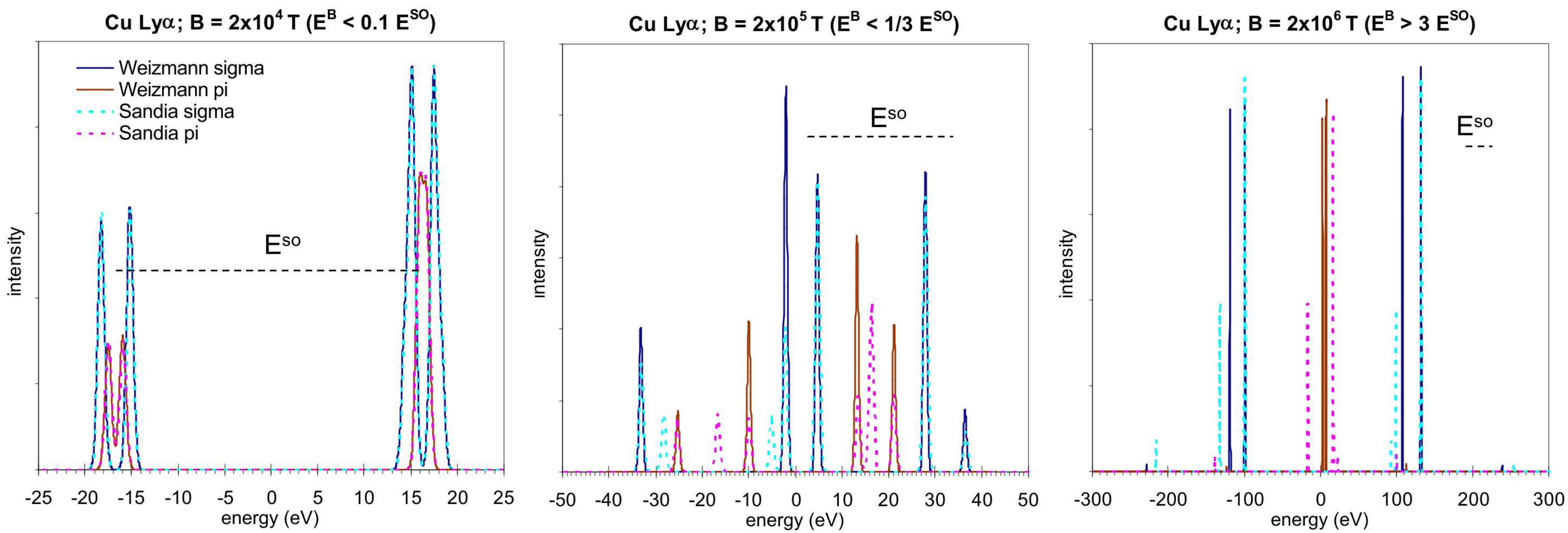
Zeeman splitting in SCRAM

For weak external magnetic fields: $\mu B << E^{so}$ (μ = 5.8e-5 eV/T)

- magnetic sublevels are shifted in energy by $\mu B g_J m$, with Lande factors g_J dependent on the LS fine structure terms; line intensities are proportional to squares of 3-j coefficients

The high-field limit is enforced through linear interpolation on $\chi = E^{SO}/(E^{SO}+\mu B)$

At intermediate field strengths, comparisons with *ab initio* Weizmann Institute calculations are used to correct perturbative weak-field energy shifts



Ar & Cu He- and H-like ions: not terrible (thanks again, Evgeny!)