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Multiconfiguration Opacities from an Average Atom Model

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Sandia National Laboratories

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Context:
emissivity and opacity spectra are critical for HEDP science

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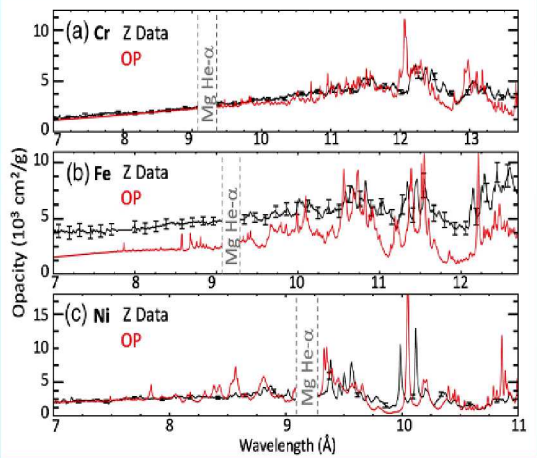
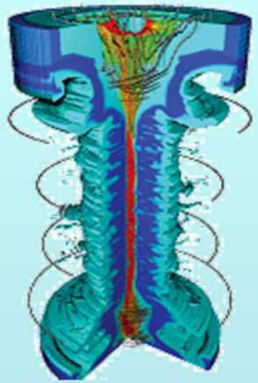
Models are constrained by experiments

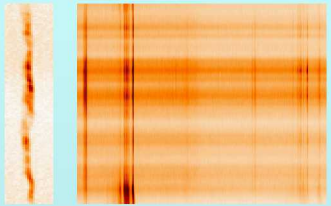


T. Nagayama *et al,*
PRL **122**, 235001 (2019);
Bailey *et al*, Nature (2015)

Models inform simulations and experimental design



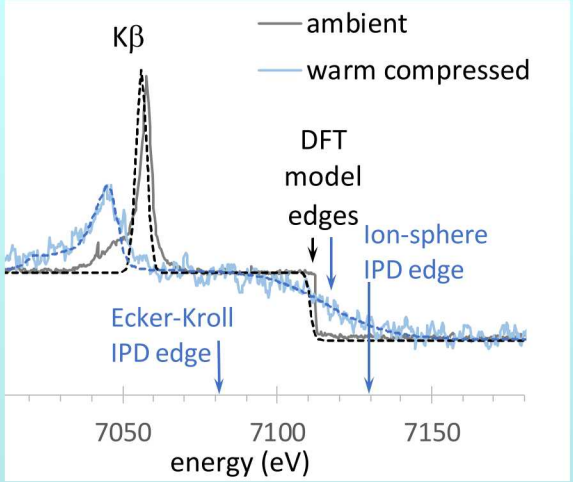
C. Jennings



E. Harding

e.g. MagLIF:
M. Gomez *et al,* PRL **113**, 155003 (2014)

Models help interpret experimental data



S. Hansen *et al,* HEDP **24**, 39 (2017)

Most spectroscopic codes include either detailed line structure or self-consistent density effects, but not both

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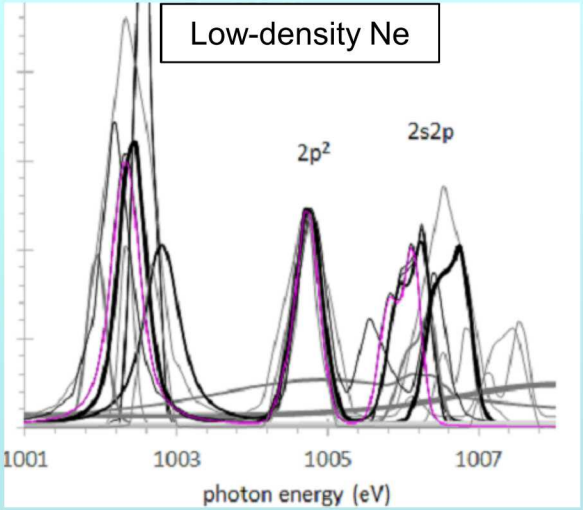
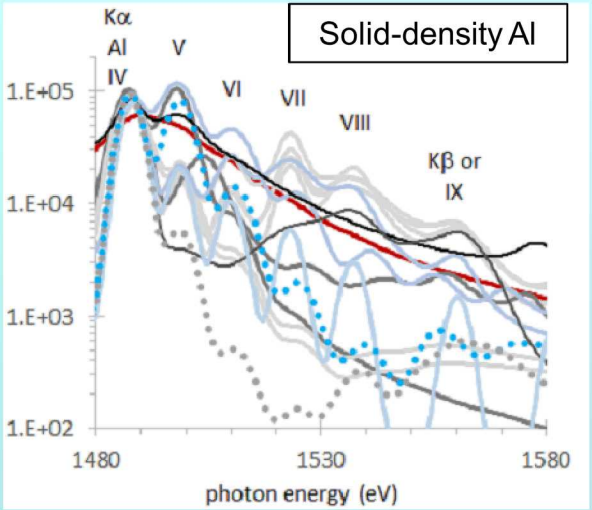
Detailed models enable precision diagnostics for plasmas at modest densities



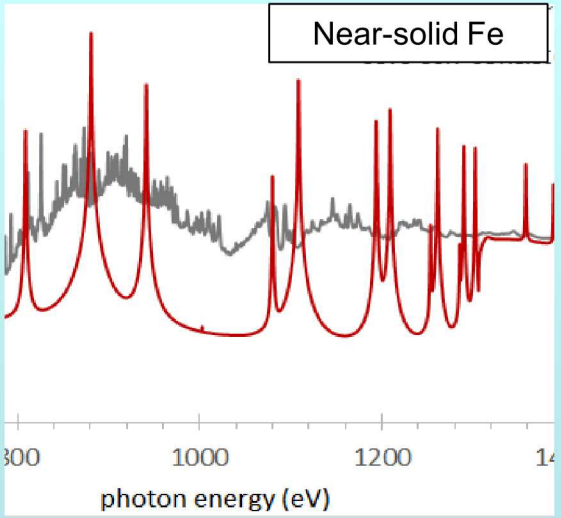
S. Hansen *et al,*
Review of the 10th NLTE code comparison workshop, HEDP (2019)

At high densities, *ad-hoc* corrections lead to incoherence



cf. O. Ciricosta *et al,*
PRL **109**, 065002 (2012)

Models that natively include density effects tend to lack detail



cf. P. Sterne *et al,* HEDP **19**, 1 (2007)

Can we combine established methods from isolated-atom physics to the self-consistent average-atom model?

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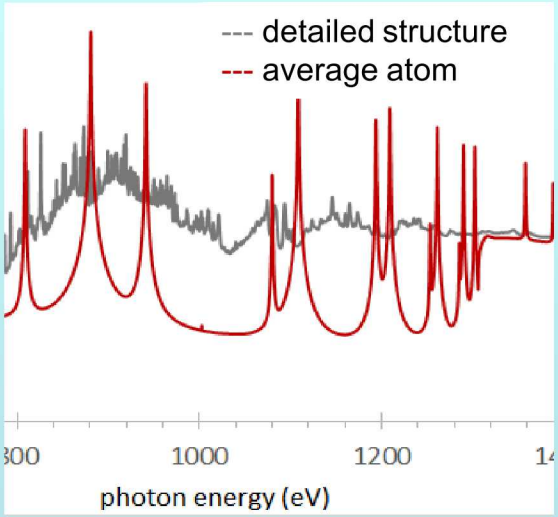
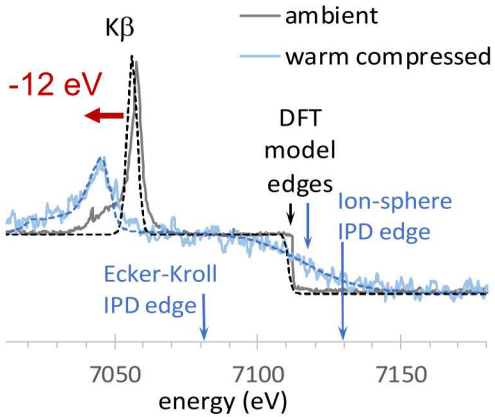
Average-atom models are terrible for spectroscopy, but they natively incorporate density effects & are inherently complete



Average-atom models fail because they lump all 1s, 2p, 3d… electrons into single-energy states
→ all transitions have the same (wrong!) ΔE

AA models capture net energy shifts due to density effects



Example: cold Fe fluorescence

	Kα 1s - 2p 6400 eV	Kβ 1s - 3p 7058 eV
AA	-115 eV	-135 eV
$4\rho_0$	-115 eV	-144 eV
ΔE	0 eV	-10 eV

S. Hansen *et al,* HEDP **24**, 39 (2017)

A multi-configuration (MC) model reduces overall error to ~50 eV (0.6%) from ~130 (1.5%)

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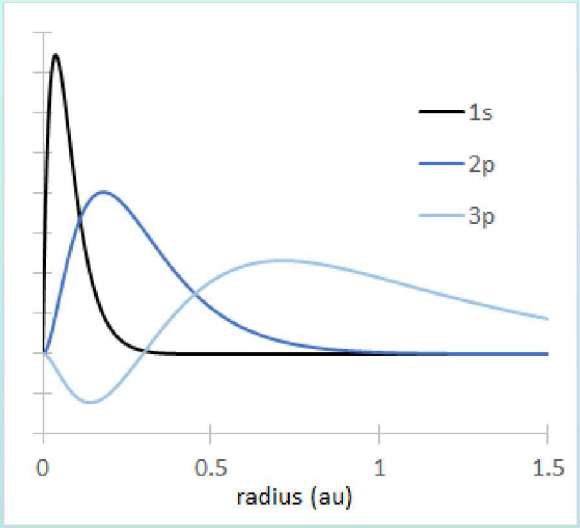
Average-atom models are terrible for spectroscopy, but they natively incorporate density effects & are inherently complete



Average-atom models fail because they lump all 1s, 2p, 3d… electrons into single-energy states
→ all transitions have the same (wrong!) ΔE

Get configuration-specific transition energies using Slater coefficients with average-atom wavefunctions

$$E_c = \sum_a \{N_a E_a^{kn} + \tfrac{1}{2} A_{aa} N_a (N_a - 1)\} + \sum_{b \neq a} \tfrac{1}{2} A_{ab} N_a N_b + E_r + E_e + E_p$$

$$Av(a,a) = F^0(a,a) - \frac{2\ell_a + 1}{4\ell_a + 1} \sum_{k>0} \begin{pmatrix} \ell_a & \ell_a & k \\ 0 & 0 & 0 \end{pmatrix}^2 F^k(a,a)$$

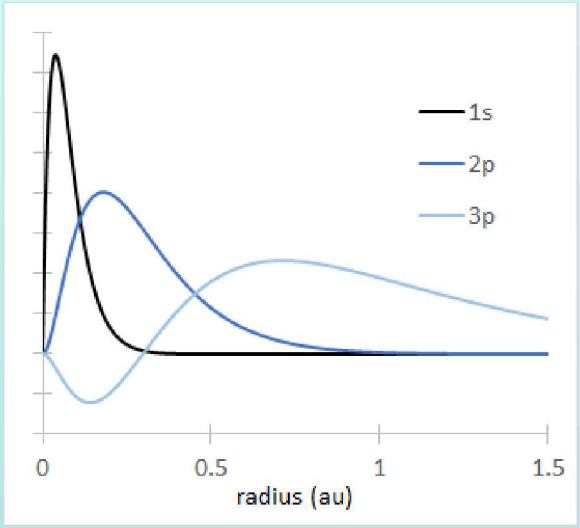
$$R^k(a,b,c,d) = \int_0^{+\infty} dr_1 \int_0^{+\infty} dr_2 P_a(r_1) P_b(r_2) P_c(r_1) P_d(r_2) \frac{r_<^k}{r_>^{k+1}}$$

Example: cold Fe fluorescence

	Kα 1s - 2p 6400 eV	Kβ 1s - 3p 7058 eV
AA	-115 eV	-135 eV
MC	+32 eV	+53 eV

An efficient Hartree-Fock (HF) extension gets much closer…

Average-atom models are terrible for spectroscopy, but they natively incorporate density effects & are inherently complete



The simple MC model does not account for changes in the wavefunctions when the configurations differ from the AA

Re-optimize AA wavefunctions under changes in occupations & Taylor-expand Slater coefficients

$$A_{aa}^{HF} = A_{aa} + \sum_b \Delta N_a \, \partial A_{aa}/\partial N_a$$

$$A_{ab}^{HF} = A_{ab} + \tfrac{1}{2} \sum_{ab} \Delta N_a \, \Delta Nb \, \partial^2 A_{ab}/\partial N_a \partial Nb$$

Example: cold Fe fluorescence

	Kα 1s - 2p 6400 eV	Kβ 1s - 3p 7058 eV
AA	-115 eV	-135 eV
MC	+32 eV	+53 eV
HF	-7 eV	-6 eV

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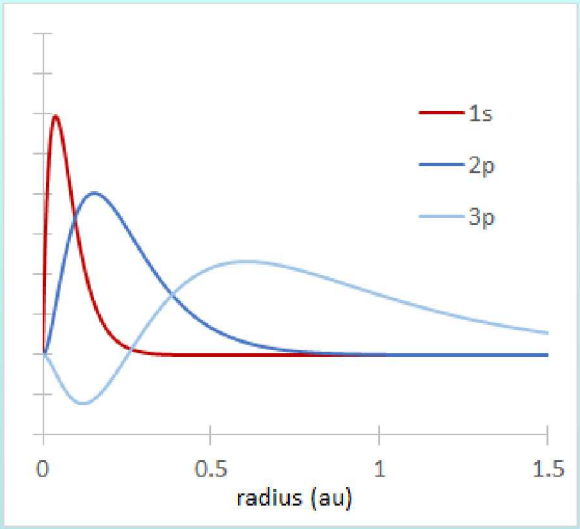

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Re-optimize AA wavefunctions under changes in occupations & Taylor-expand Slater coefficients

$$A_{aa}^{HF} = A_{aa} + \sum_b \Delta N_a \, \partial A_{aa}/\partial N_a$$

$$A_{ab}^{HF} = A_{ab} + \tfrac{1}{2} \sum_{ab} \Delta N_a \, \Delta Nb \, \partial^2 A_{ab}/\partial N_a \partial Nb$$

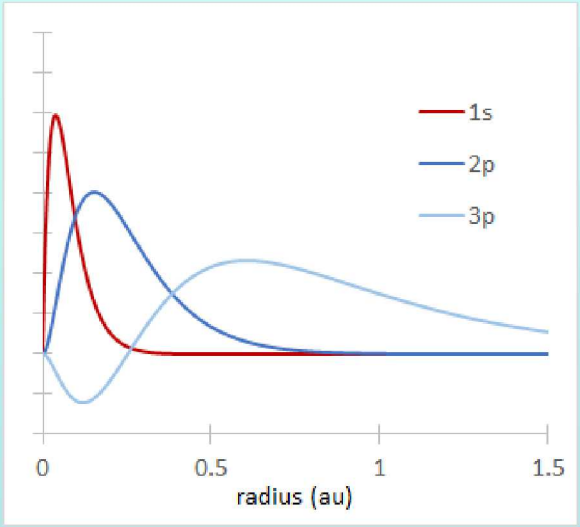
Taylor expansions have been done on binding energies, [Wilson, Liberman, and Springer JQSRT 54, 857 (1995)] but not (to our knowledge) on the Slater coefficients

Example: cold Fe fluorescence

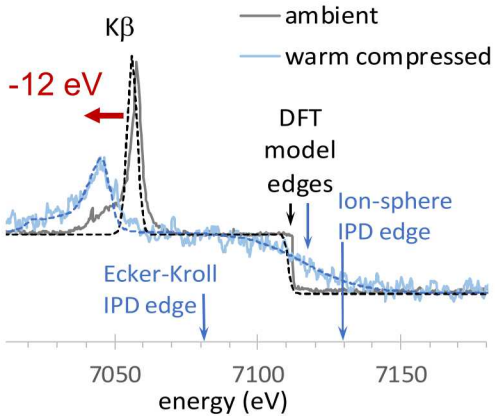
	Kα 1s - 2p 6400 eV	Kβ 1s - 3p 7058 eV
AA	-115 eV	-135 eV
MC	+32 eV	+53 eV
HF	-7 eV	-6 eV

… and extends native density effects to detailed models

Average-atom models are terrible for spectroscopy, but they natively incorporate density effects & are inherently complete



AA+MC+HF captures net energy shifts due to density effects



Example: cold Fe fluorescence

	Kα 1s - 2p 6400 eV	Kβ 1s - 3p 7058 eV
AA	-115 eV	-135 eV
MC	+32 eV	+53 eV
HF	-7 eV	-6 eV
$4\rho_0$	-9 eV	-24 eV
ΔE	-2 eV	-18 eV

We use the AA wavefunctions for radial integrals & spin-orbit splitting, increasing computational efficiency

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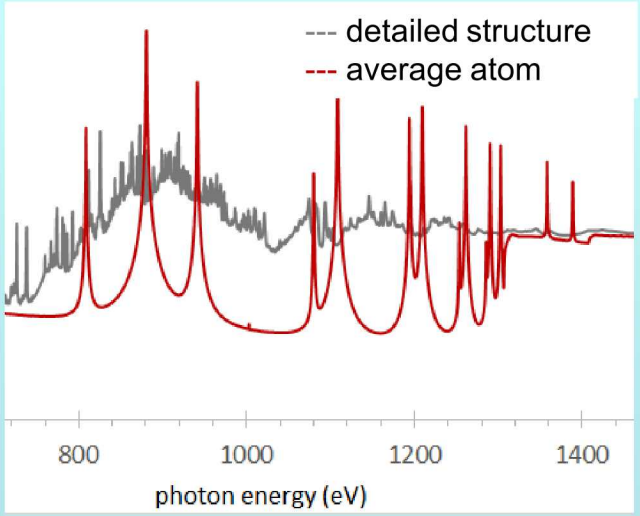
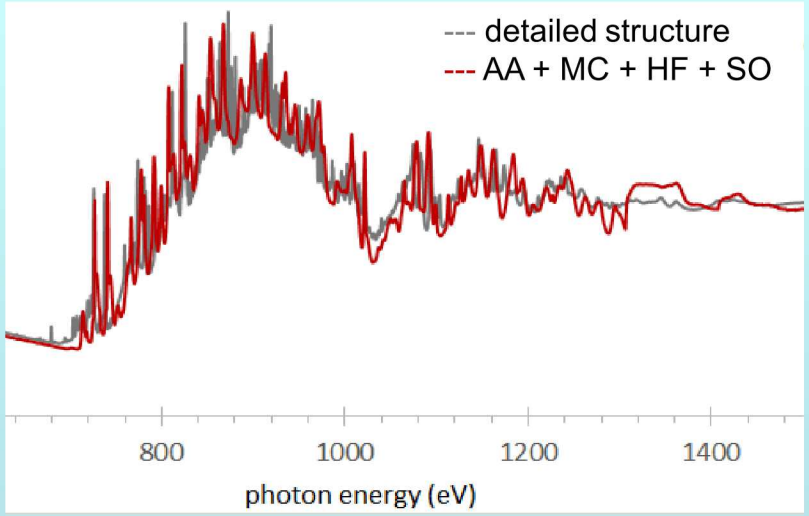
Average-atom models are terrible for spectroscopy, but they natively incorporate density effects & are inherently complete



Applying established isolated-atom physics to the wavefunctions of the average atom model gives accurate, complete, & self-consistent emission & opacity



This model is about as fast as detailed models based on pre-computed atomic data

Additional semi-relativistic effects are included through a Pauli potential and E_R in E_C (Cowan 1965)

Conclusion

- Applying established techniques from isolated-atom physics to the wavefunctions from a self-consistent average-atom wavefunctions gives a relatively detailed model that natively incorporates density effects

- This model does not resolve the discrepancies with Bailey *et al*'s Fe measurements