Atomic Calculations and Laboratory Measurements Relevant to X-ray Warm Absorbers

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X-ray spectral analysis, part 1

How did we get here?

1996: rates, codes and astrophysics
1999: atomic data needs for X-ray Astronomy
2005: XDAP
then: raymond-smith: 49.8 kbytes
now: atomdb: 135 Mbytes

Theoretical tools

Packages:
- Cowan/HFR
- Z expansion
- MCHF
- MCDF/GRASP
- Huliac
- fac
- Autotrace/superstructure
- Rmatrix

Features:
- Configuration interaction/superposition of configurations
- Non-orthogonal orbitals
- Semi-empirical corrections
- Fully relativistic or Breit-pauli approximation to relativistic hamiltonian
- Coupled to collisional-radiative code: very efficient calculation of radial part of matrix elements
- Distorted wave scattering
- Scattering: continuum wavefunctions calculated in close-coupling approximation

The algorithms are not new, but are enabled on a large scale by computing improvements

+ Databases: Chianti, atomdb, ornl, adas, topbase

Experimental tools

- Traps (ebit)
- Storage rings
- Synchrotron light sources
  • (+beams)
Dielectronic recombination challenges:
- DR is a resonant process, need accurate resonant energies
- Storage ring and ebit measurements:
  all L-shell ions of iron, M-shell under way (Savin et al.; Muller; Schippers ...)
  These are key for verifying theory, and for demonstrating the importance of accurate resonance structure

Calculations:
- Fac: total DR rates for H-Ne isosequences
- Autostructure: state-resolved rates for isosequences He-Na (?)-like ions for elements He-Zn. (Badnell, Zatsarinny, Altun et al...)
- Agreement with each other, and experiment, is ~20%

Collisional ionization
- Challenges:
  Rate from ground state is all that is needed for many purposes -- experiments can be used directly
  Lotz --> Arnaud and Rothenflug --> Arnaud and Raymond --> Mazzotta: fit to early measurements... discrepancies?
  Metastables can dominate
- Storage ring experiments (Muller et al.)
  Can eliminate metastables, due to 'cold' beam
  Reveal important effects: REDA, EA

Photoionization cross sections
Challenges
- Need for inner shells, excited states (→ RR)
- Importance of resonances
Experiment:
- Synchrotron/ion beams
- Calculations
  - Rmatrix (iron projectile)
  - Autostructure

Ionization balance
- Bryans et al. 2005
  - Put together Autostructure DR rates + collisional ionization rates for elements

Sample fit to HETG Capella spectrum; xstar ionization balance
Accurate wavelengths are key to line ids, and to anchoring semi-empirical structure calculations.

Theoretical calculations are not (generally) accurate enough to distinguish lines in rich X-ray spectra.

Lab measurements are key - Ebit has been a leader in this field.

X-ray spectral analysis

- Atomic constants
- Kinematics, geometry

"Astrophysics"

photoionized models

- Start with a single photoionized component
- Pure absorption
- Choose single turbulent width to fit majority of lines,
  \[ v_{\text{turb}} = 300 \text{ km/s} \]
- Use \( z = 0.007 \), compare with \( z_{\text{ngc3783}} = 0.00938 \)
  \[ \rightarrow v_{\text{outflow}} = 700 \text{ km/s} \]
- Best fit ionization parameter: \( \log \xi \approx 2 \).

Needs

- Auger
  - Following inner shell ionization, cascade of electrons
  - Correlated line emission?
- Charge exchange: 'non-traditional' X-ray sources: planets, solar system objects
- Trace elements
- Protons
  - Thermal: angular momentum changing collisions
  - Non-thermal: spectral signatures of cosmic rays.
- Dust/molecules/low ionization gas: inner shells
- Inner shells: inner shell lines, photoionization cross sections, collision strengths
- Collisional ionization: loose ends?
- Collisional processes away from equilibrium peak?
Fe XXI

Fe XXII

pure absorption photoionized models: multiple components

-2 Component Fit,
  - log$\xi$=-2. (as before)
  - log$\xi$= 0. (produces Fe M shell UTA)

Other parameters the same as single component:
  - z=0.007,
  - $v_{turb}$=300 km/s
What if we try a Continuous distribution of ionization parameter, $0.1 < \log\xi < 2.4$?

Complete ruled out

Comparison of photoionization models

<table>
<thead>
<tr>
<th>X-release (2.1kn)</th>
<th>X sets (2.1kn)</th>
<th>warmabs</th>
<th>Warmlabs 2.1n2</th>
<th>Other phase</th>
<th>Other titanium</th>
<th>photoion</th>
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<tbody>
<tr>
<td>Xspec interface</td>
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<td>Atomic data</td>
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<td>KB01, K04, chianti</td>
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<td>n</td>
<td>n</td>
<td>(y)</td>
<td>?</td>
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</table>

Now try absorption + thermal emission photoionized models

Add component due to 'thermal' photoionization (i.e. Recombination+collisional excitation processes): 'photemis'

Component has redshift $z = 0.009$, i.e. redshift of object

'Photoionization Models'

*Full global model
(i.e. photoionization --> synthetic spectrum --> xspec --> fit)
*Xstar version 2.1kn2
- Inner M shell 2-3 UTAs (FAC; Gu); >400 lines explicitly calculated
- Chianti v. 5 data for iron L
- Iron K shell data from R-matrix calculations (Bautista, Palmeri, Mendoza et al)
- Available from xstar website, as are ready-made tables
*Not in current release version, 2.1kn7
*Other models have similar ingredients
*Xspec 'analytic model' warmabs
- Not fully self consistent: assumes uniform ionization absorber, but this is small error for low columns.

X-ray spectral analysis

Atomic constants

Kinematics, geometry

“Astrophysics”
Now try photoionized scattering models

- Photemis model does not account for scattered emission
- To test this, we apply method from theory of hot star winds, (SEI) method (Lamers et al. 1992) assumes ordered, radial supersonic flow
- Apply SEI profile to all spectrum lines, with depth parameter proportional to depth calculated by warmabs.
- Free parameter is ratio of scattered emission to absorption, C.

Wind models

Now try multicomponent models

- UV spectra show some X-ray warm absorber lines correspond to multiple narrow components in the UV
- Multabs is an attempt to test whether multiple discrete components can mimic a single feature.
- Several identical warmabs components, each with thermal width are spread evenly across an energy interval determined by $v_{\text{turb}}$.
- The number is determined by a 'covering fraction', C=1 corresponds to a black trough, C=0 corresponds to one thermal component.

This affects the Curve of growth, e.g. For O VIII Ly$\alpha$, $v_{\text{ion}}=300$, $v_{\text{rel}}=60$, C=1, $a=0.01$
A summary of $\chi^2/8192$

<table>
<thead>
<tr>
<th>Gaussian notch</th>
<th>11945</th>
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<tr>
<td>Single component absorption</td>
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<td>2 component absorption</td>
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<td>+photemis</td>
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<tr>
<td>multabs</td>
<td>18974</td>
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</table>

The pure absorption 2 component model looks best...

dynamical models: torus winds

- Following suggestions by Balsara and Krolik (1984), Krolik and Kriss (1996)
- Assume a torus at 0.1 pc about a $10^6 M_{\odot}$ black hole
- Initial structure is constant angular momentum adiabatic (cf. Papaloizou and Pringle 1984)
- This structure is stable (numerically) for >20 rotation periods
- Choose $T<10^4 K$, $n\approx10^8 \text{ cm}^{-3}$ for unperturbed torus
- Calculate dynamics in 2.5d (2d + axisymmetry) using zeus-2d

X-ray spectral analysis: a different procedure

- Add illumination by point source of X-rays at the center
- Include physics of X-ray heating, radiative cooling --> evaporative flow (cf. Blondin 1994)
- Also radiative driving due to UV lines (cf. Castor et al. 1976; Stevens & K. 1986)
- Formulation similar to Proga et al. 2000, Proga & K. 2002, 2004

Velocity and density fields
results

- Find strong evaporative flow, $\dot{M} \sim 10^{-5} \, M_\odot/yr$
- Initial flow is inward from illuminated face
- Later flow is isotropically outward as torus shape changes
- $T_{\text{comp}} \sim 10 \, T_{\text{esc}}, \quad t_{\text{heat}} \ll t_{\text{rot}}$
- Find gas at intermediate ionization parameters
- Match to data? Region of warm flow is narrow

Extra slides

Comparison with previous work

<table>
<thead>
<tr>
<th></th>
<th>Netzer</th>
<th>Krongold</th>
<th>Blustin</th>
<th>Me</th>
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<tbody>
<tr>
<td>$\log(U)$</td>
<td>-0.6</td>
<td>0.76</td>
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<td>0.45</td>
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<tr>
<td>$\log(\tilde{\beta}_1)$</td>
<td>3.7, 3.1</td>
<td>2.25</td>
<td>2.4</td>
<td>2.2</td>
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<tr>
<td>$\log(N_1)$</td>
<td>22.2</td>
<td>22.2</td>
<td>22.45</td>
<td>21.4</td>
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<tr>
<td>$\log(U)$</td>
<td>-2.4</td>
<td>-0.78</td>
<td></td>
<td>-1.55</td>
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<tr>
<td>$\log(\tilde{\beta}_2)$</td>
<td>0.69</td>
<td>0.72</td>
<td>0.3</td>
<td>0.2</td>
</tr>
<tr>
<td>$\log(N_2)$</td>
<td>21.9</td>
<td>21.6</td>
<td>20.73</td>
<td>20.4</td>
</tr>
</tbody>
</table>
Krongold et al. 2004

>100 absorption features
- blueshifted, \( v \approx 800 \) km/s
- broadened, \( \nu \text{turb} \approx 300 \) km/s
- emission in some components
- fit to 2 photoionization model components
- Fe M shell UTA fitted using Gaussian approximation
- Full global model

Chelouche and Netzer 2005

Combined model for dynamics and spectrum
Assumes ballistic trajectories
Favors clumped wind

Blustin et al. (2004)

- Fitted the XMM RGS spectrum using global model
- Also find evidence for two components
- Omit Ca
- Include line-by-line treatment of M shell UTA, but still miss some
- Claim evidence for higher ionization parameter material
- Require large overabundance of iron

- Work so far on fitting warm absorber spectra has concentrated on the assumption of a small number of discrete components
- This places important constraints on the flow dynamics, if it is true
- There is no obvious a priori reason why outflows should favor a small number or range of physical conditions
- In this talk I will test models in which the ionization distribution is continuous rather than discrete, and discuss something about what it means
- Previous tests of this have invoked simplified models for the Fe M shell UTA which may affect the result
As a start, fit to a continuum plus Gaussian absorption lines. Choose a continuum consisting of a power law +0.1 keV blackbody + cold absorption. Absorption lines are placed randomly and strength and width adjusted to improve the fit.
Results of notch model:

- requires ~950 lines
- Ids for ~100
- 300 km/s<v<2000
- Allows line Ids
- Shows distribution of line widths, offsets

Ionization parameter of maximum ion abundance vs. line wavelength for identified lines

--> statistics of the line widths implies bound on velocity, vc<1000 km/s; small number of components of photoionized gas