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

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+
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X-ray spectral analysis, part 1

 Atomic constants

 Kinematics, geometry

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

<table>
<thead>
<tr>
<th>Packages</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cowan/HFR</td>
<td>Configuration interaction/superposition of configurations</td>
</tr>
<tr>
<td>Z expansion</td>
<td>Non-orthogonal orbitals</td>
</tr>
<tr>
<td>MCHF</td>
<td>Semi-empirical corrections</td>
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<tr>
<td>MCDF/GRASP</td>
<td>Fully relativistic or Fermi approximation to relativistic hamiltonian</td>
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<tr>
<td>Hullac</td>
<td>Coupled to collisional-radiative code, very efficient calculation of radial part of matrix elements</td>
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<tr>
<td>fac</td>
<td>Distorted wave scattering</td>
</tr>
<tr>
<td>Autostructure/superstructure</td>
<td>Scattering, continuum wavefunctions calculated in close-coupling approximation</td>
</tr>
<tr>
<td>Rmatrix</td>
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</tbody>
</table>

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%

**Sample fit to HETG Capella spectrum; DR perturbed by 30%**

**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

**Sample fit to HETG Capella spectrum; xstar ionization balance**

**Photoionization cross sections**

- **Challenges**
  - Need for inner shells, excited states (↔ RR)
  - Importance of resonances

- **Experiment:**
  - Synchrotron/ion beams
calculations
  - Rmatrix (iron project)
  - autostructure

**Ionization balance**

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

Calculated vs. measured line wavelengths

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 \( z_{\text{ngc3783}} = 0.00938 \)
  \( \rightarrow v_{\text{out/ew}} = 700 \text{ km/s} \)
- Best fit ionization parameter: \( \log \xi = -2 \).

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?
Missing lines near 16-17A: Fe M shell UTA

pure absorption photoionized models: multiple $\xi$ 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
O VIII Lα emission component
What if we try a Continuous distribution of ionization parameter, 0.1<log\(\xi<2.4\)?

\[ \text{Complete ruled out} \]

Comparison of photoionization models

<table>
<thead>
<tr>
<th>X\text{release} (2.1kn)</th>
<th>X\text{sets} (2.1kn)</th>
<th>warming</th>
<th>Warming 2.1kn</th>
<th>Other phase</th>
<th>Other titan</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>?</td>
<td>y</td>
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<td>Self consistent SED</td>
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<td>'dynamics'</td>
<td>n</td>
<td>n</td>
<td>n</td>
<td>(y)</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

"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

- Add component due to 'thermal' photoionization (i.e. Recombination-collisional excitation processes): 'photemis'
- Component has redshift z=0.009, i.e. redshift of object
Now try photoionized scattering models
- Phoebus 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
- 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 \( \nu_{turb} \)
- The number is determined by a 'covering fraction', \( C=1 \) corresponds to a black trough, \( C=0 \) corresponds to one thermal component

Now try multicomponent models
- This affects the Curve of growth; eg For O VIII Lx, \( \nu_{\text{obs}}=300, \nu_{\text{rest}}=60, C=1, a=0.01 \)
A summary of $\chi^2/8192$

<table>
<thead>
<tr>
<th>Component Absorption</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian notch</td>
<td>11945</td>
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<tr>
<td>Single component absorption</td>
<td>16093</td>
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<tr>
<td>2 component absorption</td>
<td>15186</td>
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<tr>
<td>+photemis</td>
<td>15161</td>
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<tr>
<td>Wind, C=1</td>
<td>21626</td>
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<tr>
<td>multabs</td>
<td>18974</td>
</tr>
</tbody>
</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 $T<10^4 K$, $n\sim 10^8$ cm$^{-3}$ for unperturbed torus
- Calculate dynamics in 2.5d (2d + axisymmetry) using zeus-2d

dynamical models: torus winds

- 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
Temperature and ionization parameter

Sample spectra look -like warm absorbers

results

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

Extra slides

<table>
<thead>
<tr>
<th></th>
<th>Netzer</th>
<th>Krongold</th>
<th>Blustin</th>
<th>Me</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log(U)</td>
<td>-0.6.</td>
<td>0.76</td>
<td></td>
<td>0.45</td>
</tr>
<tr>
<td>Log((\xi_1))</td>
<td>3.7, 3.1</td>
<td>2.25</td>
<td>2.4</td>
<td>2.2</td>
</tr>
<tr>
<td>Log(N_1)</td>
<td>22.2</td>
<td>22.2</td>
<td>22.45</td>
<td>21.4</td>
</tr>
<tr>
<td>Log(U)</td>
<td>-2.4</td>
<td>-0.78</td>
<td>-1.55</td>
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<tr>
<td>Log((\xi_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>
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</table>
Krongold et al. (2004)

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

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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
Examples of (2)
- How well do we do? Warm absorber example
  - What's wrong?
    - Atomic data incompleteness
    - Atomic data errors
    - Incorrect physical assumptions
- Some areas of recent progress
  - Combined emission/absorption models
  - Thermal emission
  - Scattered emission
- Things to watch out for
  - Finite resolution
  - Granularity
  - Emission/absorption tradeoffs
- Some areas of recent progress

Comparison of model properties

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1) simple models: gaussian notches
- 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/c < 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. v < 1000 km/s: small number of components of photoionized gas