Atomic Processes for Astrophysical Plasmas (Methodology)

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Goal: R-matrix effective collision strengths for isoelectronic sequences (elements up to Zn)

Completed:

- F-like (Witthoeft et al, 2007)
- Na-like, inner & outer shell (Liang et al, 2009)
- Ne-like (Liang et al, 2010)
- Li-like, inner & outer shell (Liang et al, 2010)

See poster by Guiyun Liang for further details of recent work.

Atomic Structure Methods/Codes

- Hartree/Dirac-Fock: coupled-set of radial equations result from formally varying radial orbitals to give stationary value of an energy functional — self-consistent solution: MCHF (Froese), HFR (Cowan), MCDF (Grant) etc. (Expansion coefficients may also be determined this way, MCHF.)
- Configuration Interaction (CI): radial equations (usually uncoupled) contain variational parameters (e.g. "model potentials") which are varied (numerically) to minimize a computed energy functional: AS/SS, CIV3, HULLAC
- As CI but using a self-consistent model potential: AS, HULLAC, FAC.

All approaches then, usually, construct and diagonalize the Hamiltonian to give the final e-states and e-energies.

Basis expansion is slow to converge in general. A plethora of basis functions are used: spectroscopic, psuedo (Laguerre), B-splines etc.

Pros & Cons: problems with converging HF for excited states. Local vs global minimum, flexible enough variational parameters.

Scattering codes can use only the simplest HF methods, in general: unique, orthogonal...

Hamiltonian

♣ Schrödinger equation based (AS, CIV3, MCHF):

- Non-relativistic: kinetic, nuclear & electrostatic operators.
- Breit-Pauli: as above, plus one-body fine-structure (spin-orbit), and non-fine-structure (Mass-Velocity & Darwin).
  Fine structure mixes terms, non-fine-structure can be added to NR above.
- Breit-Pauli: as above, plus two-body fine-structure (spin-spin, spin-orbit, spin-other-orbit).
- Breit-Pauli: as above, plus two-body non-fine-structure (orbit-orbit, contact-spin-spin, Darwin).

♣ Kappa-averaged Dirac equation based ($\pm$ small component): radial functions still depend only on nl, not nlj. Then using above Breit-Pauli operators. (HFR one-body only, AS.)

♣ Dirac equation based, large and small component.

- Dirac-Coulomb (HULLAC, FAC)
- $+$ (Generalized) Breit $+$QED (GRASP, Sampson/LANL)

Others: Sapirstein & Johnson, Desclaux, Chen...

Coupling schemes: LS, LSJ, jK, jj (unitary transformations).

What matters more are good quantum numbers...

Atomic Structure Data

Bound-Bound

- Energy levels, ("All")
- E_k and M_k radiative rates ("Most")

Bound-Free

- Autoionization rates, DR (AS, HULLAC, FAC, MCDF(Chen) ...)
- Photoionization cross sections, RR (ditto)

Free-Free

- Infinite and finite energy Plane-wave Born (AS, Cowan)

And More...

- Hyperfine
- Stark-mixing, DR
- ...

Atomic Collision Methods

Time-dependent methods solve the full Schrödinger equation — TDCC.

Time-independent methods expand the antisymmetric total wavefunction for the target-plus-colliding particle Ψ in terms of a known complete basis of target states ψ_ν.

$$\Psi = \mathcal{A} \sum\!\!\!\!\!\!\int_\nu \psi_\nu \phi \, . \tag{1}$$

The expansion coefficients ϕ representing the colliding particle (projectile) are then to be freely determined by a variational of the scattering matrix leading to the continuum Hartree/Dirac-Fock equations.

Coupled-channel methods

Resonances arise naturally when the scattering energy of an open-channel coincides with that of a closed-channel.

Traditional close-coupling approximation truncates the expansion to a low-lying set of closely-coupled atomic states — neglects ionization loss.

Pseudo-state expansions attempt to approximate the sum/integral over a wide range of energies and work towards practical numerical convergence — RMPS, CCC.

Complete basis expansions can be used over a limited energy range and volume (particle in a box) — B-spline R-matrix, Intermediate Energy R-matrix.

R-matrix

Probably the most successful method/code suite for electron-impact excitation and photoionization (no so much for electron-ionization).

A close-coupling method which is very efficient at mapping-out resonances, compared to CCC, UCL-IMPACT (historic) etc. (But not compared to IPIRDW...)

Need to solve the coupled integro-differential scattering equations at tens, if not hundreds, of thousands of energies and for ~ 100 angular momentum symmetries.

Complex atoms require massively parallel calculations.

Distorted-wave methods

DW methods solve (elastic) uncoupled continuum Schrödinger/Dirac equations and treat the (inelastic) coupling as a perturbation — can keep problem small, a series of 2x2 calculations: AS/HULLAC/FAC/LANL & UCL(historic - sorry, Helen)

Resonances are often neglected from electron-impact excitation, but not recombination — DR. Use of the IPIRDW approximation (Independent Processes Isolated Resonance using DW): AS/HULLAC/FAC

Simple "DW": Coulomb or plane-wave Born for EIE & EII: ATOM or AS/Cowan

Astrophysics: highly-excited states

Heavy species: we need to go beyond PWB.

AS BPDW

AS has been "extended" to calculate both LS-coupling and Breit-Pauli distorted wave collision strengths, optionally including both two-body non-fine- and fine- structure.

History & Philosophy...

Features:

- No bound (N+1) configurations - continuum-bound exchange overlaps instead
- Slater state algebra (not Racah)
- Continuum interpolation basis
- Determines $< |H - E| >$ as in BP R-matrix
- "STGF" top-up
- Metastables vs Excited states
- Delivers a type-5 (omega) *adf04* file, which can be converted to type-3 (upsilon) using `adf04_om2ups.f`

Easy to Use

Input Namelisted and free-formatted.

```
A.S. Be-like Fe DW (BP)
 &SALGEB RUN='DE' CUP='IC' NMETAJ=2
         MXVORB=2 MXCONF=3 KCOR1=1 KCOR2=1 &END
2 0 2 1
 2   0
 1   1
 0   2
 &SMINIM NZION=26 &END
 &SRADCON &END
```

Web Links

http://amdpp.phys.strath.ac.uk/

http://amdpp.phys.strath.ac.uk/tamoc/

http://amdpp.phys.strath.ac.uk/autos/

http://amdpp.phys.strath.ac.uk/UK_APAP/codes.html