Analysis of Fe XVI Spectra : Atomic Structure calculation using Relativistic Coupled Cluster Theory

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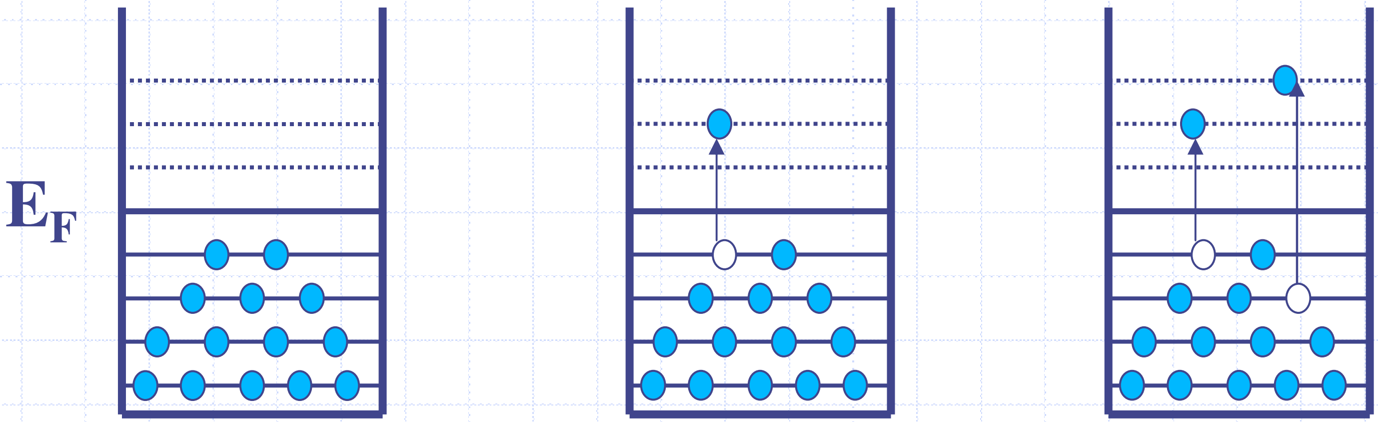
What to start with ?

- Mean field wavefunctions – *Basis sets* ; Solution of the Hartree-Fock eqn using FBSE of Gaussian Orbitals

- This will give the *reference state* $|\Phi\rangle$

- Coupled-cluster method (CCM) is equivalent to all order many-body perturbation theory (MBPT)

Coupled Cluster Methods (CCM)



$|\Phi\rangle$ $\quad\quad$ $\sigma_1|\Phi\rangle$ $\quad\quad$ $\frac{1}{2!}\sigma_1^2|\Phi\rangle$ *or* $\sigma_2|\Phi\rangle$

$$|\Psi\rangle = |\Phi\rangle + \sigma_1|\Phi\rangle + \sigma_2|\Phi\rangle + \frac{1}{2!}\sigma_1^2|\Phi\rangle + \cdots = e^{\sigma}|\Phi\rangle$$

Correlation Operator

- Divide the Hilbert space into two parts
- Correlation operator σ thus has two parts: once for the closed shell and the other for the open shell
- Use single and double excitation approximation : $T=T_1+T_2$ and $S=S_1+S_2$

Equation of motion : CC Theory

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

Coupled Cluster (CC) theory

$$\left|\Psi\right\rangle = e^{T}(1+S)\left|\Phi\right\rangle$$

In CC the EOM takes the matrix form

$$A(T)\times T = B$$
$$A'(S)\times S = B'$$

Explicit form

$$\begin{Bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \cdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{Bmatrix} \times \begin{Bmatrix} t_1 \\ t_1 \\ \vdots \\ t_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_1 \\ \vdots \\ b_n \end{Bmatrix}$$

The Coupled-cluster equations

- Amplitude determining equation
- Correlation energy determine equation

- Use the technique of ***Effective Hamiltonian***
- Use **normal ordered second quantized** form of the atomic Hamiltonian

The Iron family : FeXVI

- We start with FeXVII (*Ne* – like)
- Get the reference state
- Determine the correlation (energy and excitation → *cluster amplitudes*)
- Add electron attachment technique for specific states
- Ground and low-lying excited states
- Calculate transitions properties

Transition properties

$$\hat{O}_{fi} = \frac{\langle \Psi_f | \hat{O} | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}}$$

$$= \frac{\langle \Phi | (1 + S_f^+) e^{T^+} \hat{O} e^T (1 + S_i^+) | \Psi_i \rangle}{N_f N_i}$$

Normalization factors

$$N_{f/i} = \sqrt{\langle \Phi | (1 + S_{f/i}^+) e^{T^+} e^T (1 + S_{f/i}^+) | \Phi \rangle}$$

The form of the operator O varies for different transitions. For example O corresponds to electric (magnetic) dipole – E1(M1) or electric (magnetic) quadrupole – E2(M2) transitions and so on..

Excitation energies for *FeXVI*

States	CCM	Observation
3p $^2P_{1/2}$	277 447 (2.5283)	277 160 (2.5260)
3p $^2P_{3/2}$	299 232 (2.7268)	298 140 (2.7169)
3d $^2D_{3/2}$	677 241 (6.1715)	675 480 (6.1554)
3d $^2D_{5/2}$	680 631 (6.2023)	678 410 (6.1820)
4s $2S_{1/2}$	186 8945 (17.0310)	186 7530 (17.0182)
4p $2P_{1/2}$	197 9055 (18.0344)	197 8040 (18.0252)
4p $2P_{3/2}$	198 7499 (18.1114)	198 6100 (18.0980)
4d $2D_{3/2}$	212 6470 (19.3778)	212 4070 (19.3570)
4d $2D_{5/2}$	212 8261 (19.3942)	212 5370 (19.3677)

Excitation energies are given are in cm^{-1}. The values in parenthesis are in *Ryd*. Observed values are complied from NIST database.

Electric dipole (E1) transition

Transition Prob. (A in s^{-1}) in length gauge

Transition	CCM	Others [1]
3p $^2P_{1/2}$ – 3s $^2S_{1/2}$	0.6150(10)	0.6463(10)
3p $^2P_{3/2}$ - 3s $^2S_{1/2}$	0.7777(10)	0.8087(10)
3d $^2D_{3/2}$ – 3p $^2P_{1/2}$	0.1512(11)	0.1560(11)
3d $^2D_{3/2}$ – 3p $^2P_{3/2}$	0.2560(10)	0.2659(10)
3d $^2D_{5/2}$ – 3p $^2P_{3/2}$	0.1583(11)	0.1635(10)
4s $^2S_{1/2}$ – 3p $^2P_{1/2}$	0.1095(12)	0.1052(12)
4s $^2S_{1/2}$ – 3p $^2P_{3/2}$	0.2260(12)	0.2173(11)
4p $^2P_{1/2}$ – 3s $^2S_{1/2}$	0.2069(12)	0.1969(12)
4p $^2P_{1/2}$ – 3d $^2D_{3/2}$	0.8036(11)	0.7366(11)

[1] Aggarwal and Keenan, *Astron Astrophys,* **450**, 1249 (2006). – GRASP+DARC

Numbers (**) in parenthesis implies 10^{**}

Electric quadrupole (E2) transition

Transition Prob. (A in s^{-1}) in length gauge

Transition	CCM	Others [1]
3d $^2D_{3/2}$ – 3s $^2S_{1/2}$	0.6600(6)	0.6658(6)
4d $^2D_{3/2}$ - 3s $^2S_{1/2}$	0.1371(9)	0.1360(9)
4d $^2D_{5/2}$ – 3s $^2S_{1/2}$	0.1369(9)	0.1358(9)
3p $^2P_{3/2}$ – 3p $^2P_{1/2}$	0.2828(-1)	0.2301(-1)
4p $^2D_{3/2}$ – 3p $^2P_{1/2}$	0.3473(8)	0.3439(8)

[1] Aggarwal and Keenan, *Astron Astrophys,* **450**, 1249 (2006). – GRASP+DARC

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Conclusion

- First comparative studies of *FeXVI* results using CCM and other methods
- Other transitions – magnetic dipole / quadrupole transitions.
- Calculations are performed using length and velocity guage (*These results are not listed here*)
- Most accurate theoretical many-body calculations to our knowledge
- All the results will be compiled shortly

Collaborations

- Prof. Bhanu Pratap Das, *IIA, Bangalore, India*
- Dr. Rajat Chaudhuri, *IIA, Bangalore, India*
- Prof. Debasish Mukherjee, *IACS, Kolkata, India*