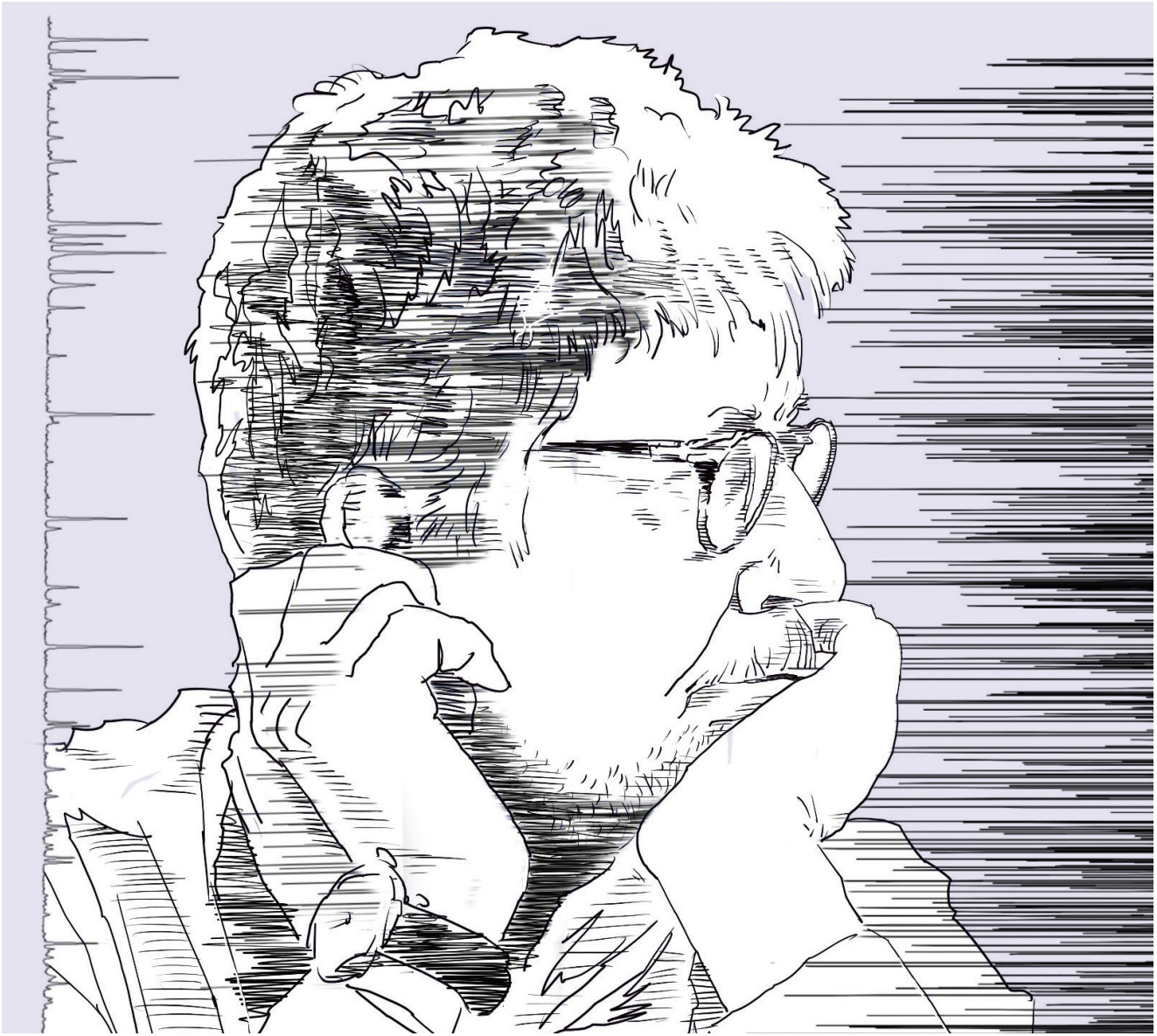
In Honour of Michel R. Godefroid on his retirement



In the 1960's

I define the beginning to be the 1960's

- Most Universities had computers
- Scientist were learning how to use them to solve problems in quantum theory
- Computers had small memory and slow disks
- Nearly all atomic studies were variations of the Hartree-Fock method
- Close collaboration between Quantum Chemists and Theoretical Physicists.

Summer of 1965 – 1s1s' (non-orthogonal approximation for $1s^2$ or $1s2s\ ^1S$
Alan Hibbert – Z-dependence of $1s2s\ ^1S$ and the saddle-point character of HF energy.

In the 1960's continued

At ULB in the mid-sixties

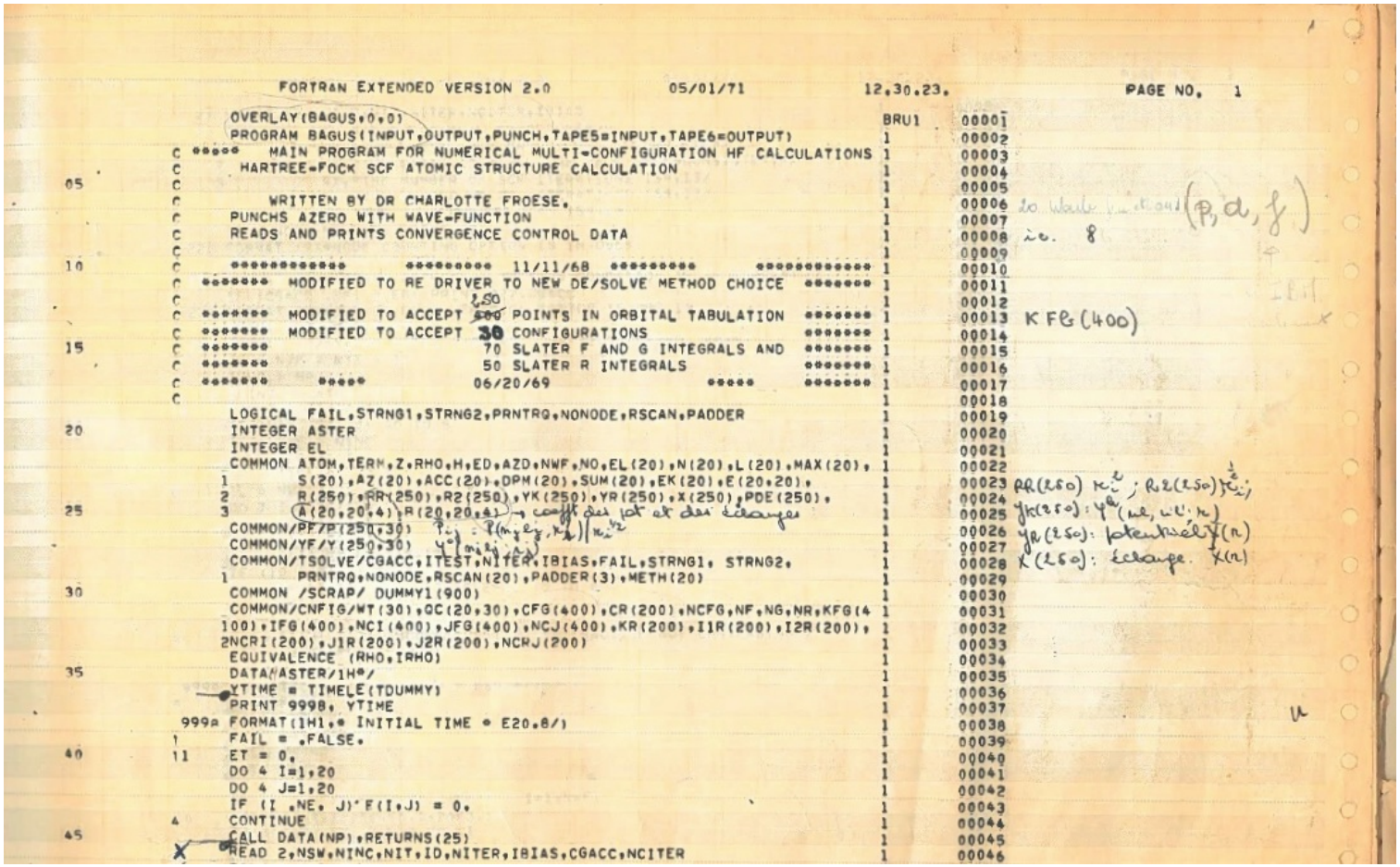
- Two quantum chemists – Reginald Colin and Georges Verhagen
- Completed PhD studies in high-temperature chemistry
- Discovered many new molecules by mass spectrometry.
- Reginald Colin went to the Herzberg Institute in Ottawa to work with A.E. Douglas on Molecular theory.
- Georges Verhaegen went to Paris to work with Carl Moser on Quantum Chemistry (CECAM)

Masters degree: 1975-77

- In Chemistry
- Professor Georges Verhaegen
- *A priori calculations of atomic oscillator strengths using transition states*
- Fractional occupation numbers for $1s(2)2s(0.5)2p(0.5)$ for a common orbital basis

Since *ab initio* calculations for molecules were much too complicated for the available computers Verhaegen and his students developed an original atom-in-molecule approach to insert correlation effects into the results. Indirectly, this prompted the beginning of studies in theoretical atomic physics in the laboratory.

MCHF programs



```
                FORTRAN EXTENDED VERSION 2.0        05/01/71        12.30.23.        PAGE NO.  1

      OVERLAY(BAGUS,0,0)                                                          BRU1   00001
      PROGRAM BAGUS(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT)                  1      00002
C *****   MAIN PROGRAM FOR NUMERICAL MULTI-CONFIGURATION HF CALCULATIONS        1      00003
C      HARTREE-FOCK SCF ATOMIC STRUCTURE CALCULATION                            1      00004
C                                                                               1      00005
C         WRITTEN BY DR CHARLOTTE FROESE,                                       1      00006
C      PUNCHS AZERO WITH WAVE-FUNCTION                                          1      00007
C      READS AND PRINTS CONVERGENCE CONTROL DATA                                1      00008
C                                                                               1      00009
C      **********       ********** 11/11/68 **********       **********        1      00010
C ********  MODIFIED TO BE DRIVER TO NEW DE/SOLVE METHOD CHOICE  ********       1      00011
C                                                                               1      00012
C ********  MODIFIED TO ACCEPT 500 POINTS IN ORBITAL TABULATION  ********       1      00013
C ********  MODIFIED TO ACCEPT 30 CONFIGURATIONS                 ********       1      00014
C ********                      70 SLATER F AND G INTEGRALS AND  ********       1      00015
C ********                      50 SLATER R INTEGRALS            ********       1      00016
C ********      *****           06/20/69            *****        ********       1      00017
C                                                                               1      00018
      LOGICAL FAIL,STRNG1,STRNG2,PRNTRQ,NONODE,RSCAN,PADDER                     1      00019
      INTEGER ASTER                                                             1      00020
      INTEGER EL                                                                1      00021
      COMMON ATOM,TERM,Z,RHO,H,ED,AZD,NWF,NO,EL(20),N(20),L(20),MAX(20),        1      00022
     1       S(20),AZ(20),ACC(20),DPM(20),SUM(20),EK(20),E(20,20),              1      00023
     2       R(250),RR(250),R2(250),YK(250),YR(250),X(250),PDE(250),            1      00024
     3       A(20,20,4),R(20,20,4)                                              1      00025
      COMMON/PF/P(250,30)                                                       1      00026
      COMMON/YF/Y(250,30)                                                       1      00027
      COMMON/TSOLVE/CGACC,ITEST,NITER,IBIAS,FAIL,STRNG1, STRNG2,                1      00028
     1       PRNTRQ,NONODE,RSCAN(20),PADDER(3),METH(20)                         1      00029
      COMMON /SCRAP/ DUMMY1(900)                                                1      00030
      COMMON/CNFIG/WT(30),QC(20,30),CFG(400),CR(200),NCFG,NF,NG,NR,KFG(4        1      00031
     100),IFG(400),NCI(400),JFG(400),NCJ(400),KR(200),I1R(200),I2R(200),        1      00032
     2NCRI(200),J1R(200),J2R(200),NCRJ(200)                                     1      00033
      EQUIVALENCE (RHO,IRHO)                                                    1      00034
      DATA/ASTER/1H*/                                                           1      00035
      YTIME = TIMELE(TDUMMY)                                                    1      00036
      PRINT 9998, YTIME                                                         1      00037
 9998 FORMAT(1H1,* INITIAL TIME = E20.8/)                                       1      00038
    1 FAIL = .FALSE.                                                            1      00039
   11 ET = 0.                                                                   1      00040
      DO 4 I=1,20                                                               1      00041
      DO 4 J=1,20                                                               1      00042
      IF (I .NE. J) F(I,J) = 0.                                                 1      00043
    4 CONTINUE                                                                  1      00044
      CALL DATA(NP),RETURNS(25)                                                 1      00045
      READ 2,NSW,NINC,NIT,ID,NITER,IBIAS,CGACC,NCITER                           1      00046
```

The MCHF program written by Charlotte Froese, modified by Paul Bagus, CECAM, Paris, compiled May 5, 1971

MCHF programs continued

- Great effort was made by the students to understand the program. This version apparently accepted 30 configurations, 70 F and G and 50 R integrals, 20 orbitals and 250 points.
- Angular coefficients – Slater determinants and linear algebra for getting eigenstates or learn Racah algebra ?
- Michel participated to some memorable contests (between them) to investigate which method was the fastest by hand. He was quickly convinced of the advantages of learning angular momentum theory and Wigner-Racah spin-angular algebra, and had the chance of learning both approaches.

PhD studies: 1977-1980

- In Chemistry
- Professor Georges Verhaegen
- *Theoretical study of electric dipole and quadrupole atomic oscillator strengths*
- *The IR-microwave double resonance technique using sealed CO lasers, should allow the high accuracy frequency measurements of new rotation transitions in the vibrationally-relaxed water molecule.*

Making Contact – July 4, 1977

1. The first concerns the definition of the potentials.
For $\psi^{MCHF} = c_1|1s2s\rangle + c_2|1s^2\rangle$ the potentials are defined by :

$$yR = 2\frac{c_2^2}{c_1^2+2c_2^2}\, y^\circ(1s1s) + 2\sqrt{2}\,\frac{c_1c_2}{c_1^2+2c_2^2}\, y^\circ(1s2s) + \frac{c_1^2}{c_1^2+2c_2^2}\, y^\circ(2s2s)$$

$$X = 2\frac{c_1^2}{c_1^2+2c_2^2}\, y^\circ(1s2s)\,\bar{P}2s + 2\sqrt{2}\,\frac{c_1c_2}{c_1^2+2c_2^2}\, y^\circ(1s1s)\,\bar{P}2s$$

$$- \sqrt{2}\,\frac{c_1c_2}{c_1^2+2c_2^2}\left[\frac{1}{r}\,\frac{d^2}{d\rho^2} + 2Z - \frac{1}{r}\,(\ell+\tfrac{1}{2})^2\right]\bar{P}2s$$

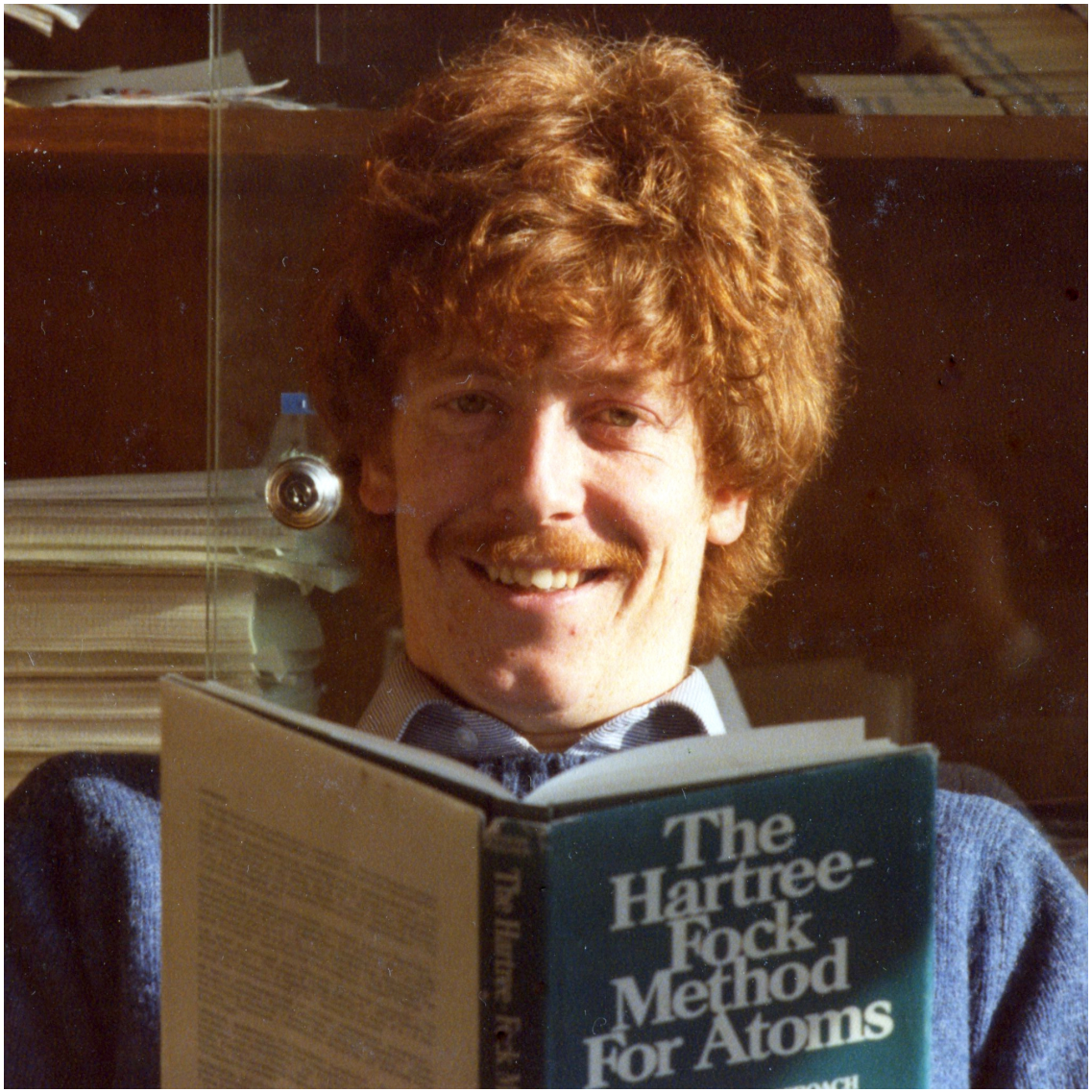
and for the 2s orbital :

$$yR = y^\circ(1s1s)$$

$$X = 2\,y^\circ(2s1s)\bar{P}1s + 2\sqrt{2}\,\frac{c_2}{c_1}\, y^\circ(1s1s)\bar{P}1s$$
$$- \sqrt{2}\,\frac{c_2}{c_1}\left[\frac{1}{r}\,\frac{d^2}{d\rho^2} + 2Z - \frac{1}{r}\,(\ell+\tfrac{1}{2})^2\right]\bar{P}1s$$

If, in these potentials, the integral L_{1s2s} appears only in the inhomogeneous parts of the 1s and 2s equations, the $R^\circ(1s1s/1s2s)$ integral appears in both homogeneous (yR) and inhomogeneous (X) parts of the 1s equation (the latter integral is involved only in the inhomogeneous part of the 2s equation).

Looking for inspiration



Postdoctoral Studies: 1981

International Conference on Fast Ion Beams Spectroscopy (Laval, Aug. 17-20, 1981). This was Michel's first oral presentation based on lifetime trends in some singlet transitions in Mg.

Angular integrations and CIV3

Figure: Alan Hibbert demonstrating data entry for his CIV3 program.

The Cray at the Free University of Brussels

Michel Godefroid, Nathalie Vaeck, and Alan Hibbert sitting on the Cray bench.

Transition Probabilities and Non-orthogonal Orbitals

- Get optimized orbitals for the initial state
- Get optimized orbitals for the final state
- Perform a biothogonal transformation such that $\langle \phi_i(initial) | \phi_j(final) \rangle = \delta_{ij}$
- Transform the wave function for the initial state
- Transform the wave function for the final state
- Compute the transition matrix element $< initial\ LS | T | final\ L'S' >$.

The ideas we based on theory developed by Jeppe Olsen, but Michel Godefroid showed how it could be applied to non-relativistic MCHF expansions. Per Jönsson, from Lund University, implemented the ideas into GRASP as part of his postdoctoral project.

The Systematic Accurate Method (SAM) group

Charlotte Froese Fischer and Alan Hibbert, with Jeppe Olsen; former postdocs Michel Godefroid, Per Jönsson, Tomas Brage; Lund Students Jörgen Carlsson, and Lennart Sturreson.

Habilitation Degree: 1981-1992

Main Topic: *The angular momenta algebra, a common method for atoms and molecules in the calculation of atomic properties*
Related Topics:

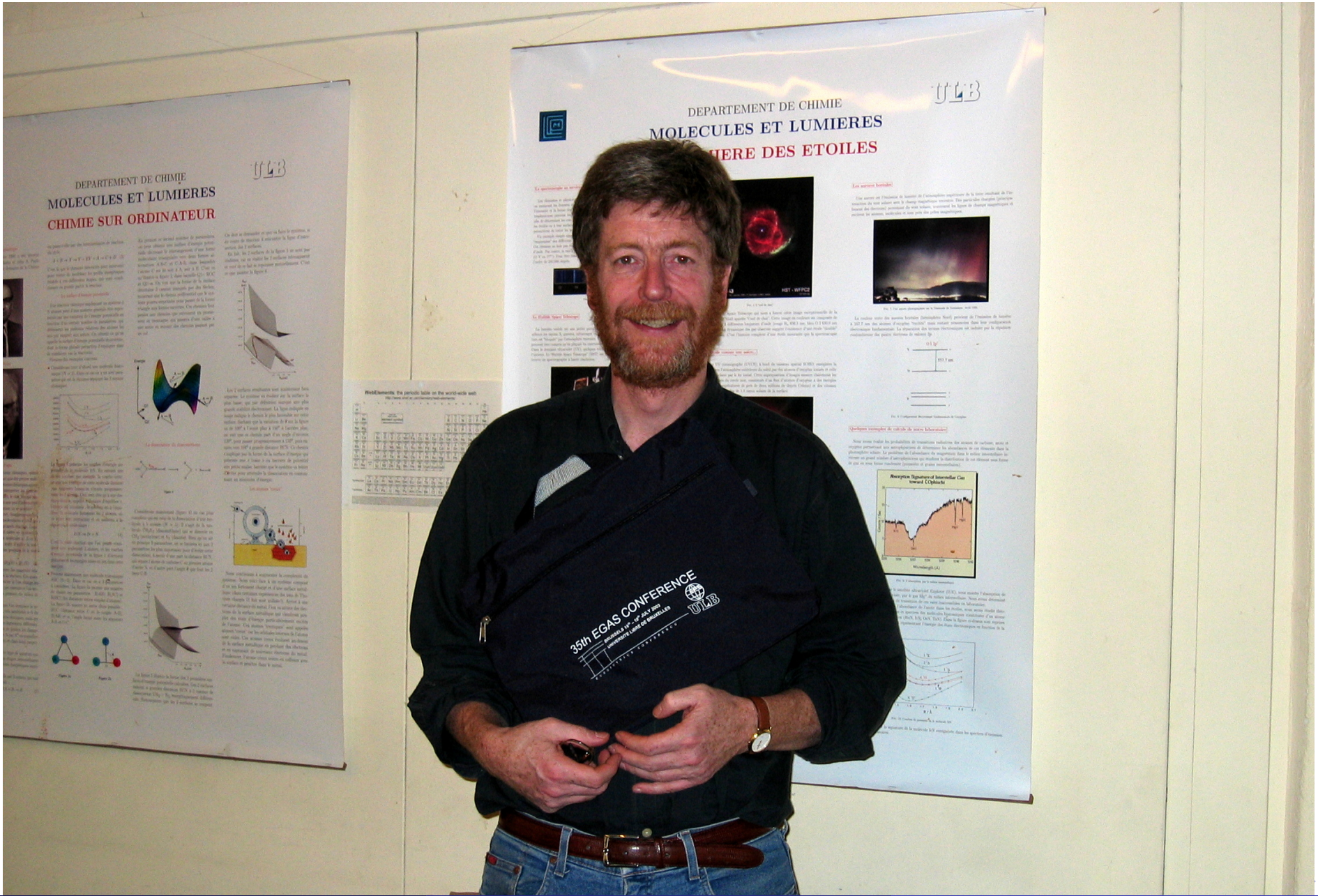
- *The quasiparticles formalism offers a global vision of the atomic electronic shell and simplifies the evaluation of matrix elements*.
  Case of the d^N configuration (with Brian Judd, 1994).
- *High resolution Fourier transform spectroscopy in the IR allows to improve the knowledge of atomic properties*.
  Application to Sc and Sc+
  (with M. Career and D. Hurtmans, and others, 1996.
- *Hartree-Fock on Lagrange meshes: an original method to study the stability of molecules immersed in high magnetic fields*
  (with a nuclear Physicists at ULB, P.H. Heenen and M. Demeur).

A ULB Professor: 2002

And now Michel transitioned into

- a Lecturer
- a Supervisor
- an Administrator, and
- a Researcher.

EGAS 2003


DEPARTEMENT DE CHIMIE
MOLECULES ET LUMIERES
CHIMIE SUR ORDINATEUR
ULB
DEPARTEMENT DE CHIMIE
MOLECULES ET LUMIERES
ULB
35th EGAS CONFERENCE
ULB

Michel's PhD Students (and Per)