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2028-1a

Joint ICTP/IAEA Workshop on Atomic and Molecular Data for Fusion

20 - 30 April 2009

Calculation of Atomic Data for Plasma Modeling: Introduction and Atomic Structure Part I

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Calculation of Atomic Data for Plasma Modeling: Introduction and Atomic Structure Part 1

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Nuclear Data Section

Overview

- Plasmas in fusion research
- Data needs for plasma modeling
- Atomic structure
- Electron impact excitation
- Electron impact ionization
- Photoionization
- Autoionization
- Applications to collisional radiative model

Fusion plasmas

- Main constituents are hydrogen isotopes
- There are impurities from variety of sources
- It is necessary to model the entire plasma for information on ionization stages, radiated power, spectrum analysis etc
- Plasma regimes include: LTE, coronal, collisional-radiative (CR)
- Large datasets are needed for a complete CR model

Hydrogen Isotopes

- Initial experiments use hydrogen
- Deuterium used to study isotope effects
- D-D cross section low, a few but non-zero fusions occur
- D-T cross section is larger, but tritium poses health risks and tritium inventory is an important issue
- Hydrogen chemistry and plasma-surface interactions are important topics

Impurities

- Plasma-wall interactions will cause sputtering
- Proposals for ITER will include Be, C and W in wall
- Gases proposed for control of edge region include: N_2, Ne, Ar and perhaps heavier inert gases
- Diagnostic beams for the plasma will mainly use Li
- Trace elements may be used in tiles to track erosion

Plasma parameters

- Edge region plasma temperatures go down to below 1 eV, molecules through C_4H_8 may form
- In the core region temperatures are ~10 keV
- Theses temperature ranges mean most ionization stages of all plasma constituents will exist
- Electron densities are ~10^{14} cm^{-3}

Plasma regimes

- At high density, collisions dominate all processes, upward and downward rates balance, the plasma is in LTE and populations are derived from energies and statistical weights.
- At very low density the excited states not significantly populated. Only transitions from ground states need be followed. This is common in astrophysics and is called coronal equilibrium.

Plasma regimes

- Moderate densities require solving the full set of rate equations, tracking populations of the excited states. Large databases are needed.
- Often the plasma is in steady state; populations are not changing, otherwise, it is necessary to carry out a time evolution calculation.

Types of data needed

- Atomic structure – energy levels, wave functions.
- Radiative processes.
- Collisional processes.
- Charge transfer processes.
- Plasma interaction with wall materials.
- Data for atoms, ions and molecules.

Atomic structure

- Relativistic versus non-relativistic.
- Notation and coupling schemes.
- Electron configurations.
- LS Terms.
- Fine structure levels.
- Mixing of basis states.

Relativistic and Non-relativistic

- For heavy elements and for high charge states full relativistic treatment is needed
- It is possible to include some relativistic features in a non-relativistic treatment; mass and darwin terms in the radial wave function, spin-orbit interaction in fine structure energy levels
- For most fusion applications the modified non-relativistic approach is adequate

Hartree-Fock Method

- Total wave function is an anti-symmetrized determinant product of one-electron orbitals (the "Slater" determinant)
- Begin with approximate orbitals for all electrons
- Use these orbitals to calculate a potential and solve the Schroedinger equation for a new one electron orbital

Hartree-Fock Method

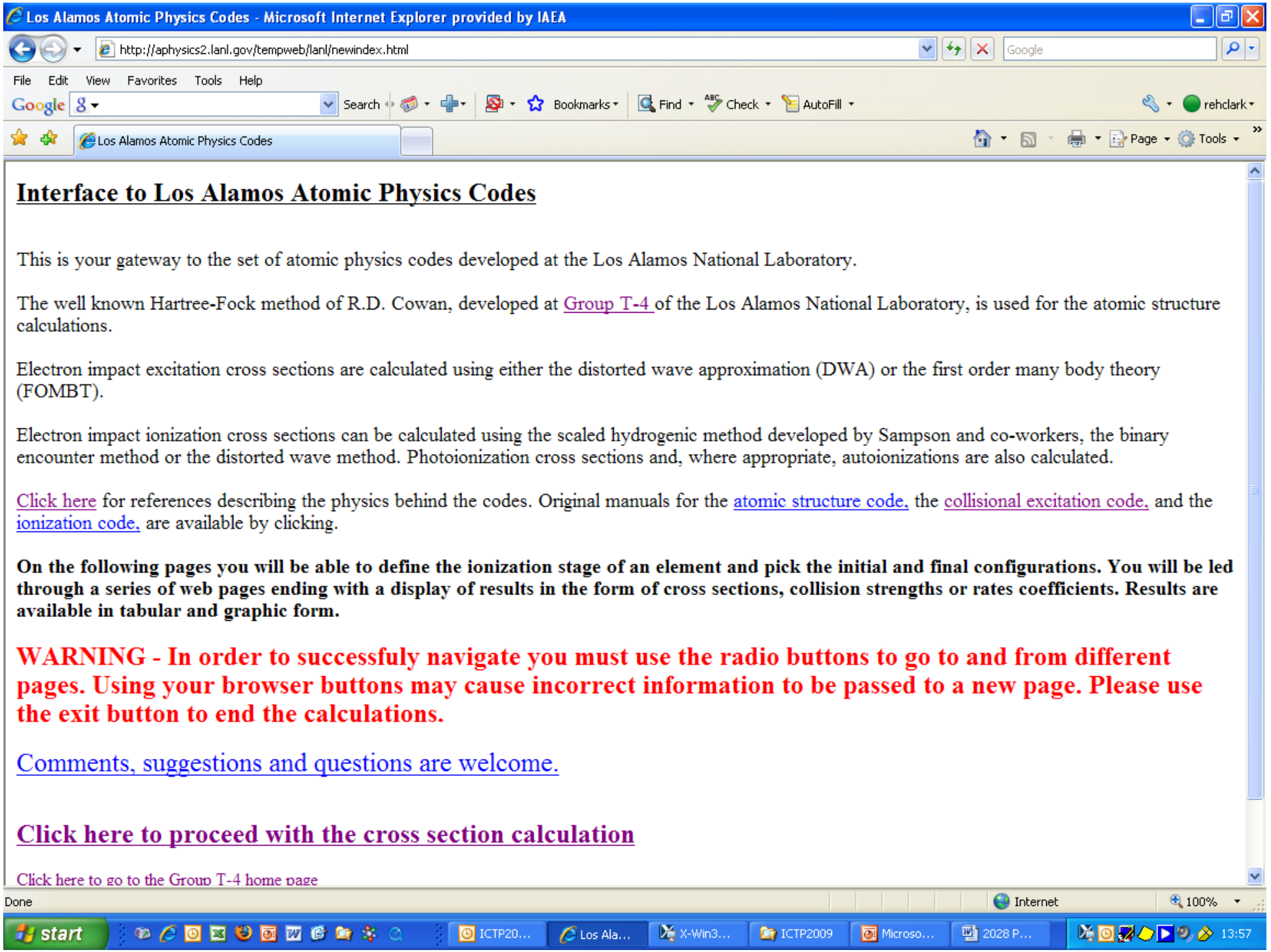
- With the new orbital, continue to the next electron orbital
- Continue through all electrons, giving a new set of orbitals
- Use the new set of orbitals to calculate a new potential and iterate until orbitals converge
- Large computer code developed by R.D. Cowan, updated and modernized by J. Abdallah, Jr. performs this calculation
- Interface allows use of structure code through Internet

Site for calculating atomic physics

http://aphysics2.lanl.gov/tempweb/lanl/

On the web

- READ the information, then proceed to calculation.
- Select ion stage, continue.
- Select configurations. More than two configurations are permitted. Enter list of configurations. Note that noble gas cores need not be entered.
- ALWAYS use the exit key to leave the program to clean file space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Los Alamos Atomic Physics Codes
Interface to Los Alamos Atomic Physics Codes
This is your gateway to the set of atomic physics codes developed at the Los Alamos National Laboratory.
The well known Hartree-Fock method of R.D. Cowan, developed at Group T-4 of the Los Alamos National Laboratory, is used for the atomic structure calculations.
Electron impact excitation cross sections are calculated using either the distorted wave approximation (DWA) or the first order many body theory (FOMBT).
Electron impact ionization cross sections can be calculated using the scaled hydrogenic method developed by Sampson and co-workers, the binary encounter method or the distorted wave method. Photoionization cross sections and, where appropriate, autoionizations are also calculated.
Click here for references describing the physics behind the codes. Original manuals for the atomic structure code, the collisional excitation code, and the ionization code, are available by clicking.
On the following pages you will be able to define the ionization stage of an element and pick the initial and final configurations. You will be led through a series of web pages ending with a display of results in the form of cross sections, collision strengths or rates coefficients. Results are available in tabular and graphic form.
WARNING - In order to successfuly navigate you must use the radio buttons to go to and from different pages. Using your browser buttons may cause incorrect information to be passed to a new page. Please use the exit button to end the calculations.
Comments, suggestions and questions are welcome.
Click here to proceed with the cross section calculation
Click here to go to the Group T-4 home page
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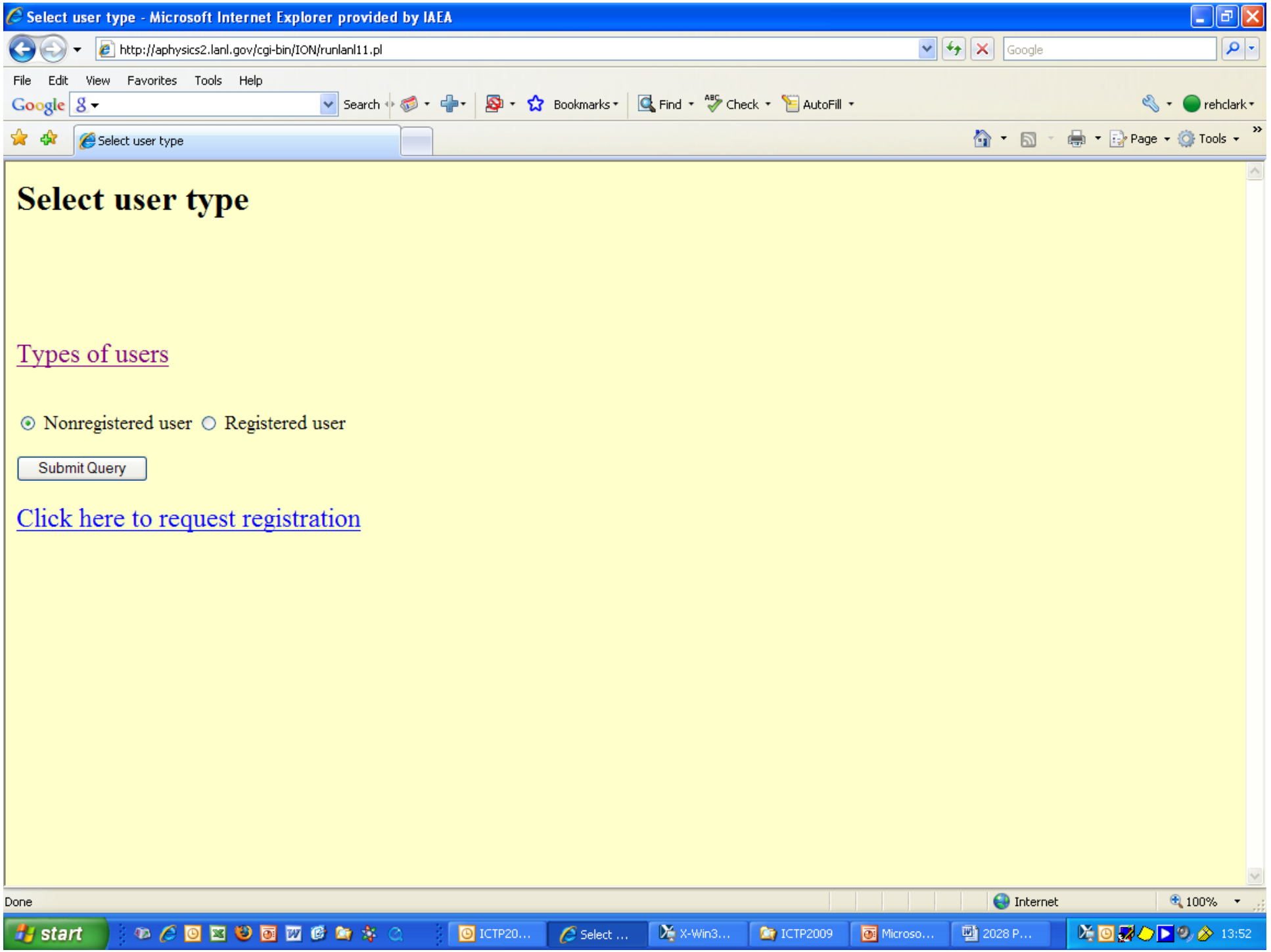
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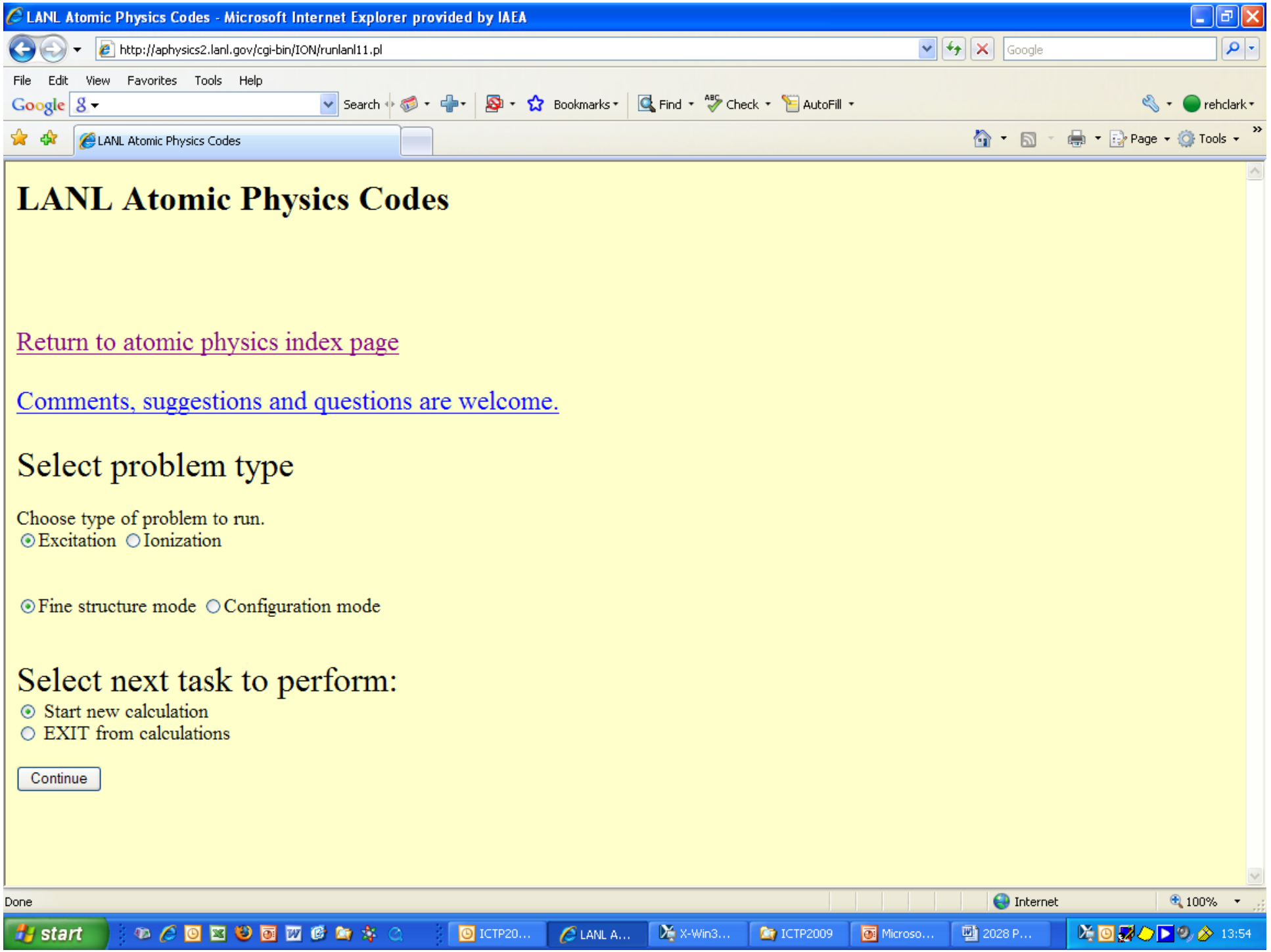
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Comments, suggestions and questions are welcome.
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Configuration notation

- Simplest specification is principle and orbital quantum numbers with occupation number: $1s^2 2s2p$ for example
- For compactness, inner noble gas core is assumed, leading to above configuration abbreviated as 2s2p
- This assumes non-relativistic orbitals; jj coupling is used by some codes

Noble gas cores

- Noble gases: He, Ne, Ar, Kr, Xe closed shell systems
- Do not change angular coupling
- For simplicity, do not need to include explicit listing of noble gas core

Examples: C I has configuration $1s^2 2s^2 2p^2$ which can be entered as $2s^2 2p^2$

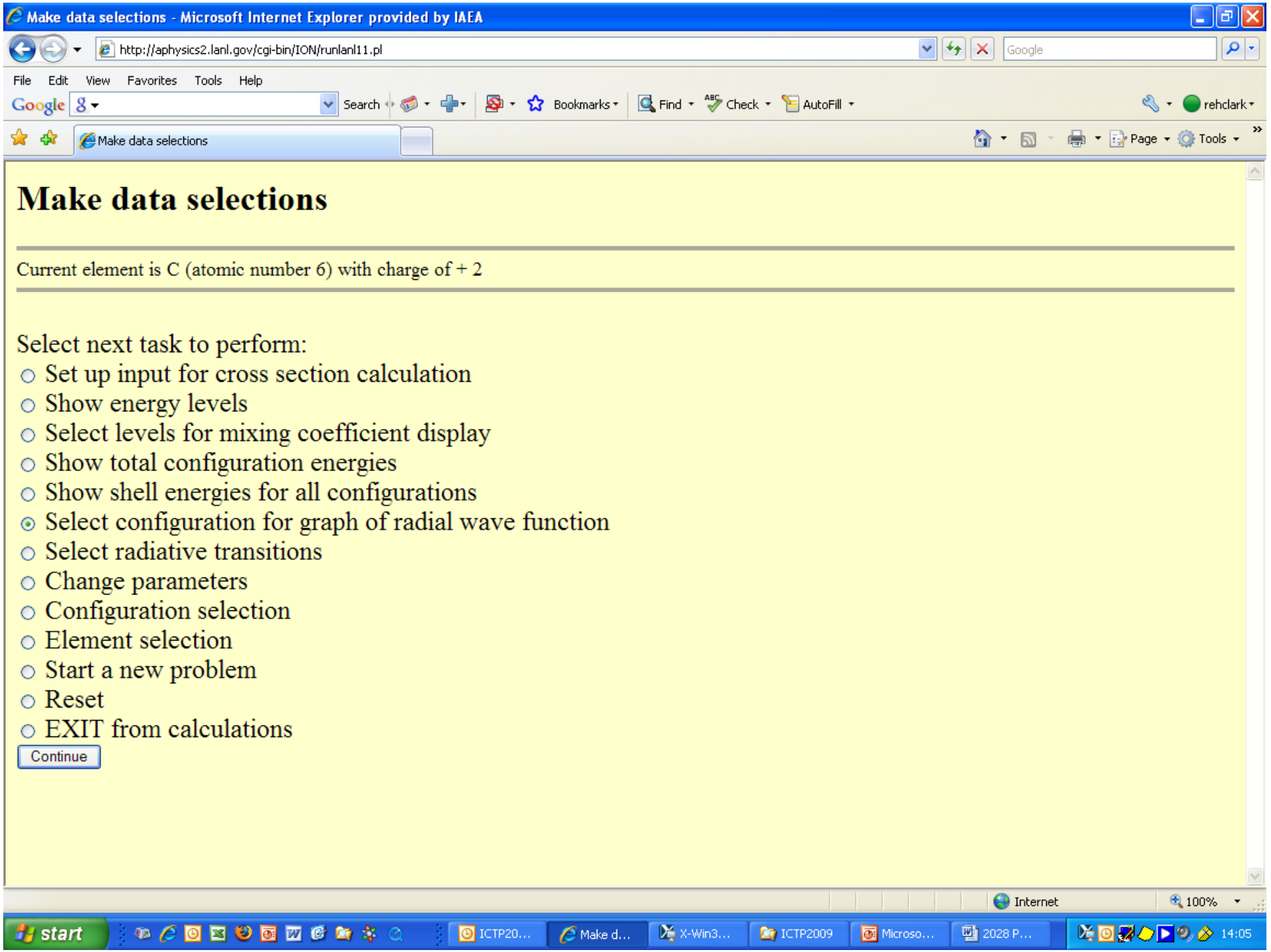
Al III may be entered as simple 3s, dropping the entire Ne-like core

Configurations

- Radial wave functions are calculated for configurations
- Radial wave functions are not changed for different couplings of angular momentum
- Influence of angular momentum coupling is included through mixing of target states

Radial wave functions

- From structure calculation each radial wave function may be displayed
- As nuclear charge increases, radius decreases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Current element is C (atomic number 6) with charge of + 2
Select next task to perform:
Set up input for cross section calculation
Show energy levels
Select levels for mixing coefficient display
Show total configuration energies
Show shell energies for all configurations
Select configuration for graph of radial wave function
Select radiative transitions
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Configuration selection
Element selection
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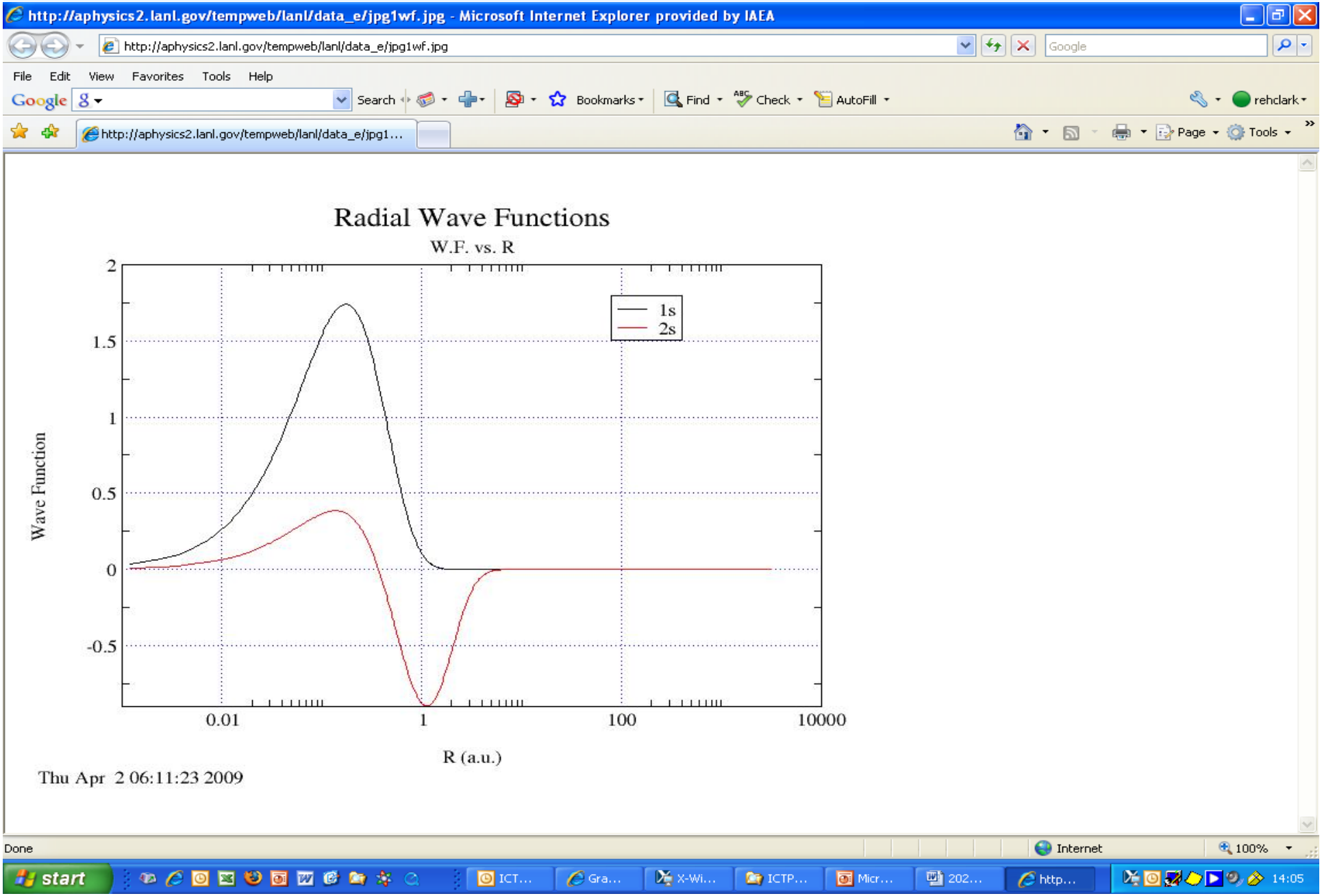
Carbon III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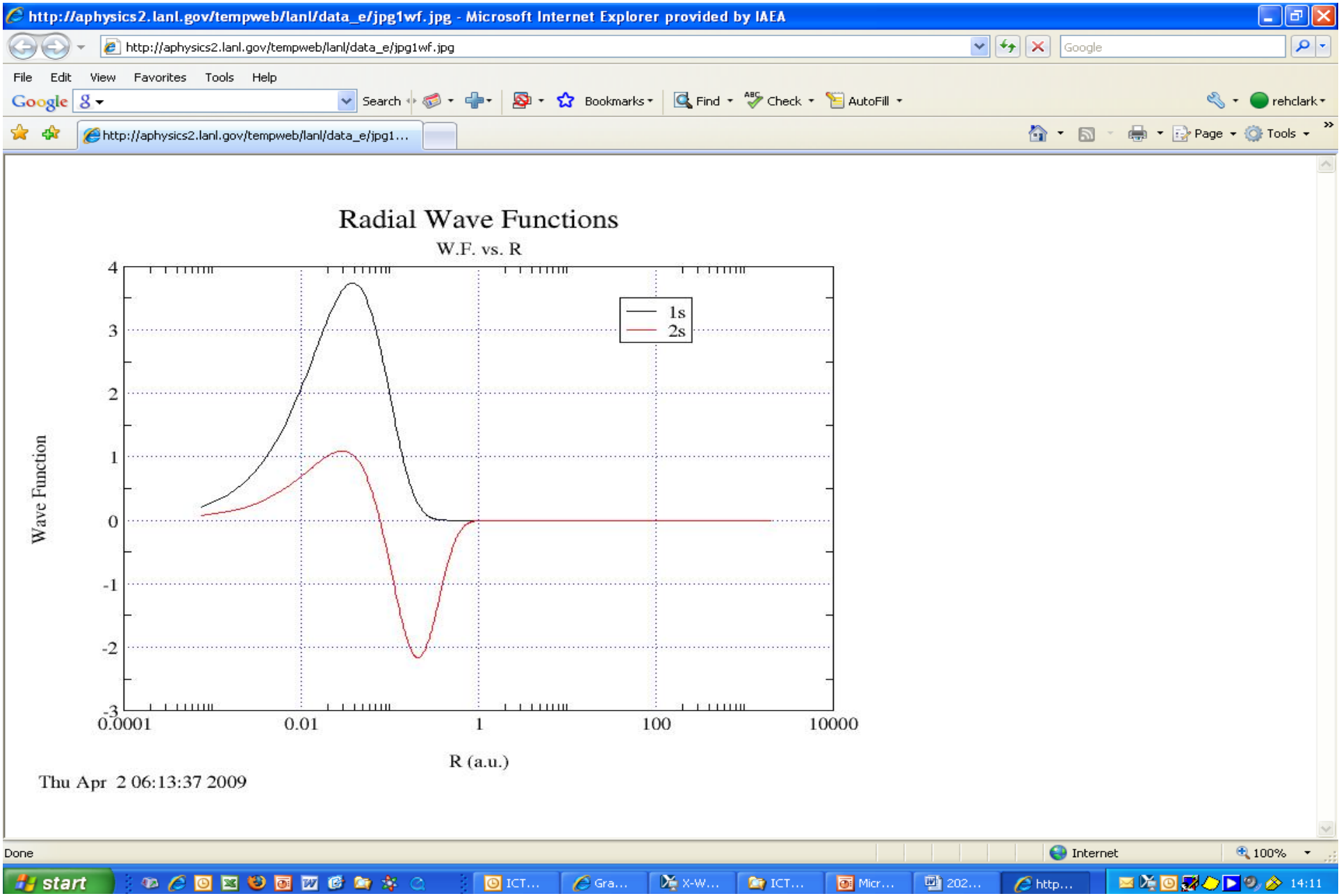
Iron XXIII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Configuration energies

- For any structure calculation, energies of all shell may be displayed
- Koopman's theory:

  Eigenenergy of an electron in a shell is equal to the ionization energy
- Theory is rigorous for hydrogenic
- It is an approximation for complex systems, actual ionization energies should be calculated by the difference of total ion energies

- ○ Change parameters
- ○ Configuration selection
- ○ Element selection
- ○ Start a new problem
- ○ Reset
- ○ EXIT from calculations

Continue

Current element is Fe (atomic number 26) with charge of + 22

Help on configuration energies

Shell energies of Fe + 22
Energy (eV) Shell

Shell energies for $2s^2$
8.5690e+03 $1s^2$
1.9459e+03 $2s^2$
Total configuration energy is 0.0000e+00
Stat. Wt. is 1

Shell energies for 2s 2p
8.5483e+03 $1s^2$
1.9491e+03 2s
1.8897e+03 2p
Total configuration energy is 5.6386e+01
Stat. Wt. is 12

Configuration energies

- **Hydrogenic orbitals:**

  Ionization energy is Z^2/n^2 where Z is the nuclear charge and n is the principle quantum number

- **Screening constants:**

  For an electron outside other orbitals, the inner electrons "screen" the nuclear charge, thus an outer bound electron has an effective nuclear charge $Z_{eff} = Z - \sigma$, where σ is a screening parameter

Screening parameters

- Approximate screening parameters were calculated in the 1950s from Coulomb theory
- Sampson used screening parameters as adjustable parameters to obtain data for complex ions from hydrogenic calculations
- Screening parameters are used in several approximate codes for atomic properties

Coupling of angular momentum

- Electrons have orbital angular momentum and spin
- These couple vectorially
- There are a number of possible methods to couple
- We will follow LSJ coupling

LSJ coupling

- Start from electron configurations
- Couple electron orbital momenta within a shell.
- Couple electron spins in shell
- Couple result to previous shell, continue through all shells
- Couple total orbital angular momentum and spin for total angular momentum
- Include target state interactions: Configuration mixing from Coulomb interaction, mixing of LS terms from spin-orbit interaction

Example

- Simple case first
- C^{+4}, helium-like
- Consider 1s2p configuration
- Total orbital angular momentum, L, must be 1 (l_1=0, l_2=1) $|l_1-l_2| \leq L \leq l_1+l_2$
- Total spin, S, can be 0 or 1 (s_1= s_2=1/2) and $|s_1-s_2| \leq S \leq s_1+s_2$
- Terms are 1s2p ^{1}P and 1s2p ^{3}P, using notation of $^{2S+1}$L

Example

- The ^1P term can only have total angular momentum, J, of 1 (S=0, L=1) $|L-S| \leq J \leq L+S$
- The ^3P can have J=0,1,2 (S=1, L=1).
- Energy levels are: 1s2p $^1P_1$, 1s2p $^3P_0$, 1s2p $^3P_1$ and 1s2p $^3P_2$.
- For more complex cases, the procedure is to couple within a shell, then couple to previous shells.

Example

- Consider case of electron configuration of $3s^2 3p^2 3d^2 4p$. This requires coupling the 3p electrons first, then coupling the 3d electrons, coupling that result to the 3p result, and finally coupling the 4p electron.
- One sample level is:
  $(3p^2\ {}^1D)^1D\ \ (3d^2\ {}^3F)^3H\ (4p^1\ \ {}^2P)\ {}^4I$.
- This single electron configuration gives rise to 604 fine structure levels.

Mixing of target states

- Configurations and LS terms form basis states
- Coulomb interaction causes mixing of configurations which have the same LS terms
- Spin-orbit causes mixing of LS terms which have the same configuration
- Mixing provides better description of energy levels

Example of Configuration Mixing

- Consider Be-like ion, Fe^{+22}.
- Consider configurations $2s^2$, 2s2p, $2p^2$, 2s3p and 2p3s.
- Configuration mixing occurs due to Coulomb interaction.
- Spin-orbit causes mixing of LS terms.
- List of make-up of energy levels:

Make-up of Energy Levels

index	j	component	configuration					
1	.0	9.8008E-01	(2s2	1S)	1S			
		2.3433E-02	(2p2	3P)	3P			
		1.9722E-01	(2p2	1S)	1S			
2	.0	1.0000E+00	(2s1	2S)	2S	(2p1	2P)	3P
3	1.0	9.8649E-01	(2s1	2S)	2S	(2p1	2P)	3P
		1.6382E-01	(2s1	2S)	2S	(2p1	2P)	1P
4	2.0	1.0000E+00	(2s1	2S)	2S	(2p1	2P)	3P
5	1.0	-1.6382E-01	(2s1	2S)	2S	(2p1	2P)	3P
		9.8647E-01	(2s1	2S)	2S	(2p1	2P)	1P
6	.0	-7.3820E-02	(2s2	1S)	1S			
		9.6485E-01	(2p2	3P)	3P			
		2.5221E-01	(2p2	1S)	1S			

Consequences of Mixing

- Configuration can allow “double electron” jumps. Since the $2s^2\ {}^1S_0$ contains some of the $2p^2\ {}^1S_0$ state, it becomes possible to have a non-zero probability for a transition to occur between those states.
- LS term mixing can cause radiative transitions between “spin-forbidden” states

Example of Effects of Mixing

- Consider He-like transition $1s^2 \rightarrow 1s2p\,^3P_1$.
- The $1s2p\,^3P_1$ is actually a mixture of $^1P_1$ and $^3P_1$ with the mixing varying with nuclear charge. For C, they mixing coefficients are 0.99995 and 0.00041, while for Fe they are 0.95922 and 0.28266.
- For carbon this is a forbidden transition, gf = 1.1851e-05

Example of Effects of Mixing

- For iron it is allowed, gf = 6.3684e-02
- This makes a difference in radiated power and for ionization balance
- For carbon, electron configuration over-estimates radiated power, underestimates ionization rates
- For iron, configuration model is better

Configuration vs fine structure

- Configuration calculation mode gives no coupling of angular momentum
- CFG mode runs fast
- CFG has few levels
- Often CFG mode makes reasonable approximation to levels
- CFG mode has no mixing effects

Data Obtained From Structure Code

- Energy levels
- Radial wave functions
- Effects of mixing (configuration and spin-orbit)
- Oscillator strengths
- Plane wave Born (PWB) collision cross sections
- Configuration and fine structure modes