ATOM manual

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A. Description

ATOM is a program which allows to calculate the ground state electron density and energy of isolated atoms and ions. It is based on the Spin Density Functional Theory (SDFT) approach to the many body problem. In most of the cases the Local Spin Density Approximation (LSDA) is used, the only exception being the choice of a source free exchange and correlation (XC) field. The basic equations underlying the solution of the atomic problem are chosen to be the Kohn-Sham-Dirac ones. As a result, the effective one electron eigenfunctions are represented by bispinors. This treatment is commonly referred to as "fully relativistic". The reader is invited to refer to the present and wide literature on the subject.

The program ATOM was written in *C* without the use of any machine dependent code and can thus be compiled on any architecture, although only *HP-UX* and *Linux* systems were personally tested. The matrix diagonalization routine is written in *Fortran77* and was imported from the *EISPACK* routines. In absence of a fortran compiler, a standard *f2c* conversion of this routine can be done before the compilation process.

B. Running the program

In the following we refer to the executable name as `ATOM`, but you may have changed it according to your personal taste. Of course the directory containing the executable must be present in your PATH environmental variable. To run the program just type its name on the command line. The program requires some input files to run. In case these files are not present, they will be created automatically. These files, the structure of which will be dealt with later, are:

- `relat.ini`, containing the list of basic options and parameters. It is a mandatory file.

- `El_structure`, containing the electronic configuration of the atom. This file may be substituted by the specification on the command line of the atom or ion symbol to be calculated.
- `niocc`, which is required in the case of a calculation with non integer occupation numbers.

C. Command line parameters

In the following we shall describe the accepted command line parameters:

-f filename The program will use the initialization file *filename* instead of the default `relat.ini`.

-pN the program will output the density of the orbital number N to a file.

-M It will output the present manual in the file `MANUAL.ps` and exit.

-h A short list of these command line options will be printed on the standard output device and exit.

:elem The ground state electronic configuration of the atom or ion *elem* will be used instead of reading the electronic configuration `El_structure` file.

As an example to run the program for the potassium plus one ion with the default settings, you could type twice:
`ATOM :K+`

D. Ini file

NRMAX Number of points in the radial mesh. The memory will be dynamically allocated.

MESH Kind of radial mesh $\{i = 0 \ldots (\mathrm{NRMAX} - 1)\}$:

0 Linear grid. $r_i = \frac{R_{\max}}{\mathrm{NRMAX}}(i+1)$

1 Quadratic grid. $r_i = \frac{R_{\max}}{\mathrm{NRMAX}^2}(i+1)^2$

2 Logarithmic grid. $r_i = R_{\min}\exp[\frac{\log(\mathrm{R_{max}/R_{min}})}{\mathrm{NRMAX}-1}\mathrm{i}]$

Since in the case of a point like nucleus, the relativistic $s_{1/2}$ and $p_{1/2}$ states are singular at the origin, the radial grid never starts with r=0.

NVERS

XCHNG

NSPIN

USESIC

NUCLEUS

NOSPH

NOCOLL

CLEAN_FIELD

NONINTOCCNUM

C

BCONST

RMIN

RMAX

MIXING

ACCRCY

ANYSHELL

NLMAX

EXTRASHELL

MAXLEXP

FIXOCCNUM

NRRECTPT

PRINT_BASE

WRITE_COUPLING

WRITE_DELTAW

NSPHORBSIC

COMPTON_PROFILE

PRINTRHO

PRINTMAGN

PRINTPOT

PRINTENRG

R_POWERS

IPRINT