

Test Report on Electron Localization Function (ELF) Implementation in Norm-Conserving Plane-Waves Formalism.

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Chapter 1

Test on an isolated H atom.

We use the Fermi-Amaldi exchange-correlation functional ($ixc = 20$) and no spin polarization (not available with this functional).

For single H atom we have the wavefunction which is $1s$ atomic orbital. For analytical approach¹ we thus use the spherical harmonic formulation which is given by:

$$\psi = \varphi_{1s}(r, \theta, \phi) = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Z \frac{|\mathbf{r}|}{a_0}} \quad (1.1)$$

with Z the atomic number and a_0 the Bohr constant.
We obtain for H atom ($Z = 1$):

- the electronic density

$$n(\mathbf{r}) = |\psi|^2 = |\varphi_{1s}(r, \theta, \phi)|^2 = \frac{1}{\pi a_0^3} e^{-\frac{2|\mathbf{r}|}{a_0}} \quad (1.2)$$

- the kinetic energy density

$$\tau(\mathbf{r}) = \frac{1}{2} |\nabla \psi|^2 = \frac{1}{2} |\nabla \varphi_{1s}(r, \theta, \phi)|^2 = \frac{1}{2\pi a_0^5} e^{-\frac{2|\mathbf{r}|}{a_0}} \quad (1.3)$$

- the square norm of the gradient of the electronic density

$$|\nabla n(\mathbf{r})|^2 = |\nabla |\psi|^2|^2 = |\nabla |\varphi_{1s}(r, \theta, \phi)|^2|^2 = \left| \frac{-2}{\pi a_0^4} e^{-\frac{2|\mathbf{r}|}{a_0}} \right|^2 = \frac{4}{\pi^2 a_0^8} e^{-\frac{4|\mathbf{r}|}{a_0}} \quad (1.4)$$

¹For theoretical and implementation details see chap. 3 in /doc/theory/ELF/

- the Weizsäcker kinetic energy density

$$\frac{1}{8} \frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})} = \frac{1}{8} \frac{\frac{4}{\pi^2 a_0^8} e^{-\frac{4|\mathbf{r}|}{a_0}}}{\frac{1}{\pi a_0^3} e^{-\frac{2|\mathbf{r}|}{a_0}}} = \frac{1}{2\pi a_0^5} e^{-\frac{2|\mathbf{r}|}{a_0}} \quad (1.5)$$

- the Thomas-Fermi kinetic energy density

$$\frac{3}{10} (3\pi^2)^{2/3} n^{5/3}(\mathbf{r}) = 2.871 \times \left(\frac{1}{\pi a_0^3} e^{-\frac{2|\mathbf{r}|}{a_0}} \right)^{5/3} \quad (1.6)$$

- the ELF

$$ELF(\mathbf{r}) = \frac{1}{1 + \left(\frac{\tau(\mathbf{r}) - \frac{1}{8} \frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})}}{2.871 \times n^{5/3}(\mathbf{r})} \right)} = \frac{1}{1 + \left(\frac{0}{2.871 \times n^{5/3}(\mathbf{r})} \right)} = 1 \quad (1.7)$$

As we can see the ELF should be 1 everywhere for the single hydrogen atom because the kinetic energy density and the Weizsäcker kinetic energy density are equal in that case² (see Eq. ?? and ??).

²the ELF is also equal to 1 everywhere for an isolated helium atom.

1.1 Standard test.

The standard input file used is the following:

```
acell 3*30
ecut 100
diemac 1.0d0
diemix 0.5d0
iscf 3
ixc 20
kpt 3*0.25
natom 1
nband 1
nkpt 1
nline 3
nspol 1
nstep 6
nsym 8
ntypat 1
occ 1
rprim 100 010 001
symrel
1 0 0 0 1 0 0 0 1
-1 0 0 0 1 0 0 0 1
1 0 0 0 -1 0 0 0 1
-1 0 0 0 -1 0 0 0 1
1 0 0 0 1 0 0 0 -1
-1 0 0 0 1 0 0 0 -1
1 0 0 0 -1 0 0 0 -1
-1 0 0 0 -1 0 0 0 -1
tnons 24*0
tolwfr 1.0d-14
typat 1
wtk 1
znucl 1
xred 3*0
prtelf 1 #output a _ELF file.
```

We observe on the following pictures the result of ABINIT compared to previous analytical formula.

First the convergence with the acell parameter (Fig.(??)).

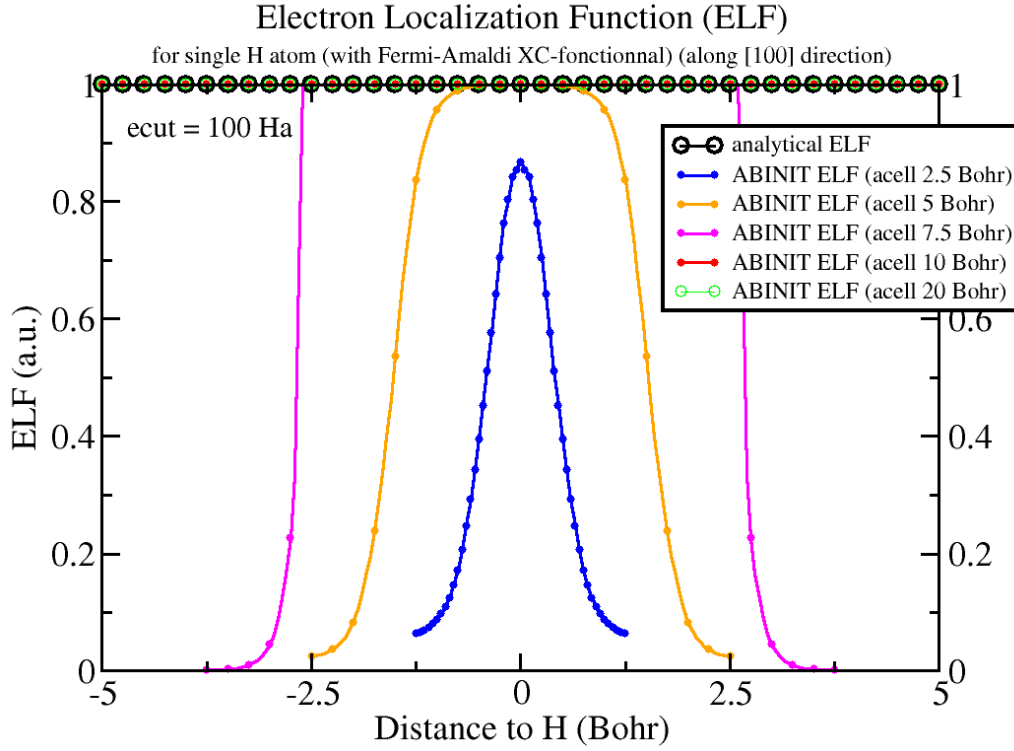


Figure 1.1: Comparison between analytical ELF and ABINIT ELF for an isolated H atom.

Then the convergence with $ecut$ parameter (Fig.(??)). The thing is that the convergence of ELF seems to be more sensitive to the $acell$ parameter than the $ecut$ parameter, at least here for the hydrogen atom. For instance with only an $ecut$ of 10 Ha but with a 10 Bohr box we already obtain 1 everywhere.

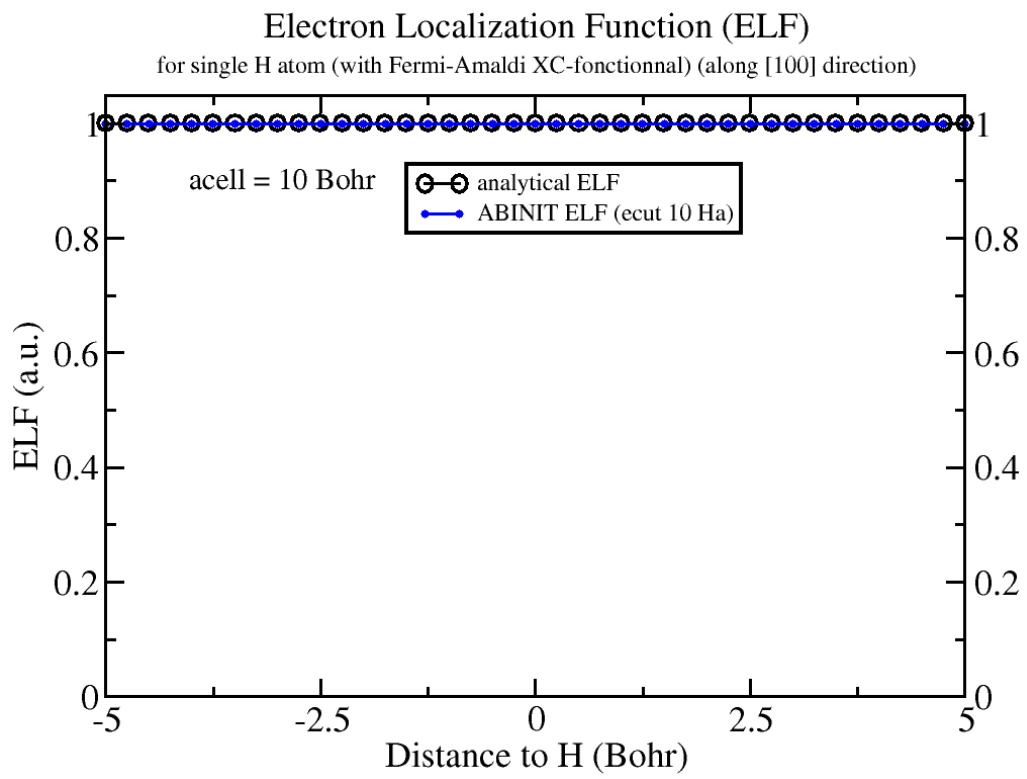


Figure 1.2: Comparison between analytical ELF and ABINIT ELF for an isolated H atom.

Chapter 2

Test on an isolated Li atom.

Since the hydrogen atom is a bit peculiar for test of *ELF* we have also performed a test with another isolated atom. We use here lithium (Li) because *ELF* which can be used to show up the shell structure of isolated atoms, is very simple for Li. Actually for Li this is just a single *s* shell. We use for that an all electron calculation¹.

First with a bare pseudopotential (Fig.(??) and Fig.(??)):

Then with **fhi** pseudopotential (Fig.(??) and Fig.(??)):

¹the pseudopotential used is 03li.pspfhi and also a by-hand constructed bare pseudopotential 03li.bare

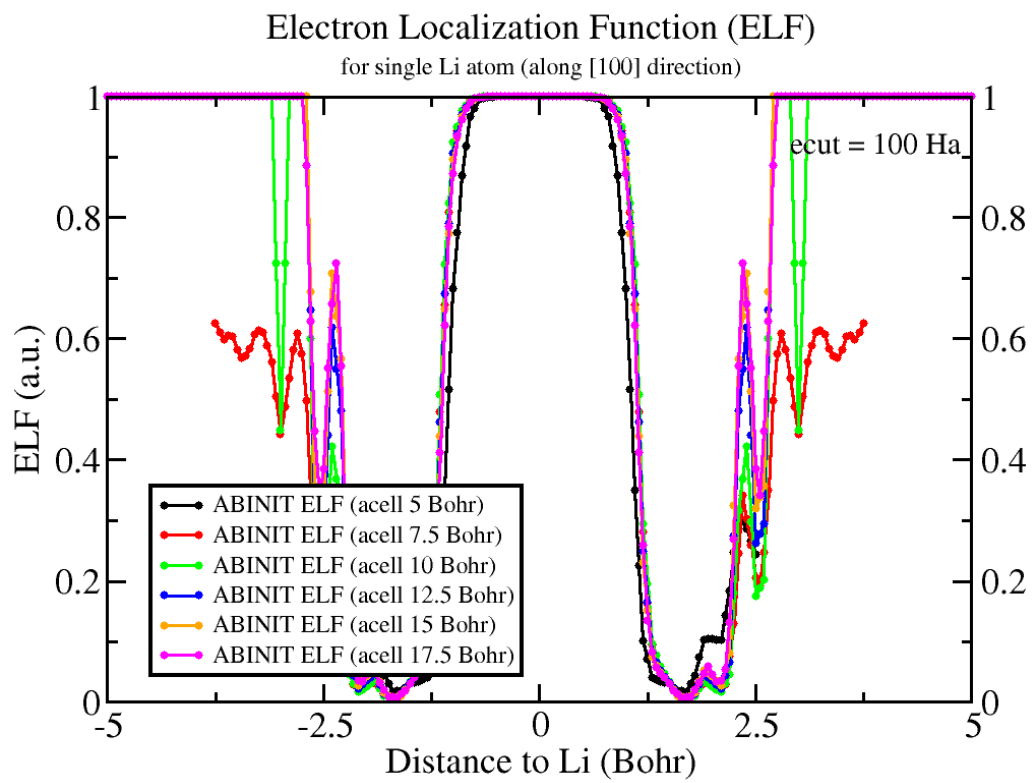


Figure 2.1: ABINIT *ELF* for an isolated Li atom with a bare pseudo.

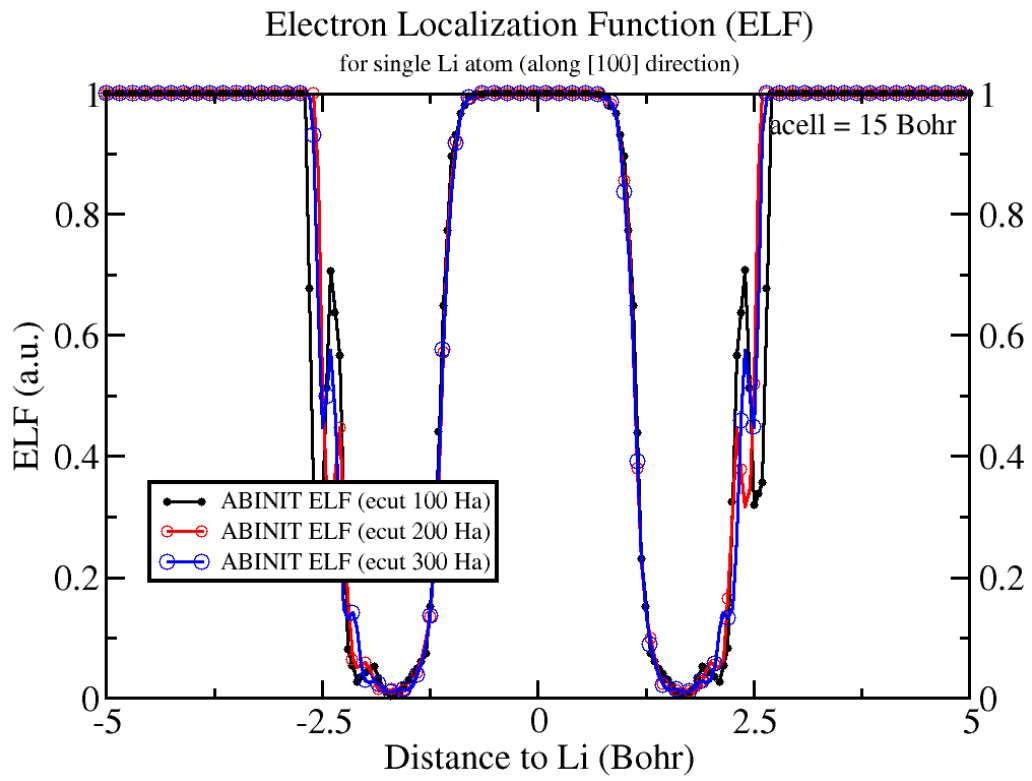


Figure 2.2: ABINIT *ELF* for an isolated Li atom with a bare pseudo.

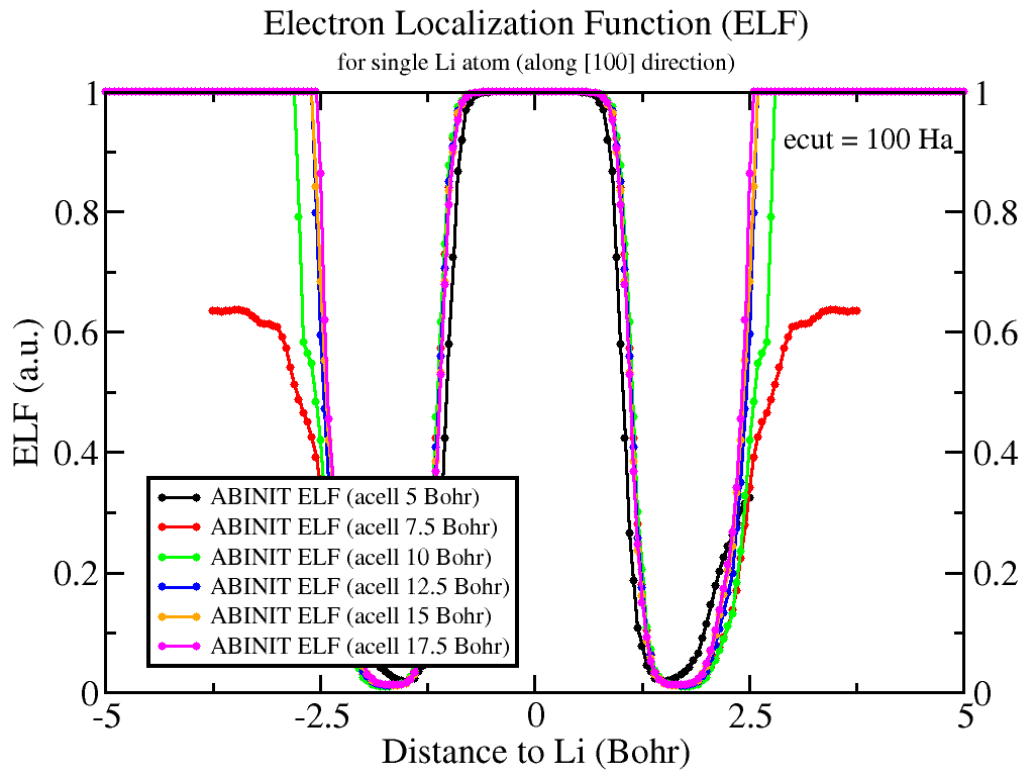


Figure 2.3: ABINIT *ELF* for an isolated Li atom with a **fhi** pseudo.

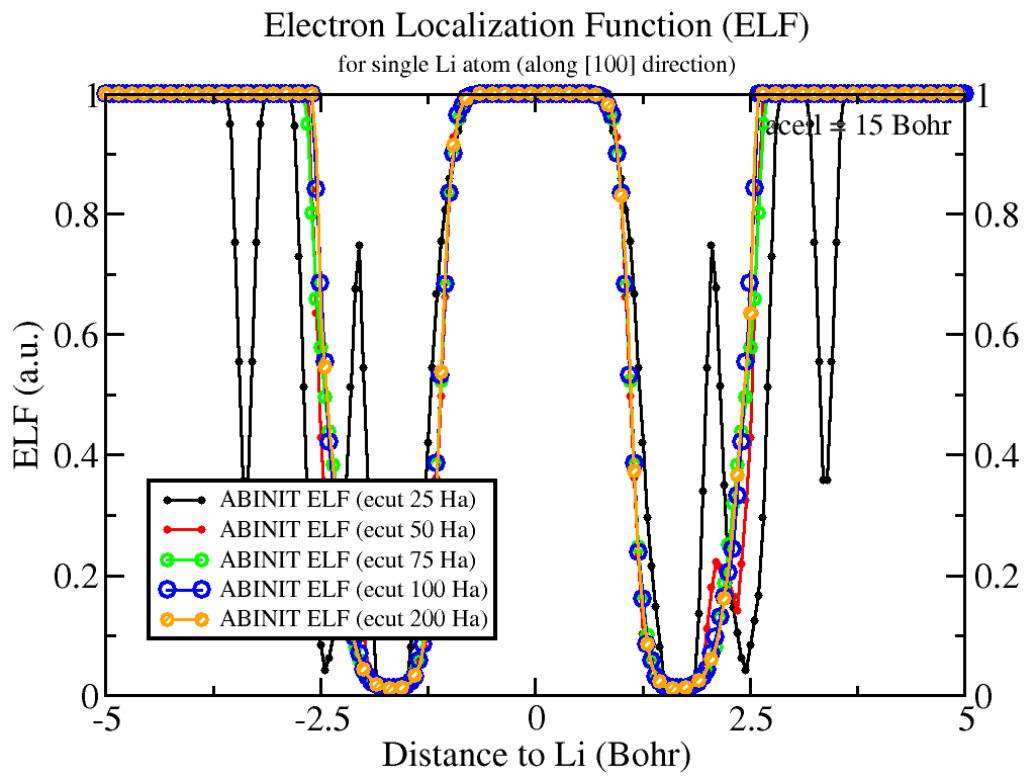


Figure 2.4: ABINIT *ELF* for an isolated Li atom with a **fhi** pseudo.