Chapter 7

Application of the LAPW method. Hands on the code

The LAPW code in the WIEN version consists of a bunch of interconnected programs, which realize different phases of the self-consistency (SCF) procedure to solve the Kohn-Sham equations.

Initialization set

The input file `case.struct` contains the atomic positions and crystal structure as well as the radii of the muffin tins.

- **NN** → checks for overlapping spheres.
- **SGROUP** → uses information from `case.struct` to determine the space group as well as all point groups of non-equivalent sites.
- **SYMMETRY** → uses information from `case.struct` to generate the space group symmetry operators. Also, the point group of each atomic site is determined and the respective symmetry operations and $LM$ values of the lattice harmonics representation are printed.
- **LSTART** → generates atomic densities, which are used by **DSTART** to be composed into a starting density for an SCF calculation. It also creates all the input files for the SCF run.
- **KGEN** → generates the $k$-mesh in the irreducible wedge of the Brillouin zone (IBZ) on a special point grid, which can be used in a modified tetrahedron integration scheme.
- **DSTART** → generates an initial crystalline charge density by a superposition of atomic densities, generated by **LSTART**.
Self-consistent field (SCF) set

\textbf{LAPW0} → computes the total potential \( V_{\text{tot}} \) as a sum of the Coulomb potential \( V_C \) (Harree) and exchange-correlation potential \( V_{xc} \) using the total electron density as an input. It generates the spherical part \( (l = 0) \) of \( V_{\text{tot}} \) and the non-spherical part as separate files. \( V_C \) is calculated by a multipolar Fourier expansion. \( V_{xc} \) is computed numerically on a grid.

\textbf{LAPW1} → sets up the Hamiltonian and overlap matrices and finds the diagonalization eigenvalues and eigenvectors.

\textbf{LAPW2} → computes the Fermi energy and expands the charge density \( \rho(\vec{r}) \) according to

\[
\rho(\vec{r}) = \begin{cases} 
\sum_{LM} \rho_{LM}(r) Y_{LM}(\hat{r}), & \text{inside sphere}, \\
\sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}, & \text{outside sphere},
\end{cases}
\]

for each occupied state and each occupied \( k \)-vector.

\textbf{LCORE} → computes the core states (relativistically or non-relativistically) for the current spherical part of the potential. It yields core eigenvalues with the corresponding core densities and core contributions to the atomic forces.

\textbf{MIXER} → adds electron densities of the core, semi-core and valence states to yield the new total density. As we commented at the beginning of the course, simply taking this composite output density leads to instabilities in the iterative SCF process. In order to stabilize the process, one mixes the output density with the old input density to obtain the new density to be used in the next iteration. Two mixing schemes are implemented:

1) the straight mixing as proposed by Pratt (1952), with mixing factor \( Q \),

\[
\rho_{\text{new}}(r) = (1 - Q) \rho_{\text{old}}(r) + Q \rho_{\text{output}}(r);
\]

2) the Broyden mixing scheme (Singh et al., 1986), in which all expansion coefficients of the density from several preceding iterations are utilized to calculate an optimal mixing fraction for each coefficient in each iteration.