Notes about the expansion of densities and potentials in the APW methods

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In WIEN2k, several functions $f(\boldsymbol{r})$ are expanded in spherical harmonics inside the spheres and in Fourier series in the interstitial region. These functions are listed below along with the name of the file where it is written and the WIEN2k module generating it.

- Valence electron density ρ_{valence} (**case.clmval**, **lapw2**)
- Core electron density ρ_{core} (**case.clmcor**, **lcore**)
- Total electron density ρ (**case.clmsum**, **mixer**)
- Effective Kohn-Sham potential $v_{\text{eff}}^{\text{KS}}$ (**case.vsp/vns**, **lapw0**)
  Remark: The Fourier expansion of $v_{\text{eff}}^{\text{KS}}$ contains the step function
- Coulomb potential v_{Coul} (**case.vcoul**, **lapw0**, for plotting)
- Exchange-correlation v_{xc} (**case.r2v**, **lapw0**, for plotting)
- Part of the kinetic-energy density (**case.vresp/val/cor/sum**, for MGGA functionals)

I. EXPANSION INSIDE THE SPHERES

A. Definition of the complex spherical harmonics

In WIEN2k, the complex spherical harmonics $Y_{\ell m}$ are defined with the Condon-Shortley convention:

$$Y_{\ell m}(\theta,\varphi) = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} P_{\ell m}(\cos\theta)e^{im\varphi} \tag{1}$$

where θ ($\in [0,\pi]$) and ϕ ($\in [0,2\pi)$) are the polar and azimuthal angles of the spherical coordinate system and $P_{\ell m}$ are the associated Legendre polynomials. The $Y_{\ell m}$ are calculated by the subroutine **ylm.f** in WIEN2k.

B. Non-cubic case

If the point group of an atom is non-cubic, i.e., negative atom index in **case.struct**, then a function $f(\boldsymbol{r})$ (density, potential, etc.) is expanded as

$$f(\boldsymbol{r}) = \sum_{\ell mp} f_{\ell mp}(r) Z_{\ell mp}(\theta, \varphi) \tag{2}$$

where $Z_{\ell mp}$ are real spherical harmonics[1]:

$$Z_{\ell 0}(\theta, \varphi) = Y_{\ell 0}(\theta, \varphi) \tag{3}$$

$$Z_{\ell m+}(\theta, \varphi) = \frac{(-1)^m}{\sqrt{2}} \left(Y_{\ell m}(\theta, \varphi) + Y^*_{\ell m}(\theta, \varphi) \right) \tag{4}$$

$$Z_{\ell m-}(\theta, \varphi) = \frac{(-1)^m}{i\sqrt{2}} \left(Y_{\ell m}(\theta, \varphi) - Y^*_{\ell m}(\theta, \varphi) \right) \tag{5}$$

and $f_{\ell mp}$ are the radial functions which are written in the files **case.clmsum**, etc. (see Sec. 4.2 of the user's guide for details). The list of non-zero (ℓ, m, p)-terms in Eq. (2) (shown in **case.in2**) depends on the point group symmetry (indicated in **case.outputs**). By default, the sum in Eq. (2) is truncated at $\ell_{\max} = 6$ and Table 7.51 in the user's guide provides the list of all (ℓ, m, p) in case the user wants to increase $\ell_{\max}$ to a larger value by adding additional terms in **case.in2**.

C. Cubic case

In the case of an atom with a cubic point group symmetry (positive atom index in **case.struct**), the expansion of a function $f(\boldsymbol{r})$ is given by

$$f(\boldsymbol{r}) = \sum_{\ell j} f_{\ell j}(r) K_{\ell j}(\theta, \varphi) \tag{6}$$

where $K_{\ell j}$ are the cubic harmonics[1] which are linear combinations of real spherical harmonics,

$$K_{\ell j}(\theta, \varphi) = \sum_{mp} k_{\ell jmp} Z_{\ell mp}(\theta, \varphi) \tag{7}$$

and the radial functions $f_{\ell j}$ are also linear combinations of the $f_{\ell mp}$ radial functions:

$$f_{\ell j}(r) = \sum_{mp} k_{\ell jmp} f_{\ell mp}(r) \tag{8}$$

TABLE I. Coefficients $k_{\ell jmp}$ in Eqs. (7) and (8).

$\ell j\backslash mp$	0	2+	2−	4+	4−	6+	6−	8+	8−	10+
0 1	1									
3 1			1							
4 1	$\frac{1}{2}\sqrt{\frac{7}{3}}$			$\frac{1}{2}\sqrt{\frac{5}{3}}$						
6 1	$\frac{1}{2}\sqrt{\frac{1}{2}}$			$-\frac{1}{2}\sqrt{\frac{7}{2}}$						
6 2		$\frac{1}{4}\sqrt{11}$				$-\frac{1}{4}\sqrt{5}$				
7 1			$\frac{1}{2}\sqrt{\frac{13}{6}}$				$\frac{1}{2}\sqrt{\frac{11}{6}}$			
8 1	$\frac{1}{8}\sqrt{33}$			$\frac{1}{4}\sqrt{\frac{7}{3}}$				$\frac{1}{8}\sqrt{\frac{65}{3}}$		
9 1			$\frac{1}{4}\sqrt{3}$				$-\frac{1}{4}\sqrt{13}$			
9 2					$\frac{1}{2}\sqrt{\frac{17}{6}}$				$-\frac{1}{2}\sqrt{\frac{7}{6}}$	
10 1	$\frac{1}{8}\sqrt{\frac{65}{6}}$			$-\frac{1}{4}\sqrt{\frac{11}{2}}$				$-\frac{1}{8}\sqrt{\frac{187}{6}}$		
10 2		$\frac{1}{8}\sqrt{\frac{247}{6}}$				$\frac{1}{16}\sqrt{\frac{19}{3}}$				$-\frac{1}{16}\sqrt{85}$

The coefficients $k_{\ell jmp}$ in Eqs. (7) and (8) are given in Table I C. Table 7.50 of the user's guide lists the non-zero (ℓ, m, p)-terms up to $\ell = 10$. Note that these are the radial functions $f_{\ell mp}$ (and not the $f_{\ell j}$) that are written in **case.clmsum**, etc.

In the WIEN2k source code, the coefficients $k_{\ell jmp}$ are stored in the array c_kub and the subroutine **cbcomb.f** makes the transformation beteween the $f_{\ell j}$ and $f_{\ell mp}$ functions.

II. EXPANSION IN THE INTERSTITIAL

A. Fourier series

In the interstitial region, a function f is expanded in Fourier series

$$f(\boldsymbol{r}) = \sum_{n=1}^{\infty} f_{\boldsymbol{G}_n} e^{i\boldsymbol{G}_n\boldsymbol{r}} \tag{9}$$

where $f_{\boldsymbol{G}_n}$ are the Fourier coefficients

$$f_{\boldsymbol{G}_n} = \frac{1}{V_{\text{cell}}} \int\limits_{\text{cell}} f(\boldsymbol{r}) e^{-i\boldsymbol{G}_n\boldsymbol{r}} d^3r \tag{10}$$

In practice, Eqs. (9) and (10) are calculated using fast Fourier transform (FFT):

$$f(\boldsymbol{r}_m) = \sum_{n=1}^{N_{\boldsymbol{G}}} f_{\boldsymbol{G}_n} e^{i\boldsymbol{G}_n \boldsymbol{r}_m} \tag{11}$$

$$f_{\boldsymbol{G}_n} = \frac{1}{V_{\text{cell}} N_{\text{FFT}}} \sum_{m=1}^{N_{\text{FFT}}} f(\boldsymbol{r}_m) e^{-i\boldsymbol{G}_n \boldsymbol{r}_m} \tag{12}$$

where $N_{\boldsymbol{G}}$ is the number of reciprocal lattice vectors such that $|\boldsymbol{G}_n| < G_{\text{max}}$ (specified in **case.in2**) and N_{FFT}, which depends on G_{max} and is multiplied by the FFT-factor in **case.in0**, is the size of the FFT arrays. In the WIEN2k source code, the FFTs are done with the statement **call c3fft**.

B. Symmetrization of plane-waves

Symmetry allows to reduce the number of stored Fourier coefficients by expanding the function f in symmetrized plane-waves:

$$f(\boldsymbol{r}) = \sum_{n=1}^{N_{\boldsymbol{G}}} f_{\boldsymbol{G}_n} e^{i\boldsymbol{G}_n \boldsymbol{r}} = \sum_{s=1}^{N_s} f_s \Phi_s(\boldsymbol{r}) \tag{13}$$

where Φ_s are the N_s ($\leqslant N_{\boldsymbol{G}}$) symmetrized plane-waves (stars) that are constructed by applying all N_{op} symmetry operations $(\boldsymbol{R}_o, \boldsymbol{t}_o)$ (those in **case.struct**) to a plane-wave:

$$\Phi_s(\boldsymbol{r}) = \frac{1}{N_{\text{op}}} \sum_{o=1}^{N_{op}} e^{i\boldsymbol{G}_{s,1}(\boldsymbol{R}_o \boldsymbol{r} + \boldsymbol{t}_o)} = \frac{1}{m_s} \sum_{n=1}^{m_s} \frac{m_s}{N_{\text{op}}} \sum_{o=1}^{N_{\text{op}}/m_s} e^{i\boldsymbol{G}_{s,1} \boldsymbol{t}_{n,o}} e^{i\boldsymbol{G}_{s,n} \boldsymbol{r}} \tag{14}$$

The coefficients f_s of the Stars are

$$f_s = \sum_{n=1}^{m_s} f_{\boldsymbol{G}_{s,n}} \frac{m_s}{N_{\text{op}}} \sum_{o=1}^{N_{\text{op}}/m_s} e^{-i\boldsymbol{G}_{s,1} \boldsymbol{t}_{n,o}} \tag{15}$$

Note that Eqs. (14) and (15) differ from those in Ref. 2 due to different ways the symmetry operations are applied. In the files **case.clmsum**, etc., N_s is written next to “NUMBER OF PW”. In the WIEN2k source code, the symmetrization of the plane-waves and coefficients is handled by the subroutines **stern.f**, **getfft.f** and **setfft.f**.

[1] M. Kara and K. Kurki-Suonio, Acta Cryst. **A37**, 201 (1981).

[2] D. J. Singh and L. Nordström, *Planewaves, Pseudopotentials and the LAPW Method*, 2nd ed. (Springer, Berlin, 2006).