Notes on pdos weight factors for PAW based on charge in augmentation sphere
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The general formula for PDOS is

$$N^a(E) = 2\sum_n \int d^3k\ \delta(E - E_n(\mathbf{k}))\ Q^a_{n\mathbf{k}}, \tag{1}$$

where 2 accounts for the spin degenercy, n denotes band index, and in our case we generally take the weighting factor $Q^a_{n\mathbf{k}}$ to be the charge of atom a within its augmentation sphere for the state $n\mathbf{k}$. In order to evaluate $Q^a_{n\mathbf{k}}$ within *PWscf*, we need the following considerations. For a particular band $|\Psi_{n\mathbf{k}}\rangle$, the full electron density is

$$|\Psi_{n\mathbf{k}}(\mathbf{r})|^2 = \left|\widetilde{\Psi}_{n\mathbf{k}}(\mathbf{r})\right|^2 + \sum_{aij} \langle\widetilde{\Psi}_{n\mathbf{k}}|p^a_{n_il_im_i}\rangle\langle p^a_{n_jl_jm_j}|\widetilde{\Psi}_{n\mathbf{k}}\rangle Y^*_{l_im_i}(\hat{\mathbf{r}})Y_{l_jm_j}(\hat{\mathbf{r}})\left(\varphi_{n_il_i}(r)\varphi_{n_jl_j}(r) - \widetilde{\varphi}_{n_il_i}(r)\widetilde{\varphi}_{n_jl_j}(r)\right). \tag{2}$$

Here $p^a_{n_il_im_i}(\mathbf{r})$ denote the projector functions while $\varphi_{n_il_i}(r)$ and $\widetilde{\varphi}_{n_il_i}(r)$ denote the radial atomic basis functions for atom a.

If we assume that the atomic pseudobasis functions are complete enough to represent the full wave function $\Psi_{n\mathbf{k}}(\mathbf{r})$ within the augmentation spheres, it is reasonable to assume that we can represent the full electron density for the state $n\mathbf{k}$ within those spheres as

$$|\Psi_{n\mathbf{k}}(\mathbf{r})|^2 \approx \sum_{aij} \langle\widetilde{\Psi}_{n\mathbf{k}}|p^a_{n_il_im_i}\rangle\langle p^a_{n_jl_jm_j}|\widetilde{\Psi}_{n\mathbf{k}}\rangle Y^*_{l_im_i}(\hat{\mathbf{r}})Y_{l_jm_j}(\hat{\mathbf{r}})\varphi_{n_il_i}(r)\varphi_{n_jl_j}(r) \quad \text{for} \quad r \le r^a_c. \tag{3}$$

In fact, we want to approximate the charge within each sphere which can be determined by performing the integral of the above expression within the augmentation sphere:

$$Q^a_{n\mathbf{k}} \approx \sum_{ij} \langle\widetilde{\Psi}_{n\mathbf{k}}|p^a_{n_il_im_i}\rangle\langle p^a_{n_jl_im_i}|\widetilde{\Psi}_{n\mathbf{k}}\rangle q^a_{n_il_i;n_jl_i}\delta_{l_il_j}. \tag{4}$$

Here we have defined

$$q^a_{n_il_i;n_jl_i} \equiv \int_0^{r^a_c} dr\ \varphi_{n_il_i}(r)\varphi_{n_jl_j}(r). \tag{5}$$

In order to put this in a form convenient for the projwfc.f90 program in quantum-espresso we can define the following decomposition:

$$Q^a_{n\mathbf{k}} \approx \sum_{n_il_im_i}\sum_{n_j} \langle\widetilde{\Psi}_{n\mathbf{k}}|p^a_{n_il_im_i}\rangle\langle p^a_{n_jl_im_i}|\widetilde{\Psi}_{n\mathbf{k}}\rangle q^a_{n_il_i;n_jl_i}\delta_{l_il_j}. \tag{6}$$

Or:

$$Q^a_{n\mathbf{k}} \approx \sum_{n_il_im_i} L^a_{n_il_im_i} \quad \text{with} \quad L^a_{n_il_im_i} \equiv \langle\widetilde{\Psi}_{n\mathbf{k}}|p^a_{n_il_im_i}\rangle \sum_{n_j} \delta_{l_il_j}\langle p^a_{n_jl_im_i}|\widetilde{\Psi}_{n\mathbf{k}}\rangle q^a_{n_il_i;n_jl_i}. \tag{7}$$

So the factors $L^a_{n_il_im_i}$ can be used as the ldos factors that are outputted in the original projwfc.f90 program.

Some details for the implementation in the 5.1 QE distribution are as follows.

- The two altered files are `projwfc.f90` ⇒ `projec_paw.f90` and `partialdos.f90` ⇒ `partialdos_paw.f90`.
- $q^a_{n_i l_i; n_j l_i}$ is calculated in the subroutine `projwave_paw` and stored in the temporary array pcharge(i,j,nt).
- The "difficulty" of the programming was that the projector functions $|p^a_{n_i l_i m_i}\rangle$ which are calculated in the subroutine `init_us_2` are stored in a particular order (thanks to Lorenzo Paulatto for pointing this out). Consequently, the nlmchi structure had to be changed accordingly (and hopefully correctly).
- the $L^a_{n_i l_i m_i}$ factors are stored in the array proj(nwfc,ibnd,ik) which are then used by the the subroutine `partialdos_paw.f90`.
- The subroutine `partialdos_paw.f90` had to be changed only in that the nlmchi datastructure has nkb elements

In principle, this implementation should give results very similar to those of abinit using the options prtdos 3 and pawprtdos 2.