NOTE: THIS PAGE UNDER CONSTRUCTION

Basis-set related quantities, general definitions

- $\vec{v}$: "Sample values of physical field $v(r)$ " - values of field at sample points r_p, $[\vec{v}]_p \equiv v_p \equiv v(r_p)$
- $\hat{\vec{v}}$: "Expansion coefficients for field $v(r) = \sum_\alpha \hat{v}_\alpha \; b_\alpha(r)$ - $[\hat{\vec{v}}]_\alpha = \hat{v}_\alpha$
- O: "Overlap operator" - overlaps of basis functions $\mathcal{O}_{\beta\alpha} \equiv \int d^3r \; b^*_\beta(r) b_\alpha(r)$
- L: "Laplacian operator" - matrix elements in the basis set of the Lapacian operator $L_{\beta\alpha} \equiv \int d^3r \;\; b^*_\beta(r) \nabla^2 b_\alpha(r)$
- I: "Forward transform" - transforms from expansion coefficient representation to real space sample representation $I_{p\alpha} \equiv b_\alpha(r_p)$
- Idag: "Dual forward transform" - $Idag \equiv I^\dagger$
- J: "Inverse transform" - transforms from real space sample representation to expansion coefficient representation - $J = I^{-1}$
- Jdag: "Dual inverse transform" - $Jdag \equiv J^\dagger = I^{-\dagger}$

Basis-set related quantities, plane wave basis

For periodic boundary conditions with lattice vectors $R \equiv [\vec{R}_0, \vec{R}_1, \vec{R}_2]$ on a grid of dimensions $\vec{S} = [S_0; S_1; S_2]$, final quantities will be on per unit cell ...

- $O = (\det R) \cdot 1$
- $L \;=\; (-\det R) Diag \;\; [|\vec{G}_0|^2; \; |\vec{G}_1|^2; \; |\vec{G}_2|^2 \ldots]$
- $I = F$, where F is the standard kernel for the discrete (fast) Fourier transform with a positive sign in the exponent. Note the following facts about this standard kernel: $F^T = F$, $F^\dagger = F^*$, $F^* F = prod \; \vec{S}$, $F^{-1} = \frac{1}{prod \; \vec{S}} F^*$, where F^* is just the standard kernel with a negative sign in the exponent.
- $I^\dagger = F^*$
- $J = \frac{1}{prod \; \vec{S}} F^*$
- $J^\dagger = \frac{1}{prod \; \vec{S}} F$

Physical quantities in density-functional theory

- $\hat{C}$: "Expansion coefficients for orthonormal wave functions" - $\psi_i(r) = \sum_\alpha \hat{C}_{\alpha i} \;\; b_\alpha(r)$
- $\hat{P}$: "Basis representation of density matrix" - $\hat{P} = f \hat{C} \hat{C}^\dagger$
- P : "Density matrix" - $P_{pq} = \rho(r_p, r_q)$, $P = I \hat{P} I^\dagger$
- $\vec{n}$: "Sample values of electron density" - $\vec{n} = diag \; P$
- $\vec{\varphi}$: "Mean field (Hartree) potential from electrons" - $\vec{\varphi} = (-4\pi) I L^{-1} O J \vec{n}$
- $\hat{W}$: "Expansion coefficients for unconstrained wave functions" - $\hat{C} = \hat{W} U^{-1/2}$
- U : "Overlaps between (unconstrained) wave functions - $U_{ij} = < W_i(r) | W_j(r) >$
- $E(\hat{W})$: "DFT energy functional" - $E(\hat{W}) = -\frac{1}{2} \triangle L \hat{P} + \vec{n}^\dagger J^\dagger O J \vec{V}_{nuc} + \frac{1}{2} \vec{n}^\dagger J^\dagger O J \vec{n} + \vec{n}^\dagger J^\dagger O J \varepsilon_{xc}(\vec{n})$