

Matrix elements of non-local pseudopotentials

Semilocal form:

$$\hat{V}^\mu = V_\mu(r) + \sum_l V_{\mu,l}(r) \hat{P}_l \quad (35)$$

where $\hat{P}_l = |l><l|$ is the projector on angular momentum l . Using the expansion of plane waves into spherical harmonics Y_{lm} and spherical Bessel functions j_l :

$$e^{-i\mathbf{k}\cdot\mathbf{r}} = (2l+1) \sum_l i^l j_l(kr) P_l(\mathbf{k} \cdot \mathbf{r}) = 4\pi \sum_l i^l j_l(kr) \sum_m Y_{lm}^*(\mathbf{k}) Y_{lm}(\mathbf{r}) \quad (36)$$

one gets

$$V_{\mu,l}(\mathbf{k}_1, \mathbf{k}_2) = \frac{1}{\Omega} \int e^{-i\mathbf{k}_1 \cdot \mathbf{r}} V_{\mu,l}(\mathbf{r}) \hat{P}_l e^{i\mathbf{k}_2 \cdot \mathbf{r}} d\mathbf{r} = \frac{4\pi}{\Omega} (2l+1) P_l(\mathbf{k}_1 \cdot \mathbf{k}_2) \int_0^\infty r^2 j_l(k_1 r) j_l(k_2 r) V_{\mu,l}(r) dr = \frac{4\pi}{\Omega} (2l+1) P_l(\mathbf{k}_1 \cdot \mathbf{k}_2) F_l^\mu(k_1, k_2) \quad (37)$$

where the P_l are Lagrange polynomials. Using Bachelet-Hamann-Schlüter parameterization:

$$\hat{V}^\mu(\mathbf{r}) = -\frac{Z_\mu e^2}{r} \sum_{n=1}^{n_c} c_n^\mu \operatorname{erf}(\sqrt{\alpha_n^\mu} r) + \sum_{l=0}^{\hat{l}} \sum_{n=1}^{n_l} \left(A_{n,l}^\mu + A_{n+3,l}^\mu r^2 \right) e^{-\alpha_{n,l}^\mu r^2} \hat{P}_l \quad (38)$$

where $n_c = 2, n_l = 3$, the $F_l^\mu(k_1, k_2)$ have an analytical expression. For the α_μ one finds

$$\alpha_\mu = \int d\mathbf{r} \left(V_{loc}(r) + \frac{Z_\mu e^2}{r} \right) = 4\pi Z_\mu e^2 \int r^2 dr \left(\frac{-c_1 \operatorname{erf}(\sqrt{\alpha_1} r) - (1-c_1) \operatorname{erf}(\sqrt{\alpha_2} r)}{r} - \frac{1}{r} \right) = 4\pi Z_\mu e^2 \left(\frac{c_1}{4\alpha_1} + \frac{1-c_1}{4\alpha_2} \right). \quad (39)$$

Separable form:

$$\hat{V}^\mu = V_\mu(r) + \sum_l \frac{1}{v_l} f_{\mu,l}(r) f_{\mu,l}^*(r'). \quad (40)$$

For simplicity, we consider just one term per value of l . Using the same expansion as above one finds

$$V_{\mu,l}(\mathbf{k}_1, \mathbf{k}_2) = \frac{1}{\Omega} \frac{1}{v_l} \int e^{-i\mathbf{k}_1 \cdot \mathbf{r}} f_{\mu,l}(\mathbf{r}) d\mathbf{r} \int e^{i\mathbf{k}_2 \cdot \mathbf{r}'} f_{\mu,l}^*(\mathbf{r}') d\mathbf{r}' = \frac{4\pi}{\Omega} \frac{1}{v_l} \sum_{m=-l}^l \int r^2 j_l(k_1 r) f_{\mu,l}(\mathbf{r})(r) dr Y_{lm}(\hat{\mathbf{k}}_1) \int r^2 j_l(k_2 r) f_{\mu,l}^*(\mathbf{r})(r) dr Y_{lm}^*(\hat{\mathbf{k}}_2). \quad (41)$$

The angular term could be summed to yield Lagrange polynomials, but it is much more convenient to keep the “separated” form in Fourier space for computational purposes.