inside muffin-tin:

$$\cancel{\psi = \sum_L A_L i^l j_l(kr) Y_L(\Omega)}$$

$$\psi = \sum_L A_L R_L(kr) Y_L(\Omega)$$

R_L is solution to radial S.E.

postulate $A_L = B_L$

OUTSIDE MUFFIN-TIN

$$\psi = \sum_L B_L\left[e^{2i\delta_l} h_l^{(1)}(kr) + h_l^{(2)}(kr)\right] Y_L(\Omega)$$

$$= \sum_L \cancel{B_l}\, \phi_L Y_L(\Omega) \qquad \phi_L = B_L\left[e^{2i\delta_l} h_l^{(1)} + h_l^{(2)}\right]$$

divide ϕ_L into scattered & unscattered waves:

$$\phi_L = \phi_L^{(0)} + \phi_L^{(s)}$$

$$\phi_L^{(s)} = B_L\left[e^{2i\delta_l} - 1\right] h_l^{(1)}$$

$$\phi_L^{(0)} = 2B_L j_l = B_L\left[h_l^{(1)} + h_l^{(2)}\right]$$

To find the w.f. for the ion core, the incoming wave must be decomposed into spherical waves centered on the ion core

$$\psi = \sum_L \left(\phi_L^{(0)} + \phi_L^{(s)} \right) Y_L(\Omega)$$

unscattered part is $\psi^{(0)} = \sum_L 2 \beta_L j_\ell(kr) Y_L(\Omega)$

compare to expansion $\sum_L \alpha_L i^\ell j_\ell(kr) Y_L(\Omega)$

where the α_L are the coefficients of the expansion

$$\int dk \sum_L |k L R_a\rangle \langle k L R_a | \psi\rangle$$

$$= \int dk \sum_L \alpha_L |k L R_a\rangle$$

which in coordinate representation is:

$$\sum_L \alpha_L \langle r | k L R_a\rangle$$

$$= \sum_L \alpha_L \sqrt{\frac{2k^2}{\pi}}\, i^\ell j_\ell Y_L(\Omega)$$

$$= \sum_L 2 \beta_L j_\ell Y_L(\Omega)$$

so $\beta_L = \frac{1}{2} \alpha_L \sqrt{\frac{2k^2}{\pi}}\, i^\ell$

$$= i^\ell \alpha_L \sqrt{\frac{k^2}{2\pi}} = \frac{1}{\sqrt{2\pi}} i^\ell k \alpha_L$$

so knowing the α_j, we know the βs..

integrated charge over the muffin-tin sphere is:

$$q = \sum_L |\beta_L|^2 \int_0^{R_{MT}} P_\ell^*(r)\, P_\ell(r)\, dr$$

where P_ℓ is the r-multiplied radial WF.

now $q(\theta,\phi) = \sum_L |\beta_L(\theta,\phi)|^2 \underbrace{\int_0^{R_{MT}} P_\ell^*(r) P_\ell(r)\, dr}_{\text{constant w/ } \theta,\phi \,\equiv\, W_\ell}$

$$q(\theta,\phi) = \sum_L |\beta_L(\theta,\phi)|^2 W_\ell$$

$$W_\ell = \int_0^{R_{MT}} P_\ell^*(r)\, P_\ell(r)\, dr$$ weight the relative importance of the β_L.

at high angular momentum, charge is excluded from the muffin-tin core and those component are relatively unimportant for the problem at hand.

$$q(\theta,\phi) = \sum_L \left| (-i)^\ell \alpha_L^* \frac{K}{\sqrt{2\pi}} \cdot (i)^\ell \alpha_L \frac{K}{\sqrt{2\pi}} \right| W_\ell$$

$$= \frac{K^2}{2\pi} \sum_L |\alpha_L|^2 W_\ell$$

$$= \frac{K^2}{2\pi} \sum_L |\alpha_L(\theta,\phi)|^2 W_\ell$$

the W_ℓ are computed as part of the phase shifts, correct?

I can choose normalization such that

$$|C_\ell|^2 \int_0^\infty P_\ell^*(r)\, P_\ell(r)\, dr \to 1$$

$$= |C_\ell|^2 \int_0^{R_{MT}} P_\ell^*(r)\, P_\ell(r)\, dr + |C_\ell|^2 \int_{R_{MT}}^\infty \left[e^{-2i\delta_\ell} h_\ell^{*(1)} + h_\ell^{*(2)}\right]\left[e^{2i\delta_\ell} h_\ell^{(1)} + h_\ell^{(2)}\right] dr$$

$$\int \psi^* \psi\, d\mathbf{r} = \int_0^\infty r^2 dr \int d\Omega \sum_{L'} \beta_{L'}^* R_{L'}^*(kr)\, Y_{L'}^*(\Omega) \sum_L \beta_L R_L(kr)\, Y_L(\Omega)$$

$$= \int_0^\infty r^2 dr \sum_{LL'} \beta_{L'}^* \beta_L R_{L'}^* R_L \underbrace{\int d\Omega\, Y_{L'}^* Y_L}_{\delta_{LL'}}$$

$$= \int_0^\infty r^2 dr \sum_L |\beta_L|^2 R_L^* R_L$$

$$= \sum_L |\beta_L|^2 \left[\int_0^{R_{MT}} P_\ell^*(r)\, P_\ell(r)\, dr + \int_{R_{MT}} r^2 \left[e^{-2i\delta_\ell} h_\ell^{*(1)} + h_\ell^{*(2)}\right]\left[e^{2i\delta_\ell} h_\ell^{(1)} + h_\ell^{(2)}\right] \right.$$

$$= \sum_L |\beta_L|^2 \left[\int_0^{R_{MT}} P_\ell^* P_\ell\, dr + \int_{R_{MT}} r^2 dr \left[h_\ell^{*(1)} h_\ell^{(1)} + e^{2i\delta_\ell} h_\ell^{*(2)} h_\ell^{(1)} + e^{-2i\delta_\ell} h_\ell^{*(1)} h_\ell^{(2)} + h_\ell^{*(2)} h_\ell^{(2)} \right] \right]$$

if I restrict to free spherical waves (potential = 0), the normalization comes out like the basis set norm: $\sqrt{\frac{2k^2}{\pi}}$, <u>which is independent of ℓ.</u>

so that would suggest normalizing to the $B_\ell = 1$ case.

- ie, once δ_ℓ is known, match radial solution to

$$e^{2i\delta_\ell} h_\ell^{(1)} + h_\ell^{(2)} \Big|_{r=R_{MT}}$$

to perhaps a factor of 2 overall

so that determines the W_ℓ, and can be done after calculating the phase shifts.

and $$q(\theta,\phi) \propto \frac{K^2}{2\pi} \sum_L |\alpha_L(\theta,\phi)|^2 |W_L|^2$$

$$\propto \frac{K^2}{2\pi} \sum_L |\langle KL | R_a | \psi \rangle|^2 |W_L|^2$$