According to Ham and Segall [8] – as discussed above – the structure constants $B_{LL'}(\mathbf{k}, z)$ can be written as

$$B_{LL'}(\mathbf{k}, z) = 4\pi \mathrm{i}^{\ell-\ell'} \sum_{L''} \mathrm{i}^{-\ell''} C_{LL'}^{L''} D_{L''}(\mathbf{k}, z) \quad , \tag{15.75}$$

where

$$D_L(\mathbf{k}, z) = D_L^{(1)}(\mathbf{k}, z) + D_L^{(2)}(\mathbf{k}, z) + D_{00}^{(3)}(z)\, \delta_{\ell 0} \delta_{m0} \quad . \tag{15.76}$$

Since $\mathbf{R}$ may be chosen arbitrarily in evaluating the $D_L(\mathbf{k}, z)$, one can also take the limit of $|\mathbf{R}| \to 0$ and obtain

$$\begin{aligned} D_L^{(1)}(\mathbf{k}, z) &= -(4\pi/\Omega)\, \mathrm{i}^{\ell} p^{-\ell} \exp(z/\eta) \\ &\times \sum_{K_n \in \mathcal{L}^{-1}} \frac{|\mathbf{K}_n + \mathbf{k}|^{\ell} \exp\left[-(\mathbf{K}_n + \mathbf{k})^2/\eta\right]}{(\mathbf{K}_n + \mathbf{k})^2 - z} Y_L^*(\widehat{\mathbf{K} + \mathbf{k}}) \quad , \end{aligned} \tag{15.77}$$

$$\begin{aligned} D_L^{(2)}(\mathbf{k}, z) &= \left[(-2)^{\ell+1}/\sqrt{\pi}\right] p^{-\ell} \sum_{\substack{\mathbf{R}_i \in \mathcal{L} \\ (\mathbf{R}_i \neq 0)}} |\mathbf{R}_i|^{\ell} \exp(\mathrm{i}\mathbf{k} \cdot \mathbf{R}_i)\, Y_L^*(\hat{\mathbf{R}}_i) \\ &\times \int_{1/2\sqrt{\eta}}^{\infty} \xi^{2\ell} \exp\left[-\xi^2 \left|\hat{\mathbf{R}}_i\right|^2 + z/4\xi^2\right] \mathrm{d}\xi \quad , \end{aligned} \tag{15.78}$$

$$D_{00}^{(3)}(z) = -\frac{\sqrt{\eta}}{2\pi} \sum_{n=0}^{\infty} \frac{(z/\eta)^n}{(2n-1)\, n!} \quad . \tag{15.79}$$

15.3.2 Three-dimensional structure constants for complex lattices

Suppose there are m atoms per unit cell with corresponding non-primitive translations $\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_m$. The explicit form of the Green function $G_0(\mathbf{r}, \mathbf{r}', z)$ is easily obtained when it is recalled that $\mathbf{r}$ and $\mathbf{r}'$ can be measured either from one and the same origin $\mathbf{a}_i$ or from two different origins $\mathbf{a}_i$ and $\mathbf{a}_j$. $G_0(\mathbf{r}, \mathbf{r}', \epsilon)$ can therefore be viewed as a matrix with respect to the different sublattices involved, i.e. as a matrix in which rows and columns refer to sublattices,

$$\underline{G}_0(\mathbf{r}, \mathbf{r}', \epsilon) = \begin{pmatrix} G_0(\mathbf{r}_i, \mathbf{r}_i', \epsilon) & G_0(\mathbf{r}_i, \mathbf{r}_j', \epsilon) \\ G_0(\mathbf{r}_j, \mathbf{r}_i', \epsilon) & G_0(\mathbf{r}_j, \mathbf{r}_j', \epsilon) \end{pmatrix} \quad , \tag{15.80}$$

for $i, j = 1, ..., m$. Note that contrary to the notation used in (15.80) the subscripts i and j refer to the origins of the sublattices and not to sites in a real space description. The advantage of (15.80) is obvious once angular momentum representations are formed, since a particular element (in momentum representation) is given by [7] as

$$G_0\left(\mathbf{r}_i,\mathbf{r}'_j,z\right) = -\Omega^{-1}\sum_{K_n\in\mathcal{L}^{-1}}\frac{\exp\left[\mathrm{i}\left(\mathbf{K}_n+\mathbf{k}\right)\cdot\left(\mathbf{a}_i-\mathbf{a}_j\right)\right]\exp\left[\mathrm{i}\left(\mathbf{K}_n+\mathbf{k}\right)\cdot\left(\mathbf{r}_i-\mathbf{r}'_i\right)\right]}{\left(\mathbf{K}_n+\mathbf{k}\right)^2-z} \quad , \tag{15.81}$$

where for $i=j: r_i < r^i_{\mathrm{MT}}$ and $i \neq j: \left(r_i+r'_j\right) < |\mathbf{a}_i-\mathbf{a}_j|$ each such element can be transformed into a partial wave representation

$$G_0\left(\mathbf{r}_i,\mathbf{r}'_j,\mathbf{k},z\right) = \mathsf{j}\left(z;\mathbf{r}_i\right)\underline{B}^{ij}\left(\mathbf{k},z\right)\mathsf{j}\left(z;\mathbf{r}'_j\right)^{\times} + \delta_{ij}p\,\mathsf{j}\left(z;\mathbf{r}_{i,<}\right)\mathsf{n}\left(z;\mathbf{r}_{j,>}\right)^{\times} \quad , \tag{15.82}$$

$$\underline{B}^{ij}\left(\mathbf{k},z\right) = \left\{B^{ij}_{LL'}(\mathbf{k},z)\right\} \quad . \tag{15.83}$$

The structure constants $B^{ij}_{LL'}(\mathbf{k},z)$ can again be expressed in coefficients $D^{ij}_L\left(\mathbf{k},z\right)$ in the following way:

$$B^{ij}_{LL'}\left(\mathbf{k},z\right) = 4\pi\mathrm{i}^{\ell-\ell'}\sum_{L''}\mathrm{i}^{-\ell''}C^{L''}_{LL'}D^{ij}_{L''}\left(\mathbf{k},z\right) \quad , \tag{15.84}$$

$$D^{ij}_L\left(\mathbf{k},z\right) = D^{ij,(1)}_L\left(\mathbf{k},z\right) + D^{ij,(2)}_L\left(\mathbf{k},z\right) + \delta_{ij}\delta_{\ell 0}\delta_{m0}D^{(3)}_{00}\left(z\right) \quad , \tag{15.85}$$

with

$$\begin{aligned} D^{ij,(1)}_L\left(\mathbf{k},z\right) &= \left(4\pi/\Omega\right)\mathrm{i}^{\ell}p^{-\ell}\exp\left(z/\eta\right) \\ &\times\sum_{K_n\in\mathcal{L}^{-1}}\left\{\frac{|\mathbf{K}_n+\mathbf{k}|^{\ell}\exp\left[-\left(\mathbf{K}_n+\mathbf{k}\right)^2/\eta\right]}{|\mathbf{K}_n+\mathbf{k}|^2-z}\right. \\ &\left.\times\ \exp\left[\mathrm{i}\left(\mathbf{K}_n+\mathbf{k}\right)\cdot\left(\mathbf{a}_i-\mathbf{a}_j\right)\right]Y^*_L(\widehat{\mathbf{K}_n+\mathbf{k}})\right\} \quad , \end{aligned} \tag{15.86}$$

$$\begin{aligned} D^{ij,(2)}_L\left(\mathbf{k},z\right) = \frac{\left(-2\right)^{\ell+1}}{\sqrt{\pi}}p^{-\ell}\sum_{\substack{\mathbf{R}_s\in\mathcal{L}\\(\mathbf{R}_s\neq 0)}}&\left\{|\mathbf{R}_s-\mathbf{a}_i+\mathbf{a}_j|^{\ell}\right. \\ &\times\exp\left[\mathrm{i}\left(\mathbf{k}\cdot\mathbf{R}_s\right)\right]Y_L(\widehat{\mathbf{R}_s-\mathbf{a}_i+\mathbf{a}_j})^* \\ &\left.\times\int_{\frac{1}{2}\sqrt{\eta}}^{\infty}\xi^{2\ell}\exp\left[-\xi^2\left(\mathbf{R}_s-\mathbf{a}_i+\mathbf{a}_j\right)^2+z/4\xi^2\right]\mathrm{d}\xi\right\} \quad . \end{aligned} \tag{15.87}$$

and $D^{(3)}_{00}\left(z\right)$ being defined in (15.79). As one can see from (15.77)–(15.78) for $i=j$ these equations reduce to the case of a simple lattice. The diagonal blocks in the structure constants refer therefore to a “propagation” within a particular sublattice, whereas the off-diagonal blocks refer to a “propagation” between sublattices.