$$V(1,\mathbf{R}_j) = [1/2\Gamma(1/2)]\sum_j{\sum_k}' Q_{jk}\sum_{\mathbf{d}}|\mathbf{R}_k + \mathbf{X}(\mathbf{d}) - \mathbf{R}_j|^{-1}$$
$$\times \Gamma(1/2, \pi w^2|\mathbf{R}_k + \mathbf{X}(\mathbf{d}) - \mathbf{R}_j|^2)$$
$$+ [1/2\Gamma(1/2)V_{\rm d}^{-1}\pi^{-1/2}\sum_{\mathbf{h}}|\mathbf{H}(\mathbf{h})|^{-2}$$
$$\times \Gamma(1/2, \pi w^{-2}|\mathbf{H}(\mathbf{h})|^2)\sum_j\sum_k Q_{jk}$$
$$\times \exp[2\pi i\mathbf{H}(\mathbf{h})\cdot(\mathbf{R}_k - \mathbf{R}_j)]$$
$$- [1/\Gamma(1/2)]\pi^{1/2}w\sum_j q_j^2,$$

which holds on conditions that the unit cell be electrically neutral and have no dipole moment. If the unit cell has a dipole moment, the limiting value discussed above depends on the direction of **H**. For methods of obtaining the Coulombic lattice sum where the unit cell does have a dipole moment, the reader is referred to the literature (DeWette & Schacher, 1964; Cummins *et al.*, 1976; Bertaut, 1978; Massidda, 1978).

3.4.7. The cases of $n = 2$ and $n = 3$

If $n = 2$ the denominator considered for the limit in the preceding section is linear in $|\mathbf{H}|$ so that only one differentiation is needed to obtain the limit by L'Hospital's method. Since a term of the type $\sum q_j \exp(2\pi i\mathbf{H}\cdot\mathbf{R}_j)$ is always a factor, the requirement that the unit cell have no dipole moment can be relaxed. For $n = 2$ the zero-charge condition is still required: $\sum q_j = 0$. When $n = 3$ the expression becomes determinate and no differentiation is required to obtain a limit. In addition, factoring the Q_{jk} sums into q_j sums is not necessary so that the only remaining requirement for this term to be zero is $\sum\sum Q_{jk} = 0$, which is a further relaxation beyond the requirement of cell neutrality.

3.4.8. Derivation of the accelerated convergence formula *via* the Patterson function

The structure factor with generalized coefficients q_j is defined by

$$F[\mathbf{H}(\mathbf{h})] = \sum_j q_j \exp[2\pi i\mathbf{H}(\mathbf{h})\cdot\mathbf{R}_j].$$

The corresponding Patterson function is defined by

$$P(\mathbf{X}) = V_{\rm d}^{-1}\sum_{\mathbf{h}}|F[\mathbf{H}(\mathbf{h})]|^2\exp[2\pi i\mathbf{H}(\mathbf{h})\cdot\mathbf{X}].$$

The physical interpretation of the Patterson function is that it is nonzero only at the intersite vector points $\mathbf{R}_k + \mathbf{X}(\mathbf{h}) - \mathbf{R}_j$. If the origin point is removed, the lattice sum may be expressed as an integral over the Patterson function. This origin point in the Patterson function corresponds to intersite vectors with $j = k$ and $\mathbf{H}(\mathbf{h}) = 0$:

$$S_n = (1/2V_{\rm d})\int|\mathbf{X}|^{-n}[P(\mathbf{X}) - P(\mathbf{X})\delta(\mathbf{X})]\,{\rm d}\mathbf{X}.$$

Using the incomplete gamma function as a convergence function, this formula expands into two integrals

$$S_n = [1/2V_{\rm d}\Gamma(n/2)]\int|\mathbf{X}|^{-n}$$
$$\times [P(\mathbf{X}) - P(\mathbf{X})\delta(\mathbf{X})]\Gamma(n/2, \pi w^2|\mathbf{X}|^2)\,{\rm d}\mathbf{X}$$
$$+ [1/2V_{\rm d}\Gamma(n/2)]\int|\mathbf{X}|^{-n}$$
$$\times [P(\mathbf{X}) - P(\mathbf{X})\delta(\mathbf{X})]\gamma(n/2, \pi w^2|\mathbf{X}|^2)\,{\rm d}\mathbf{X}.$$

The first integral is shown only for a consistent representation; actually it will be reconverted to a sum and evaluated in direct space. The first part of the second integral will be evaluated with Parseval's theorem and the second part in the limit as $|\mathbf{X}|$ approaches zero:

$$[1/2V_{\rm d}\Gamma(n/2)]\int FT_3[P(\mathbf{X})]$$
$$\times FT_3[|\mathbf{X}|^{-n}\gamma(n/2, \pi w^2|\mathbf{X}|^2)]\,{\rm d}\mathbf{H}$$
$$- \lim_{\mathbf{X}\to 0}[1/2V_{\rm d}\Gamma(n/2)][P(0)|\mathbf{X}|^{-n}\gamma(n/2, \pi w^2|\mathbf{X}|^2)].$$

The first Fourier transform (of the Patterson function) is the set of amplitudes of the structure factors and the second Fourier transform has already been discussed above; the method for obtaining the limit (for n equal to or greater than 1) was also discussed above. The result obtained is

$$[1/2V_{\rm d}\Gamma(n/2)]\pi^{n-(3/2)}\int|F[\mathbf{H}(\mathbf{h})]|^2|\mathbf{H}|^{n-3}$$
$$\times \Gamma[(-n/2) + (3/2), \pi w^{-2}|\mathbf{H}|^2]\,{\rm d}\mathbf{H}$$
$$- [1/2V_{\rm d}\Gamma(n/2)]|F(0)|^2 2\pi^{n/2}w^n n^{-1}.$$

The integral can be converted into a sum, since $|F[\mathbf{H}(\mathbf{h})]|$ is nonzero only at the reciprocal-lattice points:

$$[1/2V_{\rm d}\Gamma(n/2)]\pi^{n-(3/2)}\sum_{\mathbf{h}}|F[\mathbf{H}(\mathbf{h})]|^2|\mathbf{H}(\mathbf{h})|^{n-3}$$
$$\times \Gamma[(-n/2) + (3/2), \pi w^{-2}|\mathbf{H}(\mathbf{h})|^2].$$

The term with $\mathbf{H}(\mathbf{h}) = 0$ is evaluated in the limit, for n greater than 3, as

$$[\Gamma(n/2)]^{-1}V_{\rm d}^{-1}\pi^{n/2}w^{n-3}(n-3)^{-1}|F(0)|^2.$$

Since $|F(0)|^2 = \sum\sum q_j q_k$, this term is identical with the third term of $V(n,\mathbf{R}_j)$ as derived earlier. The case of $n = 1$ is handled in the same way as previously discussed, where the limit of this term is zero provided the unit cell has no net charge or dipole moment.

3.4.9. Evaluation of the incomplete gamma function

The incomplete gamma function may be expressed in terms of commonly available functions such as the exponential integral and the complement of the error function. The definition of the exponential integral is

$$E_1(x^2) = \int_{x^2}^{\infty} t^{-1}\exp(-t)\,{\rm d}t = \Gamma(0, x^2).$$

The definition of the complement of the error function is

$$\mathrm{erfc}(x) = \int_x^{\infty}\exp(-t^2)\,{\rm d}t = \pi^{-1/2}\Gamma(1/2, x^2).$$