

4. DIFFUSE SCATTERING AND RELATED TOPICS

1964a,b, 1987), Schulz (1982), Welberry (1985); and a series of interesting papers is collected by Collongues *et al.* (1977).

Many differences are caused by different symbols and by different ‘languages’ used in the various diffraction methods. Quite a few of the new symbols in use are not really necessary, but some are caused by differences in the experimental techniques. For example, the neutron scattering length b may usually be equated with the atomic form factor f in X-ray diffraction. The differential cross section introduced in neutron diffraction represents the intensity scattered into an angular range $d\Omega$ and an energy range dE . The famous scattering law in neutron work corresponds to the square of an (extended) structure factor; the ‘static structure factor’, a term used by neutron diffractionists, is nothing other than the conventional Patterson function. The complicated resolution functions in neutron work correspond to the well known Lorentz factors in X-ray diffraction. These have to be derived in order to include all techniques used in diffuse-scattering work.

4.2.2. Summary of basic scattering theory

Diffuse scattering results from deviations from the identity of translational invariant scattering objects and from long-range correlations in space and time. Fluctuations of scattering amplitudes and/or phase shifts of the scattered wavetrains reduce the maximum capacity of interference (leading to Bragg reflections) and are responsible for the diffuse scattering, *i.e.* scattering parts which are not located in reciprocal space in distinct spots. Unfortunately, the terms ‘coherent’ and ‘incoherent’ scattering used in this context are not uniquely defined in the literature. Since all scattering processes are correlated in space and time, there is no incoherent scattering at all in its strict sense. (A similar relationship exists for ‘elastic’ and ‘inelastic’ scattering. Here pure inelastic scattering would take place if the momentum and the energy were transferred to a single scatterer; on the other hand, an elastic scattering process would demand a uniform exchange of momentum and energy with the whole crystal.) Obviously, both cases are idealized and the truth lies somewhere in between. In spite of this, a great many authors use the term ‘incoherent’ systematically for the diffuse scattering away from the Bragg peaks, even if some diffuse maxima or minima, other than those due to structure factors of molecules or atoms, are observed. Although this definition is unequivocal as such, it is physically incorrect. Other authors use the term ‘coherent’ for Bragg scattering only; all diffuse contributions are then called ‘incoherent’. This definition is clear and unique since it considers space and time, but it does not differentiate between incoherent and inelastic. In the case of neutron scattering both terms are essential and cannot be abandoned.

In neutron diffraction the term ‘incoherent’ scattering is generally used in cases where no correlation between spin orientations or between isotopes of the same element exists. Hence, another definition of ‘incoherence’ is proposed for scattering processes that are uncorrelated in space and time. In fact there may be correlations between the spins *via* their magnetic field, but the correlation length in space (and time) may be very small, such that the scattering process appears to be incoherent. Even in these cases the nuclei contribute to coherent (average structure) and incoherent scattering (diffuse background). Hence, the scattering process cannot really be understood by assuming nuclei which scatter independently. For this reason, it seems to be useful to restrict the term ‘incoherent’ to cases where a random contribution to scattering is realized or, in other words, a continuous function exists in reciprocal space. This corresponds to a δ function in real four-dimensional space. The randomness may be attributed to a nucleus (neutron diffraction) or an atom (molecule). It follows from this definition that the scattering need not be continuous, but

may be modulated by structure factors of molecules. In this sense we shall use the term ‘incoherent’, remembering that it is incorrect from a physical point of view.

As mentioned in Chapter 4.1 the theory of thermal neutron scattering must be treated quantum mechanically. (In principle this is true also in the X-ray case.) In the classical limit, however, the final expressions have a simple physical interpretation. Generally, the quantum-mechanical nature of the scattering function of thermal neutrons is negligible at higher temperatures and in those cases where energy or momentum transfers are not too large. In almost all disorder problems this classical interpretation is sufficient for interpretation of diffuse scattering phenomena. This is not quite true in the case of orientational disorder (plastic crystals) where H atoms are involved.

The basic formulae given below are valid in either the X-ray or the neutron case: the atomic form factor f replaces the coherent scattering length b_{coh} (abbreviated to b). The formulation in the frame of the van Hove correlation function $G(\mathbf{r}, t)$ (classical interpretation, coherent part) corresponds to a treatment by a four-dimensional Patterson function $P(\mathbf{r}, t)$.

The basic equations for the differential cross sections are:

$$\frac{d^2\sigma_{\text{coh}}}{d\Omega d(\hbar\omega)} = N \frac{|\mathbf{k}| \langle b \rangle^2}{|\mathbf{k}_0| 2\pi\hbar} \int_{\mathbf{r}} \int_t G(\mathbf{r}, t) \times \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt \quad (4.2.2.1a)$$

$$\frac{d^2\sigma_{\text{inc}}}{d\Omega d(\hbar\omega)} = N \frac{|\mathbf{k}| \langle b^2 \rangle - \langle b \rangle^2}{|\mathbf{k}_0| 2\pi\hbar} \int_{\mathbf{r}} \int_t G_s(\mathbf{r}, t) \times \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt \quad (4.2.2.1b)$$

(N = number of scattering nuclei of same chemical species; \mathbf{k} , \mathbf{k}_0 = wavevectors after/before scattering).

The integrations over space may be replaced by summations in disordered crystals except for cases where structural elements exhibit a liquid-like behaviour. Then the van Hove correlation functions are:

$$G(\mathbf{r}, t) = \frac{1}{N} \sum_{\mathbf{r}_j, \mathbf{r}_j'} \delta\{\mathbf{r} - [\mathbf{r}_j(t) - \mathbf{r}_j(0)]\} \quad (4.2.2.2a)$$

$$G_s(\mathbf{r}, t) = \frac{1}{N} \sum_{\mathbf{r}_j} \delta\{\mathbf{r} - [\mathbf{r}_j(t) - \mathbf{r}_j(0)]\}. \quad (4.2.2.2b)$$

$G(\mathbf{r}, t)$ gives the probability that if there is an atom j at $\mathbf{r}_j(0)$ at time zero, there is an *arbitrary* atom j' at $\mathbf{r}_j'(t)$ at *arbitrary* time t , while $G_s(\mathbf{r}, t)$ refers to the *same* atom j at $\mathbf{r}_j(t)$ at time t .

Equations (4.2.2.1) may be rewritten by use of the four-dimensional Fourier transforms of G , and G_s , respectively:

$$S_{\text{coh}}(\mathbf{H}, \omega) = \frac{1}{2\pi} \int_{\mathbf{r}} \int_t G(\mathbf{r}, t) \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt \quad (4.2.2.3a)$$

$$S_{\text{inc}}(\mathbf{H}, \omega) = \frac{1}{2\pi} \int_{\mathbf{r}} \int_t G_s(\mathbf{r}, t) \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt \quad (4.2.2.3b)$$

$$\frac{d^2\sigma_{\text{coh}}}{d\Omega d(\hbar\omega)} = N \frac{k}{k_0} \langle b \rangle^2 S_{\text{coh}}(\mathbf{H}, \omega) \quad (4.2.2.4a)$$

$$\frac{d^2\sigma_{\text{inc}}}{d\Omega d(\hbar\omega)} = N \frac{k}{k_0} [\langle b^2 \rangle - \langle b \rangle^2] S_{\text{inc}}(\mathbf{H}, \omega). \quad (4.2.2.4b)$$

Incoherent scattering cross sections [(4.2.2.3b), (4.2.2.4b)] refer to one and the same particle (at different times). In particular, plastic crystals (see Section 4.2.4.5) may be studied by means of this

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incoherent scattering. It should be emphasized, however, that for reasons of intensity only disordered crystals with strong incoherent scatterers can be investigated by this technique. In practice, mostly samples with hydrogen atoms were investigated. This topic will not be treated further in this article (see, *e.g.*, Springer, 1972; Lechner & Riekkel, 1983). The following considerations are restricted to *coherent* scattering only.

Essentially the same formalism as given by equations (4.2.2.1a)–(4.2.2.4a) may be described by the use of a generalized Patterson function, which is more familiar to crystallographers,

$$P(\mathbf{r}, t) = \int_{\mathbf{r}'} \int_{t'=0}^{\tau} \rho(\mathbf{r}', t') \rho(\mathbf{r}' + \mathbf{r}, t' + t) d\mathbf{r}' dt', \quad (4.2.2.5)$$

where τ denotes the time of observation. The only difference between $G(\mathbf{r}, t)$ and $P(\mathbf{r}, t)$ is the inclusion of the scattering weight (f or b) in $P(\mathbf{r}, t)$. $P(\mathbf{r}, t)$ is an extension of the usual spatial Patterson function $P(\mathbf{r})$.

$$\begin{aligned} P(\mathbf{r}, t) &\leftrightarrow 2\pi S(\mathbf{H}, \omega) \equiv |F(\mathbf{H}, \omega)|^2 \\ &= \int_{\mathbf{r}} \int_t P(\mathbf{r}, t) \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt. \end{aligned} \quad (4.2.2.6)$$

One difficulty arises from neglecting the time of observation. Just as $S(\mathbf{H})$ ($\sim |F(\mathbf{H})|^2$) is always proportional to the scattering volume V , in the frame of a kinematical theory or within Born's first approximation [*cf.* equation (4.2.2.1a)], so $S(\mathbf{H}, \omega)$ [$\sim |F(\mathbf{H}, \omega)|^2$] is proportional to volume *and* observation time. Generally one does not make S proportional to V , but one normalizes S to be independent of τ as $\tau \rightarrow \infty$: $2\pi S = (1/\tau)|F|^2$. Averaging over time τ gives therefore

$$\begin{aligned} S(\mathbf{H}, \omega) &= \frac{1}{2\pi} \int_{\mathbf{r}} \int_t \left\langle \int_{\mathbf{r}'} \rho(\mathbf{r}', t') \rho(\mathbf{r}' + \mathbf{r}, t' + t) d\mathbf{r}' \right\rangle_t \\ &\quad \times \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt. \end{aligned} \quad (4.2.2.7)$$

Special cases (see, *e.g.*, Cowley, 1981):

(1) *Pure elastic measurement*

$$\begin{aligned} I_e \sim S(\mathbf{H}, 0) &= \int_{\mathbf{r}} \left[\int_t P(\mathbf{r}, t) dt \right] \exp\{2\pi i\mathbf{H} \cdot \mathbf{r}\} d\mathbf{r} \\ &= \left| \sum_j f_j \langle \exp\{2\pi i\mathbf{H} \cdot \mathbf{r}_j(t)\} \rangle_t \right|^2. \end{aligned} \quad (4.2.2.8)$$

In this type of measurement the time-averaged 'structure' is determined:

$$\langle \rho(\mathbf{r}, t) \rangle_t = \int_{\mathbf{H}} |F(\mathbf{H}, 0)| \exp\{2\pi i\mathbf{H} \cdot \mathbf{r}\} d\mathbf{H}.$$

The projection along the time axis in real (Patterson) space gives a section in Fourier space at $\omega = 0$. True elastic measurement is a domain of neutron scattering. For a determination of the time-averaged structure of a statistically disordered crystal dynamical disorder (phonon scattering) may be separated. For liquids or liquid-like systems this kind of scattering technique is rather ineffective as the time-averaging procedure gives a uniform particle distribution only.

(2) *Integration over frequency (or energy)*

$$\begin{aligned} I_{\text{tot}} \sim \int_{\omega} |F(\mathbf{H}, \omega)|^2 d\omega &= \int_{\omega} \int_{\mathbf{r}} \int_t P(\mathbf{r}, t) \\ &\quad \times \exp\{2\pi i(\mathbf{H} \cdot \mathbf{r} - \nu t)\} d\mathbf{r} dt d\omega \\ &= \int_{\mathbf{r}} P(\mathbf{r}, 0) \exp\{2\pi i\mathbf{H} \cdot \mathbf{r}\} d\mathbf{r} \end{aligned} \quad (4.2.2.9)$$

(*cf.* properties of δ functions). In such an experiment one determines

the Patterson function for $t = 0$, *i.e.* the instantaneous structure ('snapshot' of the correlation function): a projection in Fourier space along the energy axis gives a section in direct (Patterson) space at $t = 0$. An energy integration is automatically performed in a conventional X-ray diffraction experiment ($|\mathbf{k}| \sim |\mathbf{k}_0|$). One should keep in mind that in a real experiment there is, of course, an average over both the sample volume and the time of observation.

In most practical cases averaging over time is equivalent to averaging over space: the total diffracted intensity may be regarded as the sum of intensities from a large number of independent regions due to the limited coherence of a beam. At any time these regions take all possible configurations. Therefore, this sum of intensities is equivalent to the sum of intensities from any one region at different times:

$$\begin{aligned} \langle I_{\text{tot}} \rangle_t &= \left\langle \sum_j \sum_{j'} f_j f_{j'} \exp\{2\pi i\mathbf{H} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})\} \right\rangle_t \\ &= \sum_{j, j'} f_j f_{j'} \langle \exp\{2\pi i\mathbf{H} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})\} \rangle_t. \end{aligned} \quad (4.2.2.9a)$$

From the basic formulae one also derives the well known results of X-ray or neutron scattering by a periodic arrangement of particles in space [*cf.* equation (4.1.3.2) of Chapter 4.1]:

$$\frac{d\sigma}{d\Omega} = N \frac{(2\pi)^3}{V_c} \sum_{\mathbf{h}} |F(\mathbf{H})|^2 \delta(\mathbf{H} - \mathbf{h}) \quad (4.2.2.10)$$

$$F(\mathbf{H}) = \sum_j f_j(\mathbf{H}) \exp\{-W_j\} \exp\{2\pi i\mathbf{H} \cdot \mathbf{r}_j\}. \quad (4.2.2.11)$$

$F(\mathbf{H})$ denotes the Fourier transform of one cell (structure factor); the f_j 's are assumed to be real.

The evaluation of the intensity expressions (4.2.2.6), (4.2.2.8) or (4.2.2.9), (4.2.2.9a) for a disordered crystal must be performed in terms of statistical relationships between scattering factors and/or atomic positions.

From these basic concepts the generally adopted method in a disorder problem is to try to separate the scattering intensity into two parts, namely one part $\langle \rho \rangle$ from an average periodic structure where formulae (4.2.2.10), (4.2.2.11) apply and a second part $\Delta\rho$ resulting from fluctuations from this average (see, *e.g.*, Schwartz & Cohen, 1977). One may write formally:

$$\rho = \langle \rho \rangle + \Delta\rho, \quad (4.2.2.12a)$$

where $\langle \rho \rangle$ is defined to be time independent and periodic in space and $\langle \Delta\rho \rangle = 0$. Because cross terms $\langle \rho \rangle * \Delta\rho$ vanish by definition, the Patterson function is

$$\begin{aligned} [\langle \rho(\mathbf{r}) \rangle + \Delta\rho(\mathbf{r})] * [\langle \rho(-\mathbf{r}) \rangle + \Delta\rho(-\mathbf{r})] \\ = [\langle \rho(\mathbf{r}) \rangle * \langle \rho(-\mathbf{r}) \rangle] + [\Delta\rho(\mathbf{r}) * \Delta\rho(-\mathbf{r})]. \end{aligned} \quad (4.2.2.12b)$$

Fourier transformation gives

$$I \approx |\langle F \rangle|^2 + |\Delta F|^2 \quad (4.2.2.13a)$$

$$|\Delta F|^2 = \langle |F|^2 \rangle - |\langle F \rangle|^2. \quad (4.2.2.13b)$$

Since $\langle \rho \rangle$ is periodic, the first term in (4.2.2.13) describes Bragg scattering where $\langle F \rangle$ plays the normal role of a structure factor of one cell of the averaged structure. The second term corresponds to diffuse scattering. In many cases diffuse interferences are centred exactly at the positions of the Bragg reflections. It is then a serious experimental problem to decide whether the observed intensity distribution is Bragg scattering obscured by crystal-size limitations or other scattering phenomena.

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If disordering is time dependent exclusively, $\langle \rho \rangle$ represents the time average, whereas $\langle F \rangle$ gives the pure elastic scattering part [cf. equation (4.2.2.8)] and ΔF refers to inelastic scattering only.

4.2.3. General treatment

4.2.3.1. Qualitative interpretation of diffuse scattering

Any structure analysis of disordered structures should start with a qualitative interpretation of diffuse scattering. This problem may be facilitated with the aid of Fourier transforms and their algebraic operations (see, e.g., Patterson, 1959). For simplicity the following modified notation is used in this section: functions in real space are represented by small letters, e.g. $a(\mathbf{r})$, $b(\mathbf{r})$, . . . except for $F(\mathbf{r})$ and $P(\mathbf{r})$ which are used as general symbols for a structure and the Patterson function, respectively; functions in reciprocal space are given by capital letters $A(\mathbf{H})$, $B(\mathbf{H})$; \mathbf{r} and \mathbf{H} are general vectors in real and reciprocal space, respectively, $H_x + Ky + Lz$ is the scalar product $\mathbf{H} \cdot \mathbf{r}$; $d\mathbf{r}$ and $d\mathbf{H}$ indicate integrations in three dimensions in real and reciprocal space, respectively. Even for X-rays the electron density $\rho(\mathbf{r})$ will generally be replaced by the scattering potential $a(\mathbf{r})$. Consequently, anomalous contributions to scattering may be included if complex functions $a(\mathbf{r})$ are admitted. In the neutron case $a(\mathbf{r})$ refers to a quasi-potential. Using this notation we obtain the scattered amplitude and phase $A(\mathbf{H}) \exp i\varphi$

$$A(\mathbf{H}) = \int_{\mathbf{r}} a(\mathbf{r}) \exp\{2\pi i \mathbf{H} \cdot \mathbf{r}\} d\mathbf{r} \quad (4.2.3.1a)$$

$$a(\mathbf{r}) = \int_{\mathbf{H}} A(\mathbf{H}) \exp\{-2\pi i \mathbf{H} \cdot \mathbf{r}\} d\mathbf{H} \quad (4.2.3.1b)$$

(constant factors are omitted).

$a(\mathbf{r})$ and $A(\mathbf{H})$ are reversibly and uniquely determined by Fourier transformation. Consequently equations (4.2.3.1) may simply be replaced by $a(\mathbf{r}) \leftrightarrow A(\mathbf{H})$, where the double-headed arrow represents the two integrations given by (4.2.3.1) and means: $A(\mathbf{H})$ is the Fourier transform of $a(\mathbf{r})$, and *vice versa*. The following relations may easily be derived from (4.2.3.1):

$$a(\mathbf{r}) + b(\mathbf{r}) \leftrightarrow A(\mathbf{H}) + B(\mathbf{H}) \quad (\text{law of addition}) \quad (4.2.3.2)$$

$$\beta a(\mathbf{r}) \leftrightarrow \beta A(\mathbf{H}) \quad (\text{law of scalar multiplication}) \quad (4.2.3.3)$$

($\beta =$ scalar quantity).

On the other hand, the multiplication of two functions does not yield a relation of similar symmetrical simplicity:

$$\begin{aligned} a(\mathbf{r})b(\mathbf{r}) &\leftrightarrow \int A(\mathbf{H}')B(\mathbf{H} - \mathbf{H}') d\mathbf{H}' \\ &= A(\mathbf{H}) * B(\mathbf{H}) \end{aligned} \quad (4.2.3.4a)$$

$$\begin{aligned} a(\mathbf{r}) * b(\mathbf{r}) &= \int a(\mathbf{r}')b(\mathbf{r} - \mathbf{r}') d\mathbf{r}' \\ &\leftrightarrow A(\mathbf{H})B(\mathbf{H}) \end{aligned} \quad (4.2.3.4b)$$

(laws of convolution and multiplication).

Since $a(\mathbf{r})b(\mathbf{r}) = b(\mathbf{r})a(\mathbf{r})$:

$$\int A(\mathbf{H}')B(\mathbf{H} - \mathbf{H}') d\mathbf{H}' = \int B(\mathbf{H}')A(\mathbf{H} - \mathbf{H}') d\mathbf{H}'$$

and *vice versa*. The convolution operation is commutative in either space.

For simplicity the symbol $a(\mathbf{r}) * b(\mathbf{r})$ instead of the complete convolution integral is used. The distribution law $a(b + c) = ab + ac$ is valid for the convolution as well:

$$a(\mathbf{r}) * [b(\mathbf{r}) + c(\mathbf{r})] = a(\mathbf{r}) * b(\mathbf{r}) + a(\mathbf{r}) * c(\mathbf{r}). \quad (4.2.3.5)$$

The associative law of multiplication does not hold if mixed products (convolution and multiplication) are used:

$$a(\mathbf{r}) * [b(\mathbf{r})c(\mathbf{r})] \neq [a(\mathbf{r}) * b(\mathbf{r})]c(\mathbf{r}). \quad (4.2.3.6)$$

From equations (4.2.3.1) one has:

$$\begin{aligned} a(\mathbf{r} - \mathbf{r}_0) &\leftrightarrow A(\mathbf{H}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_0) \\ A(\mathbf{H} - \mathbf{H}_0) &\leftrightarrow a(\mathbf{r}) \exp(-2\pi i \mathbf{H}_0 \cdot \mathbf{r}) \end{aligned} \quad (4.2.3.7)$$

(law of displacements).

Since symmetry operations are well known to crystallographers in reciprocal space also, the law of inversion is mentioned here only:

$$a(-\mathbf{r}) \leftrightarrow A(-\mathbf{H}). \quad (4.2.3.8)$$

Consequently, if $a(\mathbf{r}) = a(-\mathbf{r})$, then $A(\mathbf{H}) = A(-\mathbf{H})$. In order to calculate the intensity the complex conjugate $A^+(\mathbf{H})$ is needed:

$$a^+(\mathbf{r}) \leftrightarrow A^+(-\mathbf{H}) \quad (4.2.3.9a)$$

$$a^+(-\mathbf{r}) \leftrightarrow A^+(\mathbf{H}). \quad (4.2.3.9b)$$

Equations (4.2.3.9) yield the relationship $A^+(-\mathbf{H}) = A(\mathbf{H})$ ('Friedel's law') if $a(\mathbf{r})$ is a *real* function. The multiplication of a function with its conjugate is given by:

$$a(\mathbf{r}) * a^+(-\mathbf{r}) \leftrightarrow |A(\mathbf{H})|^2,$$

with

$$a(\mathbf{r}) * a^+(-\mathbf{r}) = \int a(\mathbf{r}')a(\mathbf{r}' - \mathbf{r}) d\mathbf{r}' = P(\mathbf{r}). \quad (4.2.3.10)$$

Note that $P(\mathbf{r}) = P(-\mathbf{r})$ is not valid if $a(\mathbf{r})$ is complex. Consequently $|A(-\mathbf{H})|^2 \neq |A(\mathbf{H})|^2$. This is shown by evaluating $A(-\mathbf{H})A^+(-\mathbf{H})$

$$A(-\mathbf{H})A^+(-\mathbf{H}) \leftrightarrow a(-\mathbf{r}) * a^+(\mathbf{r}) = P(-\mathbf{r}). \quad (4.2.3.11)$$

Equation (4.2.3.11) is very useful for the determination of the contribution of anomalous scattering to diffuse reflections.

Most of the diffuse diffraction phenomena observed may be interpreted qualitatively or even semi-quantitatively in a very simple manner using a limited number of important Fourier transforms, given below.

4.2.3.1.1. Fourier transforms

(1) Normalized Gaussian function

$$(\pi^{3/2} \alpha \beta \gamma)^{-1} \exp\{-(x/\alpha)^2 - (y/\beta)^2 - (z/\gamma)^2\}. \quad (4.2.3.12)$$

This plays an important role in statistics. Its Fourier transform is again a Gaussian:

$$\exp\{-\pi^2(\alpha^2 H^2 + \beta^2 K^2 + \gamma^2 L^2)\}. \quad (4.2.3.12a)$$

The three parameters α , β , γ determine the width of the curve. Small values of α , β , γ represent a broad maximum in reciprocal space but a narrow one in real space, and *vice versa*. The constant has been chosen such that the integral of the Gaussian is unity in real space. The product of two Gaussians in reciprocal space

$$\begin{aligned} &\exp\{-\pi^2(\alpha_1^2 H^2 + \beta_1^2 K^2 + \gamma_1^2 L^2)\} \\ &\times \exp\{-\pi^2(\alpha_2^2 H^2 + \beta_2^2 K^2 + \gamma_2^2 L^2)\} \\ &= \exp\{-\pi^2[(\alpha_1^2 + \alpha_2^2)H^2 + (\beta_1^2 + \beta_2^2)K^2 \\ &\quad + (\gamma_1^2 + \gamma_2^2)L^2]\} \end{aligned} \quad (4.2.3.12b)$$

again represents a Gaussian of the same type, but with a sharper profile. Consequently its Fourier transform given by the convolution of the transforms of the two Gaussians is itself a Gaussian with a broader maximum. It may be concluded from this discussion that the Gaussian with $\alpha, \beta, \gamma \rightarrow 0$ is a δ function in real space, and its Fourier transform is unity in reciprocal space. The convolution of two δ functions is again a δ function.