

4.2. DISORDER DIFFUSE SCATTERING OF X-RAYS AND NEUTRONS

information about the underlying model, which can then be used for a successful interpretation of X-ray and neutron diffuse scattering. Basic aspects of electron diffraction and microscopy in structure determination are treated in Chapter 2.5 of this volume.

There is no comprehensive treatment of all aspects of diffuse scattering. Essential parts are treated in the textbooks by James (1954), Wilson (1962), Wooster (1962), Krivoglaz (1969, 1996*a,b*), Schwartz & Cohen (1977), Billinge & Thorpe (1998), Schweika (1998), Nield & Keen (2001), Fultz & Howe (2002), Frey (2003) and Welberry (2004); handbook articles have been written by Jagodzinski (1963, 1964*a,b*, 1987), Schulz (1982), Welberry (1985) and Moss *et al.* (2003), and a series of relevant papers has been collected by Collongues *et al.* (1977).

Finally, we mention that different symbols and ‘languages’ are 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 ‘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 the techniques used in diffuse-scattering work. In this article we try to preserve the most common symbols. In particular, the scattering vector will be denoted as \mathbf{H} , which is more commonly used in crystallography than $\mathbf{Q} = 2\pi\mathbf{H}$.

4.2.2. Basic scattering theory

4.2.2.1. General

Diffuse scattering results from deviations from the identity of translationally 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 that are not located in distinct spots in reciprocal space. 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, many authors use the term ‘incoherent’ systematically for the diffuse scattering away from the Bragg peaks when all diffuse maxima or minima are due to structure factors of molecules or atoms only. 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 neither can be abandoned.

In neutron diffraction, the term ‘incoherent scattering’ refers to scattering by uncorrelated nuclear spin orientations or by a random distribution of isotopes of the same element. 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 that 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 constant, 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 also true 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 the 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 as 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

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

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

where N is the number of scattering nuclei of same chemical species; \mathbf{k} , \mathbf{k}_0 are the wavevectors after/before scattering and $\omega = 2\pi\nu$.

The integrations over space may be replaced by summations in disordered crystals, except in 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 an *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 using the four-dimensional Fourier transforms of G and G_s , respectively:

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

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

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

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

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 4.2.5.5) may be studied by means of this 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 that contain H atoms have been investigated. This topic will not be treated further in this article (see, e.g., Springer, 1972; Lechner & Riekel, 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 using 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 ρ is the scattering density and 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 $P(\mathbf{r})$. Similarly, S is replaced by another function,

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

which is the Fourier transform of $P(\mathbf{r}, t)$. One difficulty arises from neglecting the time of observation. Just as $S(\mathbf{H}) [\simeq |F(\mathbf{H})|^2]$ is always proportional to the scattering volume V in the framework of kinematical theory or within Born's first approximation [cf. equation (4.2.2.1a)], so $S(\mathbf{H}, \omega) [\simeq |F(\mathbf{H}, \omega)|^2]$ is proportional to volume *and* observation time. In general, one does not make S proportional to τ , 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) are:

(1) *Pure elastic measurement*

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

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. To determine 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 only a uniform particle distribution.

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

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

(cf. the properties of δ functions). In such an experiment, one determines the Patterson function for $t = 0$, i.e. the instantaneous structure (a '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 ($|\mathbf{k}| \simeq |\mathbf{k}_0|$). One should bear 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 the 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 for X-ray or neutron scattering by a periodic arrangement of particles in space [cf. equation (4.1.3.2) of Chapter 4.1]:

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

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

$F(\mathbf{H})$ denotes the Fourier transform of one cell (structure factor); \mathbf{G} is the reciprocal-lattice vector and W is the Debye–Waller factor; the f '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.

4.2.2.2. X-ray and neutron scattering

From these basic scattering formulae some conclusions on the relative merits of X-rays and neutrons can be drawn. Both X-rays and thermal neutrons possess wavelengths of the order of interatomic distances and are thus well suited to the study of the atomic structure of condensed matter. Besides this, there are fundamental differences that make one or the other the radiation of choice for a particular problem or enable them to be used with advantage in a complementary manner. These differences are well documented in a number of textbooks on diffraction and are widely exploited in the determination of average structures. One fundamental difference is related to the interaction with matter: while X-rays are scattered by the electrons, neutrons are scat-

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tered by the atomic nuclei (we are disregarding magnetic interactions in this chapter), *i.e.* X-rays probe the distribution of charges, which (in particular for light atoms) may not coincide with that of the nuclei. This fact forms the basis for the well known X – N technique in the analysis of Bragg intensities. No such studies of disorder diffuse scattering have been performed up to now, but may be a challenge for the future. As a consequence of the different size of the scattering objects, the scattering amplitude falls off with increasing scattering vector $|\mathbf{H}| = (\sin \theta)/\lambda$ for X-rays (the form factor), while it is constant for neutrons. Since for a complete interpretation of diffuse scattering high Q values are generally required, neutrons have their advantages in this respect. The scattering intensity varies as Z^2 (Z = number of electrons) for X-rays and more-or-less erratically for neutrons, for which it also depends on the specific isotope. This imposes problems for X-rays when trying to detect light elements (in particular H and O) in the presence of heavy elements or discriminating neighbouring elements in the periodic table (*e.g.* Al/Si/Mg, Fe/Co/Ni). On the other hand, these differences in scattering power can be used to identify the atomic species taking part in the disorder by comparing the intensity distributions observed with both methods. The contrast can be further enhanced by marking selected atoms by isotope substitution for neutrons or by using anomalous dispersion for X-rays.

In many practical cases, the complementarities of the two methods can be exploited by using them simultaneously. Some illustrative examples can be found in Boysen & Frey (1998).

Another important difference is in the energies given by the dispersion laws $E_x = \hbar ck$ and $E_n = (\hbar^2/2m)k^2$ for X-rays and neutrons, respectively, where c is the velocity of light, m is the neutron mass and $k = 2\pi/\lambda$ is the wavevector. For a typical wavelength, $\lambda = 1.54 \text{ \AA}$ (Cu $K\alpha$) ($k = 4.08 \text{ \AA}^{-1}$), $E_x = 8 \text{ keV}$ and $E_n = 35 \text{ meV}$, *i.e.* the energies differ by almost six orders of magnitude. This means that neutron energies are similar to those of typical collective lattice excitations, which may therefore be determined more easily by neutron spectroscopy. The basic question of whether the underlying disorder is of static or dynamic origin can be answered using neutrons alone, *e.g.* by comparing the ‘integral’ (= elastic + inelastic) scattered intensity (*i.e.* without energy analysis, using a two-axis diffractometer) with the purely elastic intensity by placing an analyser crystal set to zero energy transfer in the diffracted beam (using a triple-axis diffractometer) or using time-of-flight methods. The high energy resolution of Mössbauer radiation can also be used for this purpose. Owing to the very low available intensities, however, this technique has only been applied occasionally. In the elastic mode, diffracted neutron intensities are also usually rather weak. The decision can, however, also be made simply by comparing the positions of the intensity maxima in reciprocal space. This follows from a consideration of the relative changes of the momentum transfer (the wavevector) in the two cases. For example, for an energy change $\Delta E = E_f - E_i$ (the subscripts refer to final and incident energies) of 1 meV, one obtains a change in the scattered wavevector Δk_f of $2 \times 10^{-6} \text{ \AA}^{-1}$ for X-rays and 0.06 \AA^{-1} for neutrons. In a two-axis experiment where the detector does not discriminate energies, *i.e.* without prior knowledge of the real energies, the distribution of diffuse intensities has to be drawn as if the scattering had been elastic ($\Delta E = 0$). In other words, the signal appears at a position displaced by Δk_f . From the estimations above it is clear that only in the neutron case can a measurable effect be expected.

Other specific features of neutrons include their magnetic moment (magnetic scattering is still a domain of neutrons, although progress is now being made with synchrotron radiation) and (nuclear) spin and isotope incoherent scattering processes (which allow the determination of the self-correlation functions). It is possible to separate the spin-incoherent part and distinguish between nuclear and magnetic scattering using polarization analysis. For most elements scattering and absorption is much

weaker for neutrons, allowing larger samples to be analysed and sample environments (furnaces, pressure cells, electric and magnetic fields, special atmospheres *etc.*) to be handled much more easily. Differences in the experimental techniques for X-ray and neutron scattering are discussed in Section 4.2.8.

4.2.3. Qualitative treatment of structural disorder

4.2.3.1. Basic mathematics

Any structure analysis of disordered structures should start with a qualitative interpretation of diffuse scattering. This may be achieved with the aid of Fourier transforms and convolutions. A thorough mathematical treatment of Fourier transforms is given in Chapter 1.3 of this volume; here we give a simple short overview of the practical use of Fourier transforms, convolutions, their algebraic operations and examples of functions which are frequently used in diffraction physics (see, *e.g.*, Patterson, 1959; Jagodzinski, 1987). For simplicity, the following modified notation is used in this section: functions in real space are represented by lower-case letters, *e.g.* $a(\mathbf{r})$, $b(\mathbf{r})$, ... except for $F(\mathbf{r})$ [also, more frequently, denoted as $\rho(\mathbf{r})$] and $P(\mathbf{r})$, which are used as general symbols for a structure and the Patterson function, respectively; functions in reciprocal space are represented by capital letters $A(\mathbf{H})$, $B(\mathbf{H})$; and \mathbf{r} and \mathbf{H} are general vectors in real and reciprocal space, respectively. H , K , L denote continuous variables in reciprocal space; integer values are given by the commonly used symbols h , k , l . $Hx + Ky + Lz$ 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

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

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

(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):

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

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

where β is a scalar quantity.

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

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

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

(the laws of convolution and multiplication).

For simplicity, the complete convolution integral is abbreviated as $a(\mathbf{r}) * b(\mathbf{r})$. 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.