The (Q, ω) Transmission Function of a Triple-Axis Neutron Spectrometer*

By G. Quittner

Institut für Physik, Reaktorzentrum, Seibersdorf, Österreichische Studiengesellschaft für Atomenergie Ges.m.b.H., Lenaugasse 10, A-1082 Wien, Austria

Formulae are given for the counting rate and the transmission function of a triple-axis neutron spectrometer for three-dimensional and two-dimensional momentum transfers starting from the known transmission functions of the monochromating and the analysing part respectively. Some problems of relating these formulae to actual spectrometers and of obtaining the necessary functions and parameters are discussed. The general formulae are then specialized to a model spectrometer with Gaussian collimators and crystals. This results in a system of non-linear equations for a point-by-point calculation of the transmission function. Special care has been taken to keep the formulae absolute, *i.e.* to avoid unknown proportionality factors. This feature allows a detailed treatment especially of the counting rate in relation to resolution and the characteristic features of the sample cross section (liquid, phonon and Bragg-peak type). Two kinds of intensity factors in the counting rate are distinguished: the 'trivial' factors are directly related to the magnitude of the illumination spot in (Q,ω) space and thus to resolution. The other factors are called 'non-trivial'. These two kinds of intensity factors are identified in the formulae. Some considerations are given on the influence of experimental conditions and parameters on each of them.

1. Introduction

The knowledge of the transmission function is useful and necessary for two purposes:

(i) Interpretation of the results of experiments already performed under specific conditions.

(ii) Planning of future experiments and choice of conditions leading to a favourable combination of intensity and resolution. This problem is rather involved in triple-axis spectrometer measurements because of the large number of degrees of freedom given in this instrument.

In § 2 we derive an expression for the (Q, ω) transmission function starting from general (*i.e.* not necessary Gaussian) transmission functions of the monochromating and the analysing part respectively. Formulae are given both for the case of three-dimensional momentum transfers (equations 7 and 8) as well as for the simpler case where only the two components of Q in the spectrometer plane are considered (equations 9 and 10). In § 3 some problems of the practical use of the formulae and of obtaining the necessary functions and/or parameters are discussed. The short § 4 gives the counting rate for the important case of phonon measurements. In § 5 the general formulae (9) and (10) are specialized to Gaussian elements (collimators and crystals) in order to obtain a system of equations useful mainly for application (ii) quoted above. § 6 gives a discussion of the Gaussian-elements formulae including the Gaussian approximation, trivial and

non-trivial intensity factors, the dependence of the counting rate on the type of cross section in the sample (smooth, phonon-like, Bragg peak), a qualitative analysis by inspection of the monochromator and analyser distributions, and the analysis by elements.

Special care has been applied to keep the formulae absolute, *i.e.* to avoid any unknown proportionality factors. Consequently besides giving more weight to application (ii) than to (i) there is more emphasis on intensity (counting rate) than on resolution, the latter being already given a good treatment in other papers. Some derivations are omitted from the main text for the sake of brevity. The interested reader may find the details of these derivations in the seven Appendices of Quittner (1970). One of them gives some checks of the formulae given here, *e.g.* by dimensional analysis.

2. Counting rate and transmission functions for general monochromator and analyser transmissions

We start from the well-known formula for the number of neutrons scattered from a sample with the cross section σ when the incident flux is φ

$$N = \sigma\varphi \text{ neutrons/sec}. \qquad (1)$$

The counting rate (CR) in a triple-axis neutron spectrometer is given by an obvious generalization of (1)

$$CR = \int I(\mathbf{k}_0)\sigma(\mathbf{k}_0,\mathbf{k}_1)R(\mathbf{k}_1)\varepsilon(\bar{k}_1)d\mathbf{k}_0 d\mathbf{k}_1 \qquad (2)$$

where the scalar quantities σ and φ of equation (1) have been replaced by densities over $\mathbf{k}$ vectors – the density $I(\mathbf{k}_0)$ of incoming neutron flux and the differential cross section $\sigma(\mathbf{k}_0,\mathbf{k}_1)$ a density over $\mathbf{k}_1$ vectors.

Moreover, the acceptance function $R(\mathbf{k}_1)\cdot\varepsilon(\bar{k}_1)$ has been added, where $R(\mathbf{k}_1)$ is the transmission probability of the analysing system and $\varepsilon(\bar{k}_1)$ the counting efficiency. [The bar over k means that a k representative of the region of interest (e.g. the nominal value) is taken.]

Another form of equation (2) is

$$\text{CR}=\frac{\varphi_0(\bar{k}_0)}{4\pi}\frac{1}{\bar{k}_0^2}\varepsilon(\bar{k}_1)\int I'(\mathbf{k}_0)\sigma(\mathbf{k}_0,\mathbf{k}_1)R(\mathbf{k}_1)\mathrm{d}\mathbf{k}_0\mathrm{d}\mathbf{k}_1 \quad (3)$$

where $\varphi_0(k)$ is the k density of the neutron source flux and $I'(\mathbf{k}_0)$ is now the transmission probability of the monochromator system. This form containing $\sigma(\mathbf{k}_0,\mathbf{k}_1)$ is not yet adapted to the usual interpretation of inelastic neutron scattering which is based on the formula

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega}=\frac{k_1}{k_0}S(\mathbf{Q},\omega) \quad (4)$$

for the differential cross section (van Hove, 1954).

$$\mathbf{Q}=\mathbf{k}_0-\mathbf{k}_1 \quad (5)$$

is the momentum transfer and

$$E=\hbar\omega=\frac{\hbar^2}{2m}(k_0^2-k_1^2) \quad (6)$$

the energy transfer in the scattering process; $S(\mathbf{Q},\omega)$ is a function depending on the scattering lengths a_{coh}^2 and a_{incoh}^2 as well as on the structure and the atomic thermal motions of the sample.

The experiment is thus interpreted in terms of momentum and energy transfers. Consequently we look for an expression giving the counting rate as an integral over $\mathbf{Q},\omega$, of the $S(\mathbf{Q},\omega)$ characteristic of the sample, multiplied by an instrumental function $F(\mathbf{Q},\omega)$:

$$\text{CR}=\frac{\varphi_0(\bar{k}_0)}{4\pi}\int F(\mathbf{Q},\omega)S(\mathbf{Q},\omega)\mathrm{d}\mathbf{Q}\mathrm{d}\omega. \quad (7)$$

This is possible and $F(\mathbf{Q},\omega)$ is given (Quittner, 1970, Appendix I) by

$$F(\mathbf{Q},\omega)=\frac{\varepsilon(\bar{k}_1)}{(\bar{k}_0)^3\cdot 2Q_0}\int_L I'(\mathbf{k}_0)R(\mathbf{k}_1)\mathrm{d}L(\mathbf{Q},\omega) \quad (8)$$

where the surface L comprises the end points of vectors $\mathbf{k}_0$ and $\mathbf{k}_1$ leading through equations (5) and (6), to a given $\mathbf{Q}$ and ω. Geometrically this is a plane perpendicular to $\mathbf{Q}$, cutting this vector at a distance M from its origin and a distance $-A$ from its end point (see e.g. Bergsma & van Dijk, 1965). (M and A are given in equations (17) and)18) below).

In many cases of practical interest the dependencies of $I(\mathbf{k}_0)$ and $R(\mathbf{k}_1)$ on the vertical components (components perpendicular to the spectrometer plane) can be factored out, resulting in a reduced transmission function $F(Q_x,Q_y,\omega)$ (Quittner, 1970, Appendix II):

$$\text{CR}=\frac{\varphi_0(\mathbf{k}_0)}{4\pi}$$

$$\times \int F(Q_x,Q_y,\omega)S(Q_x,Q_y,Q_z=0,\omega)\mathrm{d}Q_x\mathrm{d}Q_y\mathrm{d}\omega \quad (9)$$

$$F(Q_x,Q_y,\omega)=\frac{\varepsilon(\bar{k}_1)\Delta^2Q_z}{(\bar{k}_0)^3\cdot 2Q_0}$$

$$\times \int_l I'(\mathbf{k}_{0x},\mathbf{k}_{0y})R(\mathbf{k}_{1x},\mathbf{k}_{1y})\mathrm{d}l(Q_x,Q_y,\omega). \quad (10)$$

Q_x is the $\mathbf{Q}$ component, in the spectrometer plane, in the direction of $\mathbf{Q}_0$, the nominal momentum transfer, and Q_y the $\mathbf{Q}$ component perpendicular to $\mathbf{Q}_0$, also in the spectrometer plane. The integral runs now over a line $l(Q_x,Q_y,\omega)$; Δ^2Q_z is given in Appendix I.

Fig. 1 shows the scattering diagram (scattering triangle) for the nominal quantities k_{0M}, k_{0A}, etc. Fig. 2 shows the base line of scattering triangles for a general $\mathbf{Q},\omega$ and two different pairs of $\mathbf{k}_0,\mathbf{k}_1$ leading to the same $\mathbf{Q},\omega$. The end points of such pairs lie on the line $l(Q_x,Q_y,\omega)$.

When evaluating equation (10), the kinematics of inelastic neutron scattering (Figs. 1 and 2) must be taken into account; likewise the transmission probabilities, $I'(\mathbf{k}_0)$ and $R(\mathbf{k}_1)$ must be considered. For this purpose it is convenient to split off the manifold of the $\mathbf{k}_1$ vectors and to transfer it to the left-hand side so that all $\mathbf{k}$ vectors originate from the O point.

This results in the construction of Fig. 3 showing the integration in equation (10) leading to $F(Q_x,Q_y,\omega)$ for a general (Q_x,Q_y,ω).

Essential for the absolute character of the formulae (7), (8), (9) and (10) and of their later applications is the factor $1/2Q_0$, a remnant of a 'Jacobian' of the transformation of a 6-dimensional density over $(\mathbf{k}_0,\mathbf{k}_1)$ in equation (3) to the 4-dimensional density over $(\mathbf{Q},\omega)$ in equations (7) and (8). (See Quittner, 1970, Appendix I.) In many papers only the integral in equation (8)
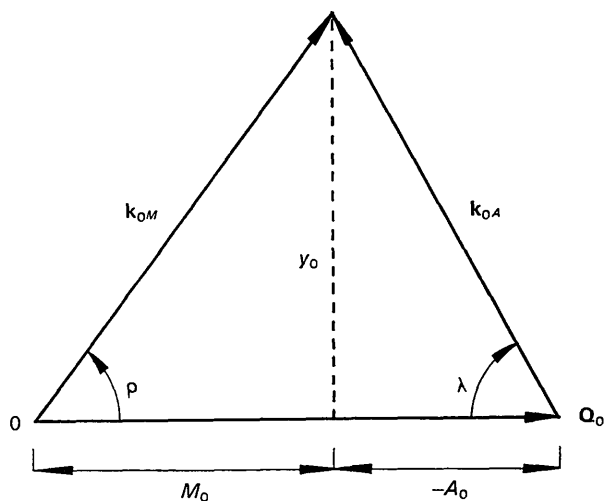

Fig. 1. The basic (nominal) scattering diagram showing the input parameters $k_{0M},k_{0A},S,\lambda,Q_0$ etc. of equations (15) to (25).

or equation (10) is considered, disregarding the slowly varying factor before it. This amounts to considering only the relative shape of the transmission function, which is usually sufficient for problem (i) of the Introduction.

We use the name 'transmission function' to point to its absolute character in contrast to the usual relative (or normalized) 'resolution function'. (A simple example of a transmission function is given by the formula $N = \varphi_0/F_1F_2 . 4\pi r^2$ for a collimating slit. The transmission $F_1F_2 . 4\pi r^2$ relates the number of transmitted neutrons to the source flux density φ_0.) This absolute feature is essential for the interpretation and prediction of both intensity and resolution.

Summarizing we see that the counting rate (CR) of the spectrometer depends on: (a) $\varphi_0(\bar{k}_0)$, the k density of source flux at the mean k value of incoming neutrons; (b) the scattering cross section of the sample (in evaluating equations (7) and (9) it is necessary to use not the scattering cross section per unit cell but this cross section multiplied by the number of elementary cells in the sample); (c) The transmission function $F(\mathbf{Q}, \omega)$ or $F(Q_x, Q_y, \omega)$ with the particular factors as given in equations (8) and (10).
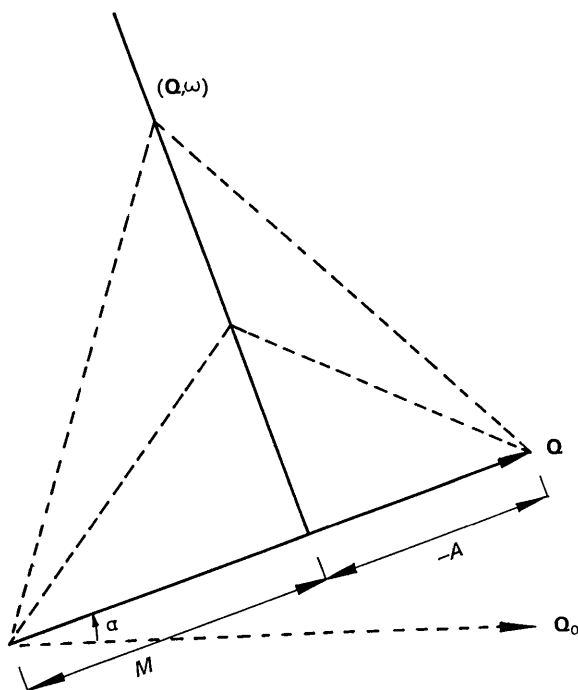

Fig. 2. The manifold of vector pairs $(\mathbf{k}_0, \mathbf{k}_1)$ leading to the same (general) values of $\mathbf{Q}$ and ω by equations (5) and (6). The common base line for such pairs is shown as a full line in the figure: its angle with respect to $\mathbf{Q}_0$ is α, [equation (16)]. M and A are defined in equations (17) and (18). The manifold of these vector pairs is represented in the Figure by two vector pairs (dotted lines). The locus of their end points is the line $l(\mathbf{Q}, \omega)$ (full line) perpendicular to the base line [see equation (10) and the text following it].
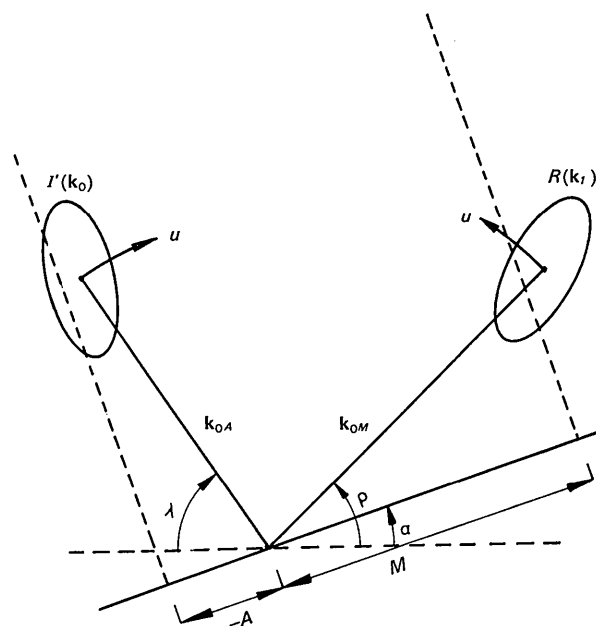
Fig. 3. Integration lines for calculating the integral in equation (10). The manifold of $\mathbf{k}_1$ vectors and the part A of the baseline have been transferred to the left-hand side. All vectors now start from the origin. The ellipses around the end points of k_{0M} and k_{0A} are representative of the distributions $I_0'(\mathbf{k}_0)$ and $R(\mathbf{k}_1)$. The integration line $l(\mathbf{Q}, \omega)$ is now represented by two (dotted) lines, one on each side. The end points of the vector pairs $(\mathbf{k}_0, \mathbf{k}_1)$ are the points on these two lines having the same distance from the base line.

3. Practical problems in the determination of the transmission function

Our formulae (8) and (10) show how the transmission function can be calculated if the two distributions $I'(\mathbf{k}_0)$ and $R(\mathbf{k}_1)$ are known. The transmission function calculated is therefore as good as the input distribution it is based on.

For the interpretation of specific experiments, application (i) of the Introduction, a reliable knowledge of the 'ready' transmission function (in its relative form), is imperative and the question of the contribution of the elements to it is of no importance. Here the method of experimental sampling of the resolution function by a δ-shaped cross section, i.e. by a Bragg reflexion from a single crystal, is applicable. (Some care must be taken in such measurements to safeguard against the influence of phonons. This is important when the resolution function is large and well-focused with respect to some phonon branch.) This method has been developed and widely applied e.g. by the Risø group (Bjerrum-Møller, 1968). We call this approach the empirical one. The approach taken in this paper which may be called the analytical is necessary for the prediction, application (ii) of the Introduction.

The transmission function is calculated from the parameters of the constituent elements; e.g. our formulae (8) and (10) combine the transmission

characteristics of the monochromator and analyser into the overall transmission function. This combination can be done once more at the next level and the characteristics of say the monochromating system derived from the parameters of the two collimators and the monochromating crystals. [See e.g. formula (A III 1) of Quittner (1970)]. To facilitate the calculations it is customary to assume Gaussian elements. [An example of a markedly non-Gaussian element is given by Novell (1969).]

It is a generally held opinion that such a calculation is sufficient for prediction. In applications, however, the question arises as to (a) how the element parameters are to be determined and (b) what is their range of applicability, e.g. over different angles and neutron wavelengths.

Certainly this problem is more difficult with crystals than with collimators. The distribution of mosaic blocks in the crystals is not always known and, even when it is, there is at present no reliable quantitative theory of neutron reflection from real single crystals (Werner, Arrot, King & Hendrick, 1966; Dietrich, 1968).

Another problem is presented by the spatial effects. Our formulae contain angular distributions only and thus suppose that the incoming flux is uniformly distributed over the sample cross section and that the sample is uniformly thick etc., which is not actually the case. These restrictions are, in principle, overcome by dividing the sample into small regions, calculating $I'(k_0)$ and $R(k_1)$ for each region e.g. by the Monte Carlo method (Dietrich, 1968) and adding the resulting counting rates. In practice, such a calculation becomes rather involved and does not seem to have been performed up to now.

There seems to be at present no satisfactory solution to the problems of this section, the main difficulties being the lack of a valid theory of neutron Bragg reflexion from crystals and the difficulties in dealing with spatial effects. However we should mention an interesting investigation (Hamasaki, 1967), where a specific spatial effect (the 'leakage') is taken into account analytically. This paper shows how spatial effects influence the angular distributions. It is also an example of how the purely formal analytical approach can be made more substantial by relating, e.g., the Gaussian parameters of the crystals to the different wavelengths.

4. Counting rates for phonon measurements

Though the phonon case is covered in principle by the general formulae (7) and (9) a separate treatment is worth while in view of the great practical importance of these measurements.

In the phonon case the following equation is approximately true:

$$S(Q,\omega) = S'[Q,\omega(Q)]\delta[\omega - \omega(Q)]$$
$$= S'_\omega(Q)\delta[\omega - \omega(Q)] . \tag{11}$$

If we define, for a particular phonon surface,

$$F_\omega(Q) = F[Q, \omega(Q)] \tag{12}$$

then

$$CR = \frac{\varphi_0(\bar{k}_0)}{4\pi} \int F_\omega(Q)S'_\omega(Q)dQ \tag{13}$$

or, if the variation of $S'_\omega(Q)$ over the range of resolution function is neglected,

$$CR = \frac{\varphi_0(\bar{k}_0)}{4\pi} S'_\omega(Q_0) \int F_\omega(Q)dQ . \tag{14}$$

In this way the intensity and shape of a phonon group during a constant Q scan, for example, can be calculated. We show in some detail such a calculation in Appendix II for a simple model of $F(Q,\omega)$ and a simple model of $\omega(Q)$, the flat phonon surface. However formulae (11) to (14), may be applied also to curved phonon surfaces both with model $F(Q,\omega)$'s and with more empirical ones, and for two-dimensional as well as for three-dimensional Q's.

5. Transmission function $F(Q_x, Q_y, \omega)$ for Gaussian elements

The transmissions of the elements are assumed to be Gaussian distributions of the angle variable u:

$$f(u) = \exp\left(-\frac{u^2}{\alpha_i^2}\right) \text{ for the collimators}$$

and

$$f(u) = P_i(\bar{k}) \exp\left(-\frac{u^2}{\beta_i^2}\right) \text{ for the crystals.}$$

The integral in equation (10) can then be evaluated analytically, resulting in a system of equations [equations (15) to (25) below] for the determination of $F(q_x, q_y, \delta E)$ a function of the relative coordinates $q_x, q_y, \delta E$.

$$\left(F(q_x, q_y, \delta E) \equiv F\left(q_x, q_y, \omega = \frac{\delta E}{E}\right)\right) ,$$

q_x is the component of $Q - Q_0$ in the direction of Q_0, and q_y the component of $Q - Q_0$ perpendicular to Q_0; likewise $\delta E = E - E_0$ is the deviation of the energy transfer from its nominal value. [For a derivation see Quittner (1970), Appendix III.]

$$Q = \sqrt{(Q_0 + q_x)^2 + q_y^2} \tag{15}$$

$$\alpha = \tan^{-1}\left(\frac{q_y}{Q}\right) \tag{16}$$

$$M = \frac{1}{2}\left(Q + \frac{E_0 + \delta E}{2 \cdot 074Q}\right) \tag{17}$$

$$A = -\frac{1}{2}\left(Q - \frac{E_0 + \delta E}{2 \cdot 074Q}\right) \tag{18}$$

(2·074 is the numerical value of $\hbar^2/2m$ [equation (3)] when the energy is given in meV and the momentum in Å^{-1}).

Monochromator

$$x_{0M} = k_{0M} \cos \varrho$$
$$y_{0M} = k_{0M} \sin \varrho$$

Definition of μ_{M_i} and α_{M_i} for equations (19) and (20)

M_i	1	2	3
μ_{M_i}	-2	-1	0
α_{M_i}	α_1	β_M	α_2

$\sqrt{U_{M_i}} = (k_{0M} \cdot \alpha_{M_i})^{-1} \cdot [\mu_{M_i} \tan \theta_{0M}$

$\times \{(M \cos \alpha - x_{0M}) \cos \varrho + (M \sin \alpha - y_{0M}) \sin \varrho\}$

$+ \{(M \cos \alpha - x_{0M})(-\sin \varrho)$

$+ (M \sin \alpha - y_{0M}) \cos \varrho\}]$

$\sqrt{W_{M_i}} = (k_{0M} \cdot \alpha_{M_i})^{-1} [\mu_{M_i} \tan \theta_{0M}$

$\times (-\sin \alpha \cos \varrho + \cos \alpha \sin \varrho)$

$+ (\sin \alpha \sin \varrho + \cos \alpha \cos \varrho)]$

and

$$V_{M_i} = \sqrt{U_{M_i}} \cdot \sqrt{W_{M_i}}$$

$$U = \sum_{M_i=1}^{3} (\sqrt{U_{M_i}})^2 + \sum_{A_i=1}^{3} (\sqrt{U_{A_i}})^2 \qquad (22)$$

$$V = \sum_{M_i=1}^{3} V_{M_i} + \sum_{A_i=1}^{3} V_{A_i} \qquad (23)$$

$$W = \sum_{M_i=1}^{3} (\sqrt{W_{M_i}})^2 + \sum_{A_i=1}^{3} (\sqrt{W_{A_i}})^2 \qquad (24)$$

$$F(q_x, q_y, \delta E) = \frac{P_M(\vec{k}_0) \cdot P_A(\vec{k}_1) \cdot \varepsilon(\vec{k}_1) \cdot \Delta^2 Q_z}{(\vec{k}_0)^3 \cdot 2 Q_0}$$

$$\times \sqrt{\frac{\pi}{W}} \cdot \exp\left[-\left(u - \frac{V^2}{W}\right)\right]. \qquad (25)$$

The input parameters φ, λ, k_{0A}, k_{0M}, Q_0 of the nominal scattering diagram are shown in Fig. 1. θ_{0M} and θ_{0A} are the nominal Bragg angles of the monochromator and the analyser, respectively. The triple of variables α, M, A is shown in Fig. 2.

To obtain the most important features of $F(q_x, q_y, \delta E)$ it is sufficient to know $F(0,0,0)$ and to have plots of the half-value contour of $F(q_x, q_y, \delta E)$ in the $(Q - \omega)$ space.

6. Discussion and some applications of formulae 15 to 25

Amplitude and shape of the transmission function

It can be shown (Quittner, 1970, Appendix IV) that for $q_x = q_y = 0$; $\delta E = 0$

$$U - \frac{V^2}{W} = 0, \text{ i.e. } \exp\left[-\left(U - \frac{V^2}{W}\right)\right] = 1$$

Analyser

$$x_{0A} - = k_{0A} \cos \lambda$$
$$y_{0A} = k_{0A} \sin \lambda$$

Definition of μ_{A_i} and α_{A_i} for equations (19) and (20)

A_i	1	2	3
μ_{A_i}	-2	-1	0
α_{A_i}	α_4	β_A	α_3

$\sqrt{U_{A_i}} = (k_{0A} \cdot \alpha_{A_i})^{-1} [\mu_{A_i} \tan \theta_{0A}$

$\times \{(A \cos \alpha - x_{0A})(-\cos \lambda) + (A \sin \alpha - y_{0A}) \sin \lambda\}$

$+ \{(A \cos \alpha - x_{0A}) \sin \lambda$

$+ (A \sin \alpha - y_{0A}) \cos \lambda\} \qquad (19)$

$\sqrt{W_{A_i}} = (k_{0A} \cdot \alpha_{A_i})^{-1} [\mu_{A_i} \tan \theta_{0A}$

$\times (\sin \alpha \cos \lambda + \cos \alpha \sin \lambda)$

$+ (-\sin \alpha \sin \lambda + \cos \alpha \cos \lambda)] \qquad (20)$

$$V_{A_i} = \sqrt{U_{A_i}} \cdot \sqrt{W_{A_i}} \qquad (21)$$

and that W is a slowly varying function of $q_x, q_y, \delta E$. Therefore, in the case of three-dimensional $\mathbf{Q}$'s, equations (7) and (8)

$$\text{NTIF} = \frac{P_M(\vec{k}_0) \cdot P_A(\vec{k}_1) \cdot \varepsilon(\vec{k}_1)}{(\vec{k}_0)^3 \cdot 2Q_0} \cdot \sqrt{\frac{\pi}{W(0,0,0)}} \qquad (26)$$

essentially determines the amplitude of the transmission function whereas the rapidly varying function

$$\exp\left[-\left(U - \frac{V^2}{W}\right)\right]$$

(which is normalized to unity) determines the relative shape of the transmission function and it this identical with the usual 'resolution function'.

Gaussian approximation

Although Gaussian elements have been assumed in the derivation the final $F(q_x, q_y, \delta E)$ of equation (25) is, strictly speaking, not a Gaussian function of $q_x, q_y, \delta E$. This is due both to the variation of W over the range of the resolution function and to the non-linear transformation of $(q_x, q_y, \delta E)$ to $(U - V^2/W)$. Bearing this in mind it is not difficult to find an approximation to equations (15) to (25) resulting in a strictly Gaussian function of $q_x, q_y, \delta E$. This is achieved if (1) W in $\sqrt{\pi/W}$ [equation (25)] is replaced by the constant $W(0,0,0) \equiv W_0$. (2) The non-linear functions in equations (15) to (25) are approximated by suitably truncated Taylor series so that the argument in equation (25) becomes:

$$U - \frac{V^2}{W} = A_{xx} q_x^2 + A_{yy} q_y^2 + A_{\varepsilon\varepsilon}(\delta E)^2$$

$$+2A_{xy}q_xq_y+2A_{x\varepsilon}q_x\delta E+2A_{y\varepsilon}q_y\delta E \qquad (27)$$

This will be considered in detail in a later publication.

Intensity and resolution

Like equations (8) and (10) formula (25) is absolute and can therefore be used to discuss both resolution and intensity. As mentioned above the resolution is determined by

$$\exp\left[-\left(U-\frac{V^2}{W}\right)\right].$$

More involved is the intensity or counting rate. The two factors outside the transmission function contributing to the counting rate are the source neutron flux density $\varphi_0(\bar{k}_0)$ and the sample cross section $S(\mathbf{Q},\omega)$. Within the transmission function we want to make a distinction between two different kinds of intensity factors based on the following consideration. Evidently, the counting rate can be increased by widening the resolution elements, thereby 'illuminating' a larger spot in the $(\mathbf{Q},\omega)$ space. We call the corresponding intensity factor a 'trivial' one.

However, there are other factors in the transmission function which influence the intensity in ways other than by widening or narrowing the resolution function, and we call these 'non-trivial' intensity factors. In the case of three-dimensional $\mathbf{Q}$'s it is exactly the amplitude of the transmission function, equation (26); hence its name NTIF (non-trivial intensity factor). (In the case of two-dimensional $\mathbf{Q}$'s, the amplitude of the transmission function is given by NTIF $\times \Delta^2 Q_z$, a factor of trivial origin in which the vertical resolution is 'buried'.) Usually one is interested in having a high counting rate and good, or at least sufficient, resolution. Therefore it is more advantageous to get intensity from non-trivial intensity factors than from trivial ones.

Trivial dependence of the counting rate on resolution function spread for different kinds of $S(\mathbf{Q},\omega)$

Qualitatively, the counting rate is larger, the larger the resolution-function spread. Quantitatively, there are important differences depending on whether $S(\mathbf{Q},\omega)$ is smooth or peaked in one or several dimensions in $(\mathbf{Q},\omega)$ space. We shall illustrate the differences in three typical cases which we call the liquid, the phonon and the Bragg-peak case, by considering the change in the counting rate due to a uniform expansion of the resolution function in the $(Q_x,Q_y,\delta E)$ space by a factor γ (Fig. 4).

(1) Liquid case: $S(\mathbf{Q},\omega)$ does not change appreciably over the extension of the resolution function. The counting rate increases by γ^3.

(2) Phonon case: $S(\mathbf{Q},\omega)$ is peaked δ-like on surfaces $\omega(Q_x,Q_y)$. The counting rate increases by γ^2.

(3) Bragg-peak case: $S(\mathbf{Q},\omega) \simeq \delta(\mathbf{Q}-\mathbf{Q}_0)\delta(\omega)$. The counting rate remains unchanged.

In case (1) the influence of the trivial intensity factor is maximum, and it is minimum (zero) in case (3). The

phonon case is intermediate and also the most complicated (e.g. owing to focusing effects).

Influence of the magnitudes and shapes of the $I'(k_0)$ and $R(k_1)$ distributions

We consider Fig. 5, showing the integration leading to $F(q_x,q_y,\delta E)$, specialized to $q_x=q_y=0$, $\delta E=0$, and remember that for $(0,0,0)$, $\exp[-(U-V^2/W)]=1$. This integration gives, except for the factor

$$\frac{\varepsilon(\bar{k}_1)\Delta^2 Q_z}{(\bar{k}_0)^3.2Q_0},$$

the non-trivial intensity factor of equation (26). We see that the extensions of the $I_0(k_0)$ and $R(k_1)$ distributions perpendicular to $\mathbf{Q}_0$ determine the non-trivial intensity factor while the extensions parallel to $\mathbf{Q}_0$ has
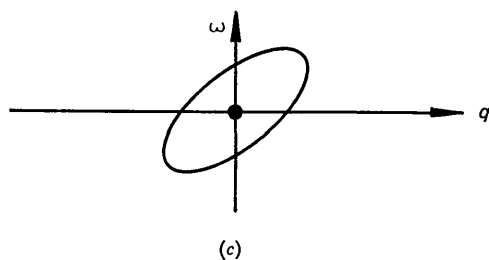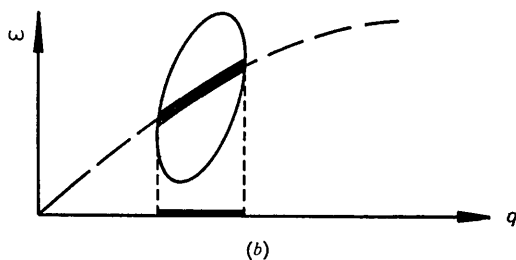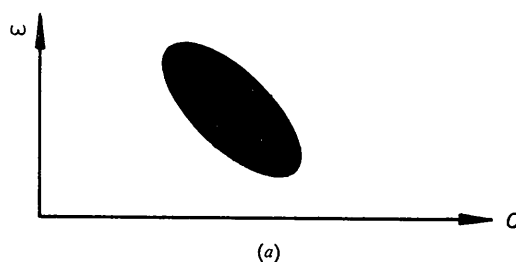

(a)

(b)

(c)

Fig. 4. Schematic drawings illustrating the trivial dependence of counting rate on the character of $S(\mathbf{Q},\omega)$. (a) 'Liquid' case; counting rate proportional to the volume within the half-value surface of $F(\mathbf{Q},\omega)$. (b) 'Phonon' case; counting rate proportional to the surface cut out from the phonon dispersion surface $\omega(\mathbf{Q})$ by the half-value surface of $F(\mathbf{Q},\omega)$ and projected onto the $\mathbf{Q}$ space (solid line on the q axis). (c) 'Bragg-reflexion' case. Counting rate not dependent on the extension of $F(\mathbf{Q},\omega)$.

no influence on it. More quantitatively, if both $I^0(\mathbf{k}_0)$ and $R(\mathbf{k}_1)$ are stretched by $\gamma_\perp$ perpendicular to $\mathbf{Q}_0$ the counting rate increases (in the liquid case) by $\gamma_\perp^2$, one $\gamma_\perp$ being non-trivial and the other trivial (increase of resolution width in the Q_y direction). On the other hand if both distributions are stretched by $\gamma_\parallel$ in the $\mathbf{Q}_0$ direction the counting rate in the liquid case increases again by $\gamma_\parallel^2$, this times both $\gamma_\parallel$ being trivial because of an increase of resolution spread in Q_x and ΔE directions.

Another application of a consideration of this kind to the 'inner focusing' will be given in a separate publication (Quittner, 1971a).

Analysis by elements

The equations (15) to (25) can be used to calculate numerically the resolution and intensity in a particular spectrometer configuration. However, they can also be used to compare different configurations from suitably chosen families of them, thus allowing important conclusions to be drawn without making detailed numerical calculations. One example is the similarity analysis showing the 'global' effects of choosing a scale for the neutron wavelengths and angular widths of the resolution elements. This is described in another publication (Quittner, 1971b).

Here we discuss another important kind of analysis, the analysis of the contribution of the different elements, collimators and crystals, to intensity and resolution. Such an analysis for the resolution has been already done by Stedman (1968) and in more detail by Nielsen & Bjerrum-Møller (1969).

The contribution of angular widths α_i to resolution can be conveniently considered within the Gaussian approximation. As we do not discuss this latter here
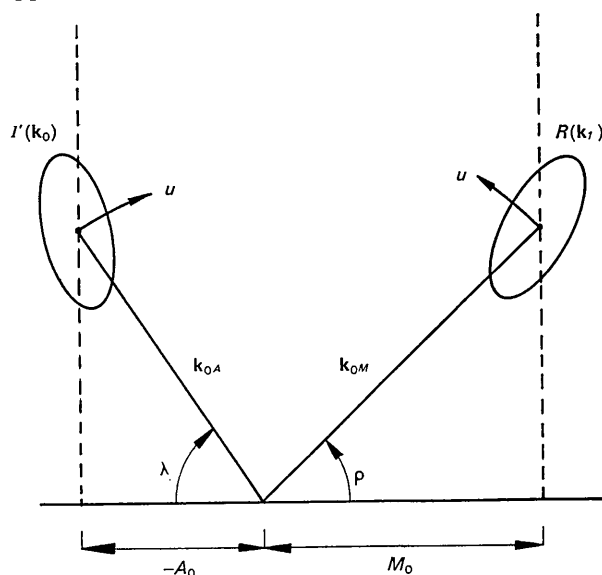

Fig. 5. The integration of Fig. 3, now specialized to $q_x = q_y = 0$; $\Delta E = 0$. For $P_M(k_0) = P_A(k_1) = 1$ it is directly related to $\sqrt{\pi/W_0}$ and thus to the non-trivial intensity factor [equations (26) and (27)].

we will only give some general remarks on this topic. The general form of the coefficients A_{xx}, A_{xy} [equation (27)] is

$$A_{xx} = \frac{c_{11}}{\alpha_1^2} + \frac{c_{12}}{\alpha_1 \alpha_2} + \frac{c_{22}}{\alpha_2^2} + \cdots$$

Such an expression can be considered as a sum of contributions of element widths to the reciprocal width in the Q_x direction (although the mixed terms like $c_{12}/\alpha_1\alpha_2$ complicate this interpretation). The variables here are the reciprocal angular widths, $1/\alpha_i$. This is in contrast to the approach of Nielsen & Bjerrum-Møller (1969), who consider the contributions to the width of the resolution function. In their analysis they start from infinitely narrow elements whereas in the present approach it is logical to start from infinitely wide elements.

The dependence of the amplitude of the transmission function and thus of the non-trivial intensity on the element widths α_i is given by $\sqrt{\pi/W_0}$ with

$$W_0 = \frac{(2 \tan \theta_{0M} \sin \varrho - \cos \varrho)^2}{k_{0M}^2 \alpha_1^2} + \frac{(\tan \theta_{0M} \sin \varrho - \cos \varrho)^2}{k_{0M}^2 \beta_M^2}$$
$$+ \frac{(\cos \varrho)^2}{k_{0M}^2 \alpha_2^2} + \frac{(2 \tan \theta_{0A} \sin \lambda - \cos \lambda)^2}{k_{0A}^2 \alpha_4^2}$$
$$+ \frac{(\tan \theta_{0A} \sin \lambda - \cos \lambda)^2}{k_{0A}^2 \beta_A^2} + \frac{(\cos \lambda)^2}{k_{0A}^2 \alpha_3^2}. \quad (28)$$

7. Relation to other papers on the same subject

Several papers have appeared since Collins (1963), dealing with different aspects of the resolution function, with different degrees of sophistication. We pick out only two of them simply because they are the most detailed ones.

Cooper & Nathans (1967) treat the (normalized) resolution function in detail and perform also the (trivial) integration over a phonon surface. Their resolution function is Gaussian and thus contains additional approximations over that inherent in equations (15) to (25). A comparison with the Gaussian approximation should be possible. Absolute intensity has not been discussed in this approach.

Peckham, Saunderson & Sharp (1967) have considered intensity in their starting formulae but these have been developed further with respect to focusing effects only. As shown in Appendix II, a reduced consideration (as compared with the full absolute treatment) is sufficient for this particular purpose. A comparison is also difficult because they do not give the transmission function as an intermediate result, but only the counting rate. At first glance, the structure of the formulae is different from that of this paper's formulae.

The absolute character of the present approach allows a full discussion of all factors contributing to intensity in its relation to resolution. Without this absolute feature several discussions of this paper and of Quittner (1971a, 1971b) would not be feasible.

The author is grateful to G. Ernst for writing and elaborating a computer program on the transmission function.

APPENDIX I

Transition from three-dimensional momentum transfers, equations (7), (8), to two-dimensional ones in equations (9), (10). Definition of $\Delta^2 Q_z$

This transition can be readily performed if the distributions $I_0'(\mathbf{k}_0)$ and $R(\mathbf{k}_1)$ for three-dimensional $\mathbf{k}_0$ and $\mathbf{k}_1$ factorize into:

$$I_0'(k_{0x}, k_{0y}, k_{0z}) = I_0'(k_{0x}, k_{0y}, 0) \cdot i_0'(k_{0z})$$
$$R(k_{1x}, k_{1y}, k_{1z}) = R(k_{1x}, k_{1y}, 0) \cdot r(k_{1z}) \ .$$

$\Delta^2 Q_z$ is then

$$\Delta^2 Q_z = \int i_0'(k_z) r(k_z - Q_z) dk_z dQ_z \ . \quad \text{(AI1)}$$

The connection between the $F(\mathbf{Q}, \omega)$ of equation (8) and $F(Q_x, Q_y, \omega)$, equation (10), is

$$\left. \begin{array}{l} F(\mathbf{Q}, \omega) \equiv F(Q_x, Q_y, Q_z, \omega) = V(Q_z) F(Q_x, Q_y, \omega), \\[2mm] V(Q_z) = \int i_0'(k_z) r(k_z - Q_z) dk_z \end{array} \right\} . \text{(AI2)}$$

For $i_0'(k_{0z})$ and $r(k_{1z})$ Gaussian,

$$i_0'(k_{0z}) = \exp - \left[\frac{k_{0z}^2}{\Delta^2 k_{zM}} \right] \ ; \quad r(k_{1z}) = \exp - \left[\frac{k_{1z}^2}{\Delta^2 k_{zA}} \right] ,$$

$$\Delta^2 Q_z = \pi \cdot \Delta k_{zM} \cdot \Delta k_{zA} = \pi \cdot k_{0M} \cdot k_{0A} \cdot \gamma_M \cdot \gamma_A \quad \text{(AI3)}$$

where γ_M and γ_A are the angular widths of vertical collimation. For a more detailed account of this transition see Quittner (1970), Appendix II.

APPENDIX II

Calculation of the counting rate for a linearized phonon surface in a constant-Q scan

Once the coefficients A_{xx}, A_{xy}, etc. of equation (27) are available the counting rate can be calculated as follows. We assume that the dispersion relation $E(q_x, q_y)$ can be approximated by a linear form

$$E(q_x, q_y) = E_0 + \Delta E + \frac{\partial E}{\partial q_x} q_x + \frac{\partial E}{\partial q_y} q_y \quad \text{(AII1)}$$

over the extension of the resolution function, where E_0 corresponds to the nominal spectrometer setting and

$$E_0 + \Delta E = E(Q_0) = E(q_x = 0; \quad q_y = 0) \ .$$

Substituting

$$\Delta E + \frac{\partial E}{\partial Q_x} q_x + \frac{\partial E}{\partial Q_y} q_y$$

for δE in equation (27) and collecting terms in q_x^2, $2q_x q_y$, q_y^2 we obtain three new coefficients

$$B_{xx} = A_{xx} + A_{\varepsilon\varepsilon} \left(\frac{\partial E}{\partial q_x} \right)^2 + 2A_{x\varepsilon} \frac{\partial E}{\partial q_x} \quad \text{(AII2)}$$

$$B_{xy} = A_{xy} + A_{\varepsilon\varepsilon} \frac{\partial E}{\partial q_x} \cdot \frac{\partial E}{\partial q_y} + A_{x\varepsilon} \frac{\partial E}{\partial q_y} + A_{y\varepsilon} \frac{\partial E}{\partial q_x} \quad \text{(AII3)}$$

$$B_{yy} = A_{yy} + A_{\varepsilon\varepsilon} \left(\frac{\partial E}{\partial q_y} \right)^2 + 2A_{y\varepsilon} \frac{\partial E}{\partial q_y} , \quad \text{(AII4)}$$

two coefficients for terms linear in q_x, q_y, and a constant, $A_{\varepsilon\varepsilon}(\Delta E)^2$. According to equation (12) this non-centric Gaussian function in Q_x, Q_y must be integrated over Q_x, Q_y.

After some lengthy calculations we obtain the peak counting rate

$$\text{PCR} = \frac{\varphi_0(\bar{k}_0)}{4\pi} \cdot \frac{P_M(\bar{k}_0) P_A(\bar{k}_1) \varepsilon(\bar{k}_1) \Delta^2 Q_z}{(\bar{k}_0)^3 \cdot 2Q_0}$$

$$\times S_\omega'(\bar{Q}_0) \cdot \sqrt{\frac{\pi}{W_0}} \cdot \frac{\pi}{(B_{xx}B_{yy} - B_{xy}^2)^{1/2}} \quad \text{(AII5)}$$

$[S_\omega'(Q)$ is defined in equation (11)], whereas the decrement S in a constant Q scan,

$$\text{CR}(\Delta E) = (\text{PCR}) \cdot \exp\left[-S(\Delta E)^2 \right]$$

is given by

$$S = A_{\varepsilon\varepsilon} - \frac{(B_{yy}C_x^2 - 2B_{xy}C_xC_y + B_{xx}C_y^2)}{B_{xx}B_{yy} - B_{xy}^2} \quad \text{(AII6)}$$

where

$$C_x = A_{\varepsilon\varepsilon} \frac{\partial E}{\partial q_x} + A_{x\varepsilon} \quad \text{(AII7)}$$

$$C_y = A_{\varepsilon\varepsilon} \frac{\partial E}{\partial q_y} + A_{y\varepsilon} \quad \text{(AII8)}$$

Focusing effects can be studied quantitatively in a way similar to Peckham et al. (1967) by considering the last factor in equation (AII5).

References

BERGSMA, J. & VAN DIJK, C. (1965). Report RCN 34. Reactor Centrum, Netherlands.

BJERRUM-MØLLER, H. (1968), Risø Report. 178.

COLLINS, H. F. (1963). Brit. J. Appl. Phys. **14**, 805.

COOPER, H. J. & NATHANS, R. (1967). Acta Cryst. A**23**, 357.

DIETRICH, O. W. (1968). Nucl. Instrum. Meth. **61**, 296.

HAMASAKI, S. (1967). Thesis, Univ. of Wisconsin.

HOVE, L. VAN (1954). Phys. Rev. **95**, 249.

NIELSEN, N. & BJERRUM-MØLLER, H. (1969). Acta Cryst. A**25**, 547.

NOVELL, J. C. (1969), Phys Rev. **186**, 567.

PECKHAM, G. E., SAUNDERSON, D. H. & SHARP, R. J. (1967). Brit. J. Appl. Phys. **18**, 73.

QUITTNER, G. (1970), SGAE-PH-1970. (This is a preprint to the present paper with more detailed Appendices). Studiengesellschaft für Atomenergie G.m.b.H., A-1082 Wien.

QUITTNER, G. (1971a). To be published.

QUITTNER, G. (1971b). To be published.

STEDMAN, R. (1968). Rev. Sci. Instrum. **39**, 878.

WERNER, S. A., ARROT, A., KING, J. S. & HENDRICK, H. (1966). J. Appl. Phys. **37**, 2343.