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Focusing Effects for Three-Crystal Neutron Diffractometers

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The factors which are important in determining the focusing properties of a three-crystal neutron diffractometer are discussed and a simplified resolution function is used to derive expressions for the orientation of the resolution ellipsoid which can be used when considering focusing effects for a particular experiment.

Introduction

Resolution and focusing properties of neutron diffractometers have been considered by a number of workers and recently Cooper & Nathans (1967, 1968*a*) have presented derivations of analytical expressions for the resolution functions of both three-crystal and two-crystal diffractometers, assuming Gaussian mosaic and collimation functions. Under these conditions the loci of constant probability for a three-crystal diffractometer are ellipsoids in $\omega,\mathbf{Q}$ space and can be defined by a four-dimensional matrix, which can be used to predict the widths of experimental peaks.

The matrix elements are involved functions of the mosaic spread values of the monochromator and analyser crystals, the divergence angles of the collimators and the parameters defining the settings of the diffractometer. One of the main requirements in the study of inelastic neutron scattering is for a knowledge of the focusing effects which arise from the detailed shape of the resolution function so that appropriate parameters may be chosen to enable the measurements to be made under suitable focusing conditions. In the present paper we discuss the factors which are important in determining the focusing properties of the diffractometer and show how a simplified consideration of the resolution function can be used to study these, thus avoiding much of the computation involved when using the full resolution function. We shall use the same notation and conventions as used in the paper by Cooper & Nathans (1967), which we shall refer to as paper I.

Focusing effects

It was shown in paper I that intensity focusing effects for a three-crystal diffractometer can be considered to be of two types, 'Q' focusing and 'gradient' focusing. 'Q' focusing arises because of the eccentricity of the resolution ellipsoid in the $\Delta\omega=0$, $\Delta Q_z=0$ plane and 'gradient' focusing arises because of the marked asphericity ofthe ellipsoid in the ω, Q_x, Q_y sub-space. Of these, 'gradient' focusing is the much more important since intensity focusing will be strongest when the gradient of the elliospid coincides with that of the scattering surface. In order to determine what parameters play an important role in this focusing we shall consider firstly how the various parameters affect the shape of the resolution ellipsoid.

Fig. 1 shows a vector diagram in reciprocal (Q_x, Q_y) space, in which typical resolution ellipsoids are indicated for the monochromator and analyser systems. The two sections are separated for clarity and the resolution is represented as the projections of the resolution ellipsoids onto the $\Delta\omega=0$ plane. The resolution function for the whole system is obtained by superimposing the two parts of the diagram for all possible wave-vectors $\mathbf{k}_I$ and $\mathbf{k}_f$ and hence determining the resultant probability function around Q, which will then have the form indicated by the resolution ellipsoid shown in Fig. 2(*a*).

In order to determine how the shape of the resolution ellipsoid is affected by the various instrumental parameters we shall consider first all the case of a perfect monochromator with $\eta_M=0$. For such a monochromator we shall have a range of k_I values, as allowed by

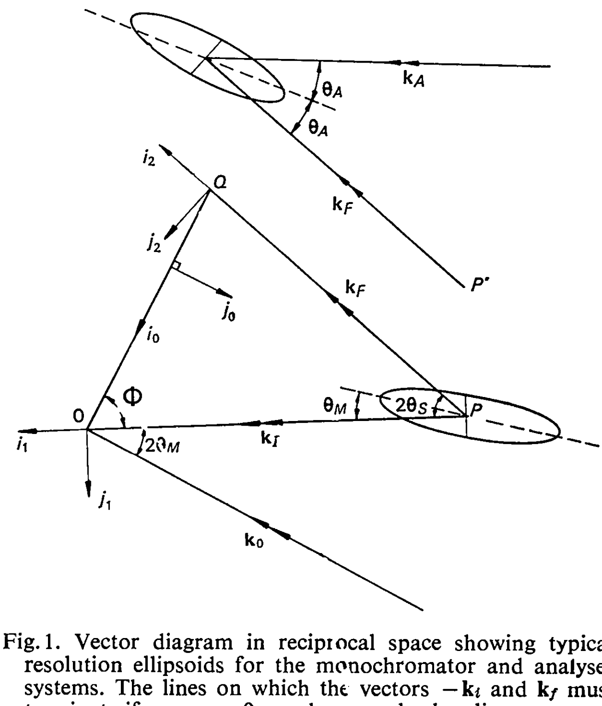

Fig. 1. Vector diagram in reciprocal space showing typical resolution ellipsoids for the monochromator and analyser systems. The lines on which the vectors $-\mathbf{k}_I$ and $\mathbf{k}_f$ must terminate if $\eta_M=\eta_A=0$ are shown as broken lines.

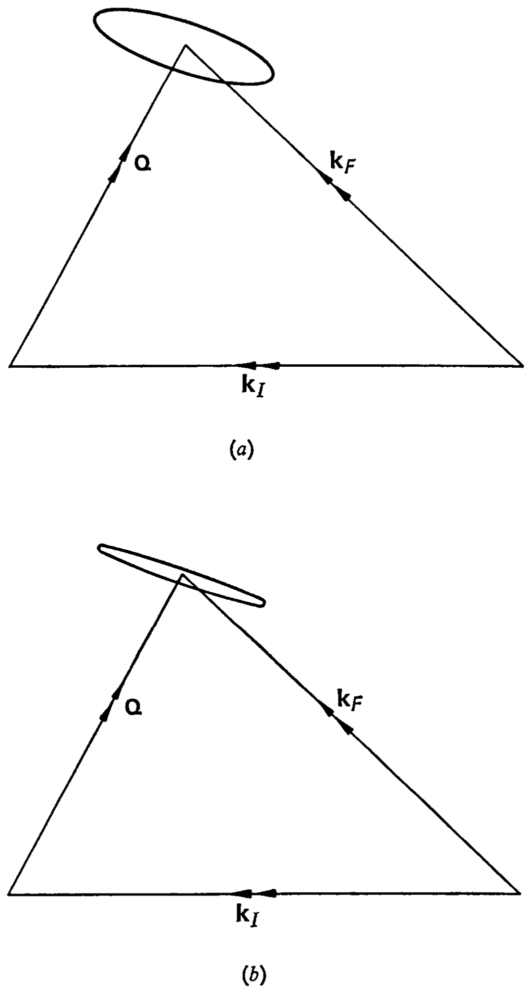

Fig. 2. Overall resolution for (a) monochromator and analyzer crystals with finite mosaic spread, and (b) monochromator and analyzer crystals with zero mosaic spread.

the finite collimation before and after the monochromator, but there will be a direct correlation between k_i and direction because of the perfect alignment of the reflecting planes. All $-\mathbf{k}_i$ vectors will therefore terminate on a line through P at an angle $-\theta_M$ to $\mathbf{k}_I$ (see next section). If we consider the monochromator to have a finite mosaic spread each possible k_i can occur over a range of angle on either side of the $\mathbf{k}_i$ for a perfect monochromator, corresponding to $-\mathbf{k}_i$ vectors terminating on a line perpendicular to $\mathbf{k}_I$ on either side of the line at $-\theta_M$ to $\mathbf{k}_I$. The probability function for various $\mathbf{k}_i$ vectors then results in a resolution ellipsoid whose longer principal axis makes an angle μ_1 to $\mathbf{k}_I$, where $\mu_1 \simeq \theta_M$ and an expression for tan $2\mu_1$ is given by equation (2) of Cooper & Nathans (1968b). We may note, however, that μ_1 tends to θ_M for $\alpha_0, \alpha_1 \gg \eta_M$, *i.e.* relaxed collimation or small mosaic spread. A similar resolution ellipse can be derived for $\mathbf{k}_f$, depending on the mosaic spread of the analyser and the collimation before and after the analyser. The resultant ellipse for the overall resolution will then have principal axes which lie along directions between those of the monochromator and analyser ellipses. For a normal focusing geometry, with alternating senses of rotation for θ_m, θ_S and θ_A as illustrated in Fig. 1 of paper I, $\Delta\omega$ will vary most rapidly in a direction which is fairly close to that perpendicular to **Q**. (For identical monochromator and analyser systems this directions would be exactly perpendicular to **Q**.)

It is clear from the above considerations that under normal circumstances the mosaic spread of the monochromator and analyser crystals affects primarily the magnitude of the resolution ellipsoid and not the direction of its principal axes.

We can therefore consider the main features of the focusing by considering a model for which $\eta_M = \eta_A = 0$. In this case the resolution functions for $\mathbf{k}_i$ and $\mathbf{k}_f$ reduce to Gaussian functions along the directions making angles of $-\theta_M$ to $\mathbf{k}_I$ and θ_A to $\mathbf{k}_F$, shown as broken lines in Fig. 1, and the overall resolution gives a resolution ellipse whose principal axis lies between these two directions, as illustrated in Fig. 2(b). Although the width of the ellipse is much less than for the case for finite mosaic spread, shown in Fig. 2(a), it can be seen that the orientation of the ellipse is essentially the same. Because of the direct correlation between wave number and direction this ellipse lies in an inclined plane in ω, **Q** space and the 'gradient' focusing will be determined by the orientation of this plane, which is dependent on geometrical factors such as the relative magnitude and sense of rotation of θ_S, θ_M and θ_A, and the relative magnitude of $\mathbf{k}_I$ and $\mathbf{k}_F$. For any given configuration we can calculate the orientation of the plane containing the resolution ellipse, as discussed in the next section, and hence evaluate the focusing conditions.

Simplified resolution function

The probability of reflexion of a neutron by the monochromator is given by equation (4) of paper I, *viz.*

$$P(\Delta k_i, y_1) = P_M \exp\left\{ -\tfrac{1}{2} \left(\frac{(\Delta k_i/k_I)\tan\theta_M + y_1}{\eta_M} \right)^2 \right\} \quad (1)$$

and it can be seen that if $\eta_M = 0$ this is only finite if $y_1 = -(\Delta k_i/k_I)\tan\theta_M$, when it has the value P_M. This condition defines a straight line in reciprocal (Q_x, Q_y) space give by

$$y_1 = -\tan\theta_M x_1 \quad (2)$$

where x_1 and y_1 are the components of $\Delta\mathbf{k}_i$ along and perpendicular to $\mathbf{k}_I$ respectively. Equations (2) thus defines a line making an angle of $-\theta_M$ to $\mathbf{k}_I$ on which all allowed $-\mathbf{k}_i$ vectors must terminate.

A similar condition arises for the analyser, namely

$$y_2 = \tan\theta_A x_2 \quad (3)$$

which defines a line making an angle of θ_A to $\mathbf{k}_F$ on which all detectable $\mathbf{k}_F$ vectors must terminate.

The probability of a neutron being detected [equation (6) of paper I] then becomes

$$P(\Delta k_i, \Delta k_f, \delta_1, \delta_2)=P_M P_A P_0 \times \left\{-\tfrac{1}{2}\left[\left(\frac{1}{\alpha_0^2}+\frac{1}{\alpha_1^2}\right)\tan^2\theta_M x_1^2 + \left(\frac{1}{\alpha_2^2}+\frac{1}{\alpha_3^2}\right)\tan^2\theta_A x_2^2 + \left(\frac{1}{\beta_0^2}+\frac{1}{\beta_1^2}\right)\delta_1^2 + \left(\frac{1}{\beta_2^2}+\frac{1}{\beta_3^2}\right)\delta_2^2\right]\right\}. \quad (4)$$

As before the terms involving δ_1 and δ_2 are independent of the others and we can write

$$P(\Delta k_i, \Delta k_f, \delta_1, \delta_2) = P(\Delta k_i, \Delta k_f).\ P(\delta_1, \delta_2)\ . \quad (5)$$

The factor $P(\delta_1, \delta_2)$ does not enter into the focusing and we shall therefore not consider it further.

Because of the correlation between wave number and direction there is only one possible path to a given point in Q_x, Q_y space ($\mathbf{Q}+\Delta\mathbf{Q}$). The resolution function is therefore simply the probability for this path, which can be determined by splitting $\Delta\mathbf{Q}$ into its two allowed components $\Delta\mathbf{k}_i$ and $\Delta\mathbf{k}_f$ along the directions defined by equations (2) and (3) respectively.

If we substitute for y_1 and y_2 from equations (2) and (3) into equations (30) of paper I we can derive the following equations for x_1 and x_2 in terms of ΔQ_x and ΔQ_y where a, b, A and B are defined by equations (13):

$$x_1= -\frac{(A-B\tan\theta_A)\Delta Q_x+(B+A\tan\theta_A)\Delta Q_y}{(b-a\tan\theta_M)(A-B\tan\theta_A)+(a+b\tan\theta_M)(B+A\tan\theta_A)} \quad (6a)$$

$$x_2= \frac{(a+b\tan\theta_M)\Delta Q_x-(b-a\tan\theta_M)\Delta Q_y}{(a+b\tan\theta_M)(B+A\tan\theta_A)+(b-a\tan\theta_M)(A+B\tan\theta_A)} \quad (6b)$$

which thus define $\Delta\mathbf{k}_i$ and $\Delta\mathbf{k}_f$ respectively. The resolution function is then obtained by substituting these values into equation (4).

The change in angular frequency, $\Delta\omega$, is given from equation (31a) of paper I as

$$\Delta\omega=\frac{\hbar}{m}(x_1 k_I - x_2 k_F) \quad (7)$$

and the gradient of the plane containing the resolution function will be given by the maximum value of $\Delta\omega/\Delta Q$.

We can write $\Delta\omega/\Delta Q$ from equations (6) and (7) in the form

$$\frac{\Delta\omega}{\Delta Q}=\frac{\hbar}{m}\frac{(F\Delta Q_x+G\Delta Q_y)}{\Delta Q} \quad (8)$$

and the maximum value of $\Delta\omega/\Delta Q$ is then

$$\left(\frac{\Delta\omega}{\Delta Q}\right)_{\max}=\frac{\hbar}{m}\sqrt{F^2+G^2} \quad (9)$$

and occurs for a direction defined by

$$G\Delta Q_x=F\Delta Q_y\ . \quad (10)$$

F and G are defined by the following equations

$$F=-\frac{C k_I}{Cd+cD}-\frac{ck_F}{cC+dD} \quad (11a)$$

$$G=-\frac{Dk_I}{Cd+cD}+\frac{dk_F}{cC+dD} \quad (11b)$$

with

$$c=a+b\tan\theta_M \qquad C=A-B\tan\theta_A$$
$$d=b-a\tan\theta_M \qquad D=B+A\tan\theta_A \quad (12)$$

and

$$a=\sin\Phi \qquad A=\sin(2\theta_s+\Phi)$$
$$b=\cos\Phi \qquad B=\cos(2\theta_s+\Phi) \quad (13)$$

Φ being the angle between $\mathbf{k}_I$ and $-\mathbf{Q}$.

Equations (9) and (10) can therefore be used directly to determine the orientation of the plane containing the resolution ellipse which can be compared directly with the orientation of the scattering surface in order to consider the focusing properties for a given experiment.

Summary

The focusing properties of a three-crystal neutron diffractometer are determined to a large extent by the orientation of the resolution ellipsoid, which is itself determined primarily by geometrical factors. The orientation of the resolution ellipsoid can be determined quite easily by considering the case for which both the monochromator and analyser crystals have zero mosaic spread. The resolution is then restricted to a plane in ω, Q_x, Q_y space and the orientation of this plane is determined by equations (9) and (10). Focusing effects will occur when the gradient of this plane coincides in magnitude and direction with the gradient of the scattering surface (*e.g.* the dispersion surface for phonon scattering) and the best configuration of the diffractometer for a particular measurement can be determined by calculating the orientation of the plane for sets of possible instrumental parameters.

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