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On the Resolution of Slow-Neutron Spectrometers. IV. The Triple-Axis Spectrometer Resolution Function, Spatial Effects Included

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The procedure for computing the resolution function of triple-axis spectrometers is reformulated to make allowance for the spatial configuration of the experimental set-up and for the curvature of the monochromator and analyser crystals. Simple formulae are given for computing the resolution function of conventional instruments as well as of spectrometers with focusing crystals.

Introduction

The calculation of the resolution function for slow-neutron spectrometers has received considerable attention during the last decade and especially since the paper of Cooper & Nathans (1967). The usual computation technique is based on the concept of the angular transmission function introduced in the pioneering work of Sailor, Foote, Landon & Wood (1956) and developed by Caglioti, Paoletti & Ricci (1958). Although it has been recognized occasionally that the description of experimental arrangements in terms of angular distributions only is incomplete and that spatial distributions should also be considered [see Dietrich (1968) and Dorner (1970), for instance], little progress has been made in the technique of accounting for spatial effects when considering the optics of neutron crystal spectrometers.

Recently there has been an increased interest in exploiting spatial focusing effects occurring when bent crystals are used. Riste (1970) and Nunes & Shirane (1971) have reported substantial gains in neutron fluxes from vertically bent monochromators. Curved crystals and related effects have also been recently investigated experimentally by Karas, Rauch & Seidl (1971), Antonini, Corchia, Nicotera & Rustichelli (1972), Kalus, Gobert & Schedler (1973) and others.

The influence of crystal curvature on the spectrometer resolution cannot be described properly within the usual computation technique in which only angular variables are used. Attempts have been made by Maier-Leibnitz (1970), Dachs (1970), Nunes & Shirane (1971), Currat (1973) to calculate the effect of crystal curvature on the resolution or luminosity of crystal spectrometers. The results reported so far do not seem to offer a suitable basis for a consistent treatment of the resolution function problem.

Meanwhile, a new computation procedure has been proposed in part II of this series by Stoica (1975*b*) for calculating the resolution (which is particularly sensitive to spatial effects) of time-of-flight instruments. This procedure [see also Popa (1974)] consists in using as initial variables the spatial coordinates describing the geometry of the experiment and then in making a transformation to angular variables. It is at once obvious that the method should also be suitable for treating effects related to the crystal shape and curvature in neutron crystal spectrometers.

However, in this case the initial variables of the problem are not independent, owing to the constraints imposed by Bragg reflexion optics. For this reason the general calculation method developed in the part I of this series by Stoica (1975*a*) cannot be applied directly: one has to operate first a reduction to independent variables. The aim of this paper is to develop the procedure for computing the normal approximation to the triple-axis spectrometer resolution function in the general case, spatial effects included.

The problem under consideration is the determination of the resolution function defined in the $\mathbf{Q},\omega$ space, $\mathbf{Q}=\mathbf{k}_i-\mathbf{k}_f$ being the wave-vector transfer and $\hbar\omega=\hbar^2(k_i^2-k_f^2)/(2m)$ the energy transfer in the scattering process. For a nominal setting of the spectrometer at $\mathbf{Q}_0$ and $\hbar\omega_0$ (defined by the most probable wave-vectors $\mathbf{k}_I$ and $\mathbf{k}_F$) the probability of measuring the transfers $\mathbf{Q}$ and $\hbar\omega$ is given by $R(\mathbf{X})/R_0$, $R(\mathbf{X})$ being the resolution function. In the normal approximation this function has the form:

$$R(\mathbf{X})=R_0(2\pi)^{-2}\sqrt{\det \mathbf{M}}\,\exp\left(-\tfrac{1}{2}\mathbf{X}^T\mathbf{M}\mathbf{X}\right). \qquad (1)$$

Here $\mathbf{X}$ is the column matrix of the four-component vector $\mathbf{X}=(\mathbf{Q}-\mathbf{Q}_0,\omega-\omega_0)$, $\mathbf{X}^T$ is the row matrix transpose of $\mathbf{X}$, and $\mathbf{M}$ is the resolution matrix, the inverse of which is the covariance matrix $\mathbf{M}^{-1}=\{\langle X_iX_j\rangle\}$ of the resolution function.

The general formulation of the resolution function problem advanced by Stoica (1975*a*) reduces the calculation of the normal approximation (1) to the determination of the covariance matrix of the distribution $P(\mathbf{k}_i,\mathbf{k}_f)$ of the incident and scattered neutron wave-vectors allowed to pass through the spectrometer. Having introduced the six-component vector $\mathbf{Y}=(\mathbf{k}_i-\mathbf{k}_I,\mathbf{k}_f-\mathbf{k}_F)=(\Delta k_i,k_I\gamma_1,k_I\delta_1,\Delta k_f,k_F\gamma_2,k_F\delta_2)$ one can express the normal approximation to $P(\mathbf{k}_i,\mathbf{k}_f)$ in the form:

$$P(\mathbf{Y})=P_0(2\pi)^{-3}\sqrt{\det \mathbf{N}}\,\exp\left(-\tfrac{1}{2}\mathbf{Y}^T\mathbf{N}\mathbf{Y}\right) \qquad (2)$$

where $\mathbf{N}^{-1}=\{\langle Y_iY_j\rangle\}$. With the aid of the matrix $\mathbf{B}$ of

the linearized relation $\mathbf{X}=\mathbf{BY}$ the covariance matrix of the resolution function is constructed through the relation:

$$\mathbf{M}^{-1}=\mathbf{BN}^{-1}\mathbf{B}^T. \tag{3}$$

This relation, which would be obvious if the matrix $\mathbf{B}$ were quadratic, results as a particular case from the general expression of the resolution function moments derived in part I. The matrix $\mathbf{B}$ is known (see Appendix 1) so that the problem is reduced to the calculation of the matrix $\mathbf{N}^{-1}$ and the normalization factor R_0.

The conventional case of a triple-axis spectrometer with Soller collimators is considered in § 1. The usual calculation procedure is reformulated to allow a generalization to be made. This generalization, which includes spatial effects and lattice spacing spread is presented in § 2. Some consequences of the formulae obtained are discussed in § 3.

1. The conventional triple-axis spectrometer

In the classical calculation procedure the distribution $P(\mathbf{k}_i,\mathbf{k}_f)$ is computed by using the angular transmission functions $T_i(\gamma_i,\delta_i)$ of the Soller collimators [γ_i and δ_i are horizontal and vertical divergence angles denoted as in the paper of Cooper & Nathans (1967)] and the reflectivity functions $r_M(\xi_M,\xi'_M)$ and $r_A(\xi_A,\xi'_A)$ of the monochromator and analyser crystals (ξ and ξ' are angular deviations of the mosaic blocks in the horizontal and vertical planes, respectively). To generalize this procedure, let us reformulate it in matrix language.

We define the following vectors of the angular variables: $\mathbf{U}=(\gamma_0,\gamma_1,\delta_0,\delta_1,\gamma_2,\gamma_3,\delta_2,\delta_3)$ and $\mathbf{W}=(\xi_M,\xi'_M,\xi_A,\xi'_A)$. The distribution of these variables is $P(\mathbf{U},\mathbf{W})=r_M(\xi_M,\xi'_M)r_A(\xi_A,\xi'_A)\prod_{i=0}^{3}T_i(\gamma_i,\delta_i)$. In the normal approximation this distribution has the form:

$$P(\mathbf{U},\mathbf{W})=P_0\frac{\sqrt{\det\mathbf{G}}}{(2\pi)^4}\exp\left(-\tfrac{1}{2}\mathbf{U}^T\mathbf{G}\mathbf{U}\right)\times\frac{\sqrt{\det\mathbf{F}}}{(2\pi)^2}\exp\left(-\tfrac{1}{2}\mathbf{W}^T\mathbf{F}\mathbf{W}\right). \tag{4}$$

The diagonal matrix $\mathbf{G}$ has the form $\mathbf{G}=\{\alpha_0^{-2},\alpha_1^{-2},\beta_0^{-2},\beta_1^{-2},\alpha_2^{-2},\alpha_3^{-2},\beta_2^{-2},\beta_3^{-2}\}$, α_i,β_i being the standard deviations of γ_i,δ_i, respectively. The matrix $\mathbf{F}$ is also diagonal, $\mathbf{F}=\{\eta_M^{-2},\eta_M'^{-2},\eta_A^{-2},\eta_A'^{-2}\}$, the quantities η and η' being the standard deviations of the differential reflectivities dependences on ξ and ξ' [for crystals of simple shape η and η' can be calculated as functions of mosaic spread and neutron energy, see Grabcev & Stoica (1975) and also Popovici, Gheorghiu & Gelberg (1969)].

The normalization constant P_0 in (4) is given by:

$$P_0=R_M^{\mathbf{k}}R_A^{\mathbf{k}}(2\pi)^4/\sqrt{\det\mathbf{G}} \tag{5}$$

where $R_M^{\mathbf{k}}$ and $R_A^{\mathbf{k}}$ are the monochromator and analyser crystal reflectivities after integration over $\mathbf{k}_i$ and $\mathbf{k}_f$ respectively, $R_M^{\mathbf{k}}=\mathbf{k}_I^3\operatorname{ctg}\theta_M R_M^{\theta}$ and $R_A^{\mathbf{k}}=\mathbf{k}_F^3\operatorname{ctg}\theta_A R_A^{\theta}$. R_M^{θ} and R_A^{θ} are the integrated crystal reflectivities defined as usual. The quantity $(2\pi)^4/\sqrt{\det\mathbf{G}}$ is the product of the solid angles defined by the collimators.

As the optics of the Bragg reflexion imposes some constraints on the angular variables, the vectors $\mathbf{U}$ and $\mathbf{W}$ are not independent. The constraints may be expressed as $\mathbf{W}=\mathbf{CU}$. The elements of the matrix $\mathbf{C}$ are given in Appendix 1. The distribution of the variables u_i, constraints taken into account, is calculated through the relation:

$$P(\mathbf{U})=(16\sin\theta_M\sin\theta_A)^{-1}\int P(\mathbf{U},\mathbf{W})\delta(\mathbf{W}-\mathbf{CU})\mathrm{d}\mathbf{W}. \tag{6}$$

The factor $(16\sin\theta_M\sin\theta_A)^{-1}$ here ensures the proper normalization of the $\delta(\mathbf{W}-\mathbf{CU})$ function. After performing the integration one obtains:

$$P(\mathbf{U})=\frac{P_0}{16\sin\theta_M\sin\theta_A}\times\frac{\sqrt{\det\mathbf{G}}}{(2\pi)^4}\frac{\sqrt{\det\mathbf{F}}}{(2\pi)^2}\exp\left(-\tfrac{1}{2}\mathbf{U}^T\mathbf{H}\mathbf{U}\right) \tag{7}$$

where $\mathbf{H}$ is given by:

$$\mathbf{H}=\mathbf{G}+\mathbf{C}^T\mathbf{F}\mathbf{C}. \tag{8}$$

The distribution (7) is normalized to $\int P(\mathbf{U})\mathrm{d}\mathbf{U}=R_0$ with

$$R_0=\frac{P_0}{64\pi^2\sin\theta_M\sin\theta_A}\frac{\sqrt{\det\mathbf{G}\det\mathbf{F}}}{\sqrt{\det\mathbf{H}}}. \tag{9}$$

As the normalization does not change in what follows, this factor propagates up to the relation (1).

The components of the vector $\mathbf{Y}=(\mathbf{k}_i-\mathbf{k}_I,\mathbf{k}_f-\mathbf{k}_F)$ can be expressed through the variables u_i with the aid of a linearized relation $\mathbf{Y}=\mathbf{AU}$. The matrix $\mathbf{A}$ of this relation is specified in Appendix 1. As u_i are already independent variables, one may apply the prescription of part I to obtain the covariance matrix $\mathbf{N}^{-1}$ of the distribution $P(\mathbf{Y})$ in the form:

$$\mathbf{N}^{-1}=\mathbf{AH}^{-1}\mathbf{A}^T. \tag{10}$$

The matrix $\mathbf{N}^{-1}$ obtained in this way is cell-diagonal, consisting of two 3×3 blocks $\mathbf{N}_M^{-1}$ and $\mathbf{N}_A^{-1}$ on the main diagonal, $\mathbf{N}^{-1}=\{\mathbf{N}_M^{-1},\mathbf{N}_A^{-1}\}$. This means that the distribution $P(\mathbf{k}_i,\mathbf{k}_f)$ can be expressed as a product of two functions $p_M(\mathbf{k}_i)$ and $p_A(\mathbf{k}_f)$ referring to the monochromator and analyser units, respectively. In the normal approximation the equal probability surfaces of $\mathbf{k}_i$ and $\mathbf{k}_f$ are ellipsoids in the wave-vector space.

The determination of the resolution function is now complete: the covariance matrix is obtained through (8), (10) and (3), that is:

$$\mathbf{M}^{-1}=\mathbf{BA}(\mathbf{G}+\mathbf{C}^T\mathbf{F}\mathbf{C})^{-1}\mathbf{A}^T\mathbf{B}^T \tag{11}$$

and the normalization factor is given by (9), (5) and (8).

To obtain the normalization factor $R_0(\mathbf{Q}_0, \omega_0)$ as defined by Dorner (1972), Chesser & Axe (1973) and also [up to a factor $1/(2\pi\eta'_M\eta'_A)$] by Tucciarone, Lau, Corliss, Delapalme & Hastings (1971) one has to multiply by $(2\pi)^{-2}\sqrt{\det \mathbf{M}}$ the quantity given by (9). The difference is due to the normalization convention used here. Besides, the reflectivity factors P_M and P_A of these authors must be identified with the quantities $R^{\theta}_M/(\sqrt{2\pi}\eta_M)$ and $R^{\theta}_A/(\sqrt{2\pi}\eta_A)$, respectively.

The results obtained in the above manner are fully equivalent to those derived by Cooper & Nathans (1967), Bjerrum-Møller & Nielsen (1970), Quittner (1971), Werner & Pynn (1971), Grabcev (1973), if allowance is made for several minor mistakes appearing occasionally in some of these papers [see Dorner (1972) and Chesser & Axe (1973) for rectifications to the papers of Cooper & Nathans (1967) and Tucciarone, Lau, Corliss, Delapalme & Hastings (1971)].

As to the fact that one has first to calculate $\mathbf{M}^{-1}$ and then to invert it, this is not actually an inconvenience, but rather the right sequence, as it is the elements of $\mathbf{M}^{-1}$ that have a clear physical meaning. The resolution function properties are best visualized at the covariance matrix level.

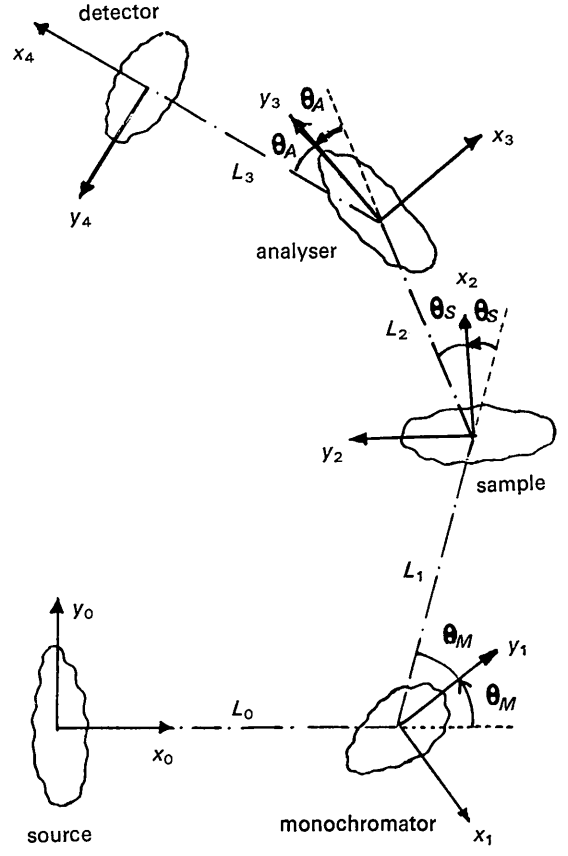

Fig. 1. The geometry of the neutron scattering experiment. The angles $2\theta_M$, $2\theta_S$ and $2\theta_A$ are positive in the arrangement shown. The coordinate systems used in computations are indicated.

2. The general case, spatial effects included

The above derivation will be now generalized to include the spatial arrangement of the spectrometer elements and the curvature of crystals. In place of the angular variables of the preceding section we shall use as initial variables the coordinates $\mathbf{r}_i$ of the points where the neutron is emitted from the source ($\mathbf{r}_0$), reflected in the monochromator ($\mathbf{r}_1$), scattered in the sample ($\mathbf{r}_2$), reflected again in the analyser ($\mathbf{r}_3$) and finally detected ($\mathbf{r}_4$). The reference systems for these coordinates are shown in Fig. 1. The axes y_1 and y_3 of the crystal reference frames are directed along the bisectors of the angles $2\theta_M$ and $2\theta_A$, respectively, and the x_2 axis of the sample reference frame is directed along the bisector of the scattering angle $2\theta_S$. The distances between the origins of the reference systems are denoted by L_i ($i=0,1,2,3$). The shape of the crystals and the sample will be described by probability distributions $p_i(\mathbf{r}_i)$. The normal approximation to $p_i(\mathbf{r}_i)$ will be used.

Let us define the following vector $\mathbf{V}$ of the relevant spatial coordinates: $\mathbf{V}=(y_0, z_0, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, y_4, z_4)$ and let $\mathbf{S}^{-1}=\{\langle v_i v_j\rangle\}$ be the covariance matrix of the distribution of these variables. For given crystals and sample this matrix is known. Its structure is given explicitly in Appendix 2. The initial, linearly dependent, variables of the problem are now v_i and w_i. Their distribution $P(\mathbf{V},\mathbf{W})$ is approximated by:

$$P(\mathbf{V},\mathbf{W})=P'_0\frac{\sqrt{\det \mathbf{S}}}{(2\pi)^{13/2}}\exp\left(-\tfrac{1}{2}\mathbf{V}^T\mathbf{S}\mathbf{V}\right)$$
$$\times\frac{\sqrt{\det \mathbf{F}}}{(2\pi)^2}\exp\left(-\tfrac{1}{2}\mathbf{W}^T\mathbf{F}\mathbf{W}\right). \quad (12)$$

The angular variables u_i can be expressed through the spatial variables v_i by considering the scattering geometry in real space. The relation between $\mathbf{U}$ and $\mathbf{V}$ has the form $\mathbf{U}=\mathbf{D}\mathbf{V}$ with the matrix $\mathbf{D}$ specified in Appendix 2. The covariance matrix of the distribution of angular variables in the absence of constraints is $\mathbf{D}\mathbf{S}^{-1}\mathbf{D}^T$, which is the analogue of the matrix $\mathbf{G}^{-1}$ of the preceding section. Correspondingly, the normalization constant P'_0 in (12) is obtained from an expression similar to (5), that is:

$$P'_0=R^{\mathbf{k}}_M R^{\mathbf{k}}_A(2\pi)^4\sqrt{\det(\mathbf{D}\mathbf{S}^{-1}\mathbf{D}^T)}. \quad (13)$$

As before, the constraints imposed by the optics of Bragg reflexion will be used to eliminate the variables w_i through an integration. For the case of curved crystals these constraints may be easily shown to have the form:

$$\gamma_1=-\gamma_0+2(\xi_M+y_1/\varrho_M);\quad \delta_1=\delta_0-2\sin\theta_M(\xi'_M+z_1/\varrho'_M)$$
$$\gamma_3=-\gamma_2+2(\xi_A+y_3/\varrho_A);\quad \delta_3=\delta_2-2\sin\theta_A(\xi'_A+z_3/\varrho'_A). \quad (14)$$

The angular variables in (14) may be expressed through the spatial ones. The expression for the constraints then becomes $\mathbf{W}=\mathbf{TV}$. The matrix $\mathbf{T}$ is specified explicitly in Appendix 2. By integrating the distribution (12) with respect to w_i, constraints taken into account, one obtains the distribution

$$P(\mathbf{V})=R_0(2\pi)^{-13/2}\sqrt{\det \mathbf{K}}\exp\left(-\tfrac{1}{2}\mathbf{V}^T\mathbf{K}\mathbf{V}\right)$$

with the matrix $\mathbf{K}$ given by

$$\mathbf{K}=\mathbf{S}+\mathbf{T}^T\mathbf{F}\mathbf{T} \tag{15}$$

and the normalization factor R_0 given by the expression:

$$R_0=\frac{P_0'}{64\pi^2\sin\theta_M\sin\theta_A}\,\frac{\sqrt{\det \mathbf{S}\det \mathbf{F}}}{\sqrt{\det \mathbf{K}}} \tag{16}$$

which is the analogue of (9).

The next step is to apply to $P(\mathbf{V})$ the transformation $\mathbf{U}=\mathbf{DV}$ from spatial to angular variables. One then obtains the distribution

$$P(\mathbf{U})=R_0(2\pi)^{-4}\sqrt{\det \mathbf{H}}\exp\left(-\tfrac{1}{2}\mathbf{U}^T\mathbf{H}\mathbf{U}\right)$$

with the matrix $\mathbf{H}$ given by

$$\mathbf{H}^{-1}=\mathbf{D}\mathbf{K}^{-1}\mathbf{D}^T. \tag{17}$$

At this stage the presence of Soller collimators, if any, may be accounted for in a simple way: one has to multiply the distribution $P(\mathbf{U})$ by the transmission function of these collimators. The effect of this operation is to change the matrix $\mathbf{H}$ into $\mathbf{H}+\mathbf{G}$. The normalization constant P_0' also changes into

$$P_0'=R_M^{\mathbf{k}}R_A^{\mathbf{k}}(2\pi)^4/\sqrt{\det\left[\mathbf{G}+(\mathbf{D}\mathbf{S}^{-1}\mathbf{D}^T)^{-1}\right]}. \tag{13a}$$

The covariance matrix of the distribution (2) is now obtained through the relation:

$$\mathbf{N}^{-1}=\mathbf{A}(\mathbf{H}+\mathbf{G})^{-1}\mathbf{A}^T \tag{18}$$

where $\mathbf{A}$ is the matrix defined earlier. The matrix $\mathbf{N}^{-1}$ has the following structure (the elements specified are different from zero):

$$\mathbf{N}^{-1}=\begin{pmatrix}
\langle Y_1^2\rangle & \langle Y_1Y_2\rangle & 0 & \langle Y_1Y_4\rangle & \langle Y_1Y_5\rangle & 0\\
\langle Y_1Y_2\rangle & \langle Y_2^2\rangle & 0 & \langle Y_2Y_4\rangle & \langle Y_2Y_5\rangle & 0\\
0 & 0 & \langle Y_3^2\rangle & 0 & 0 & \langle Y_3Y_6\rangle\\
\langle Y_1Y_4\rangle & \langle Y_2Y_4\rangle & 0 & \langle Y_4^2\rangle & \langle Y_4Y_5\rangle & 0\\
\langle Y_1Y_5\rangle & \langle Y_2Y_5\rangle & 0 & \langle Y_4Y_5\rangle & \langle Y_5^2\rangle & 0\\
0 & 0 & \langle Y_3Y_6\rangle & 0 & 0 & \langle Y_6^2\rangle
\end{pmatrix}. \tag{19}$$

In comparison with the conventional case, the structure of this matrix has changed: the finite sample dimensions have introduced a coupling between the monochromator and analyser units. The smaller the monochromator or analyser mosaic spread, the stronger is the coupling. The coupling is expressed by the cross-correlation between the components Y_i referring to different units. As a result, one can no longer, except for very small samples, express $P(\mathbf{k}_i,\mathbf{k}_f)$ as a product of two independent transmission functions; nor can one define rigorously separate monochromator and analyser ellipsoids in the wave-vector space.

At this point the crystal lattice spacing spread may be introduced most easily: it can be shown that the only change to be made is the modification of the elements $\langle Y_1^2\rangle$ and $\langle Y_4^2\rangle$ of the above matrix to $\langle Y_1^2\rangle+k_I^2\langle\Delta\tau_M^2\rangle/\tau_M^2$ and $\langle Y_4^2\rangle+k_F^2\langle\Delta\tau_A^2\rangle/\tau_A^2$, respectively. Here $\langle\Delta\tau_M^2\rangle$ and $\langle\Delta\tau_A^2\rangle$ are the dispersions of the deviations $\Delta\tau_M$ and $\Delta\tau_A$ of the lattice vector moduli from the corresponding mean values τ_M and τ_A (for imperfect crystals these deviations come from the mosaic block size). The modification described has to be operated by all means for crystals in back reflexion: the additional term then becomes dominant even for perfect crystals [see Alefeld, Birr & Heidemann (1968)].

The final expression for the resolution matrix becomes, for the general case:

$$\mathbf{M}^{-1}=\mathbf{BA}\{[\mathbf{D}(\mathbf{S}+\mathbf{T}^T\mathbf{F}\mathbf{T})^{-1}\mathbf{D}^T]^{-1}+\mathbf{G}\}^{-1}\mathbf{A}^T\mathbf{B}^T. \tag{20}$$

This is the desired generalization of (11). If there are no Soller collimators then $\mathbf{G}=0$ and (20) simplifies to $\mathbf{M}^{-1}=\mathbf{BAD}(\mathbf{S}+\mathbf{T}^T\mathbf{F}\mathbf{T})^{-1}\mathbf{D}^T\mathbf{A}^T\mathbf{B}^T$. The normalization factor is obtained through (16), (13*a*) and (15). The new factor computed in this way takes into account automatically the absolute intensity dependence on the distances L_i, the dimensions and shape of the crystals and sample and the exposed areas of the neutron source and detector, as well as on the divergence of Soller collimators, if any. All the matrices necessary for the computations are defined in Appendices 1 and 2. The computations are performed easily with the aid of standard subroutines available in computer libraries.

3. Discussion

It is beyond the scope of this paper to evaluate explicit expressions for the resolution-function covariance-matrix elements in the general case. These expressions are cumbersome and little can be derived at their level without numerical computations (which, in turn, are most conveniently performed in matrix form). The matrix formulation allows one to handle in a simple manner the complicated expressions involved in the problem under consideration.

To illustrate, however, the way in which the focusing effects arise from the results, let us consider the simplified case when there are no Soller collimators and the crystals and the sample have the form of plates of negligible thickness. Because the x_i and y_i coordinates for thin plates are coupled, the number of spatial coordinates is reduced and one has to redefine the matrices $\mathbf{S}$, $\mathbf{T}$ and $\mathbf{D}$ of the preceding section. This is done in Appendix 3. The expressions for the elements of the covariance matrix of the distribution $P(\mathbf{k}_i,\mathbf{k}_f)$ are rather complicated even in this simple case, because of the coupling between the monochromator and analyser units. If this coupling is neglected, then the monochromator transmission function $p_M(\mathbf{k}_i)$ may be de-

fined. For this function, the explicit expressions of the normalization factor and of the elements of the covariance matrix are given in Appendix 3.

The normalization factor P_{M0} gives the total monochromatic neutron flux falling onto the sample. The expression of P_{M0} contains in the denominator the product $f(\varrho_M)f'(\varrho'_M)=(\eta_M^2+t_{11}^2\langle y_0^2\rangle+t_{12}^2\langle y_1^2\rangle+t_{13}^2\langle y_2^2\rangle)^{1/2}$ $[(\eta_M'^2+t_{26}^2\langle z_0^2\rangle+t_{27}^2\langle z_1^2\rangle+t_{28}^2\langle z_2^2\rangle)^{1/2}$, the coefficients t_{ij} being those defined in Appendix 3. The coefficients in front of $\langle y_1^2\rangle$ and $\langle z_1^2\rangle$ depend on the curvature radii ϱ_M and ϱ'_M and can be cancelled by a suitable choice of these radii. This corresponds to the spatial focusing. The explicit expression of the horizontal focusing condition $t_{12}=0$ is:

$$\sin(\theta_M+\chi_1)/L_0+\sin(\theta_M-\chi_1)/L_1=2\cos\chi_1/\varrho_M\,. \quad (21)$$

Here χ_1 is the inclination angle of the monochromator thin plate with respect to the reflecting planes. By noting that the curvature radius of the thin plate is $R_M=\varrho_M/\cos\chi_1$ one recognizes the familiar relation of horizontal focusing as given, for instance, by Maier-Leibnitz (1970). The vertical focusing condition is $t_{27}=0$, that is:

$$1/L_0+1/L_1=2\sin\theta_M/\varrho'_M \quad (22)$$

which is the relation discussed by Riste (1970).

The flux gain of the bent crystal over the plane one is given by the ratio $f(\infty)/f(\varrho_M)$ for horizontally bent crystals and by $f'(\infty)/f'(\varrho'_M)$ for vertically bent ones [f and f' being given by (A3.3 and (A3.4) in Appendix 3]. The gain factor for vertically bent crystals has been calculated also by Nunes & Shirane (1971) and Currat (1973) from simple geometrical considerations for crystals of zero mosaic spread. The expression $f'(\infty)/f'(\varrho'_M)$ and the formulae of Currat (1973) describe equally accurately the experimental data of Nunes & Shirane (1971).

The expression (A3.2) of the factor P_{M0} may be used to calculate the intensity dependence on the crystal cutting angle χ_1. When doing this, care should be taken to account also for the crystal reflectivity dependence on χ_1. For crystals in reflexion geometry, to a first approximation (strong extinction, weak absorption) $R_M^{\mathbf{k}}$ is proportional to $|\sin(\theta_M-\chi_1)/\sin(\theta_M+\chi_1)|$ for χ_1 between zero and θ_M and is independent of χ_1 elsewhere.

The expressions for the monochromator transmission covariance matrix elements given in Appendix 3 contain in the denominators just the factors which are minimized by the spatial focusing conditions. Therefore the gain in intensity at focusing implies generally a dilatation of the monochromator ellipsoid. However, it can be seen that the element $\langle Y_1^2\rangle$ can be minimized by fulfilling the conditions $d_{12}=d_{22}=1/\varrho_M$. These are the conditions of energy focusing, as $\langle Y_1^2\rangle=\langle\Delta k_i^2\rangle$ gives the energy spread of the neutron beam falling on the sample. If they are fulfilled, both spatial and energy focusing take place. The explicit conditions are:

$$L_0/\sin(\theta_M+\chi_1)=L_1/\sin(\theta_M-\chi_1)=R_M\,. \quad (23)$$

It may be ascertained that (23) coincides with the condition of monochromatic focusing as given by Maier-Leibnitz (1970). When (23) is satisfied the monochromator ellipse in the Y_1, Y_2 plane orientates with its major axis almost normally to $\mathbf{k}_I$. This is also evident from the expression for $\langle Y_1Y_2\rangle$.

The expression for $\langle Y_2^2\rangle$ shows also that for very small samples and small monochromator mosaic spread the energy focusing still occurs when the condition $d_{22}=1/\varrho_M$ only is satisfied. In this case one can use the coefficient d_{12} as a free parameter to minimize the matrix element $\langle Y_2^2\rangle$, *i.e.* to keep at a minimum the angular spread of the neutron beam. The corresponding condition is $d_{12}=2/\varrho_M$.

The above formulae may be applied also to the analyser unit. The simplest way to operate the necessary changes is to imagine the neutron motion reversed in time: the detector may be viewed then as a neutron source and the analyser unit becomes a monochromator.

In the fixed-energy back-reflexion spectrometer of Alefeld (1972) all the four conditions (21), (22) and (23) are fulfilled. To keep the focusing conditions satisfied while varying the neutron energy one can change either the distances L_i or the crystal curvature. Procedures for varying the crystal curvature have been described by Kalus *et al.* (1973) and Karas *et al.* (1974). However, the exact fulfilment of the focusing conditions is not always critical, as shown by the results of Nunes & Shirane (1971).

Let us consider now the energy transfer resolution of the triple-axis spectrometer as a whole. This resolution is given by the element $\langle X_4^2\rangle=\langle\Delta\omega^2\rangle$ of the resolution function (1) covariance matrix. This element has the following expression:

$$\langle X_4^2\rangle=(\hbar^2/m^2)\,(k_I^2\langle Y_1^2\rangle+2k_Ik_F\langle Y_1Y_4\rangle+k_F^2\langle Y_4^2\rangle) \quad (24)$$

(it may be recalled that $Y_1=\Delta k_i$ and $Y_4=\Delta k_f$). Owing to the correlation between the monochromator and analyser units the mixed term is no longer zero. This fact may be exploited to reach a new kind of focusing, when $\langle X_4^2\rangle$ is minimized by a negative mixed term $\langle Y_1Y_4\rangle$. Good energy-transfer resolution may then be obtained at relatively coarse energy resolutions in the incident and scattered beams, that is at high luminosity. This is an interesting effect which deserves special attention. It will be discussed in detail elsewhere.

I should like to acknowledge useful discussions with my colleague, A. D. Stoica, on the fundamental aspects of the computation method.

APPENDIX 1

The conventional spectrometer case

The matrices needed for computing the resolution function of the conventional spectrometer with Soller collimators are defined below.

G is an 8×8 diagonal matrix of the form $\mathbf{G}=\{\alpha_0^{-2},\alpha_1^{-2},\beta_0^{-2},\beta_1^{-2},\alpha_2^{-2},\alpha_3^{-2},\beta_2^{-2},\beta_3^{-2}\}$. $\mathbf{G}^{-1}$ is the covariance matrix of the distribution of angular variables.

F is a 4×4 diagonal matrix: $\mathbf{F}=\{\eta_M^{-2},\eta_M'^{-2},\eta_A^{-2},\eta_A'^{-2}\}$. $\mathbf{F}^{-1}$ is the covariance matrix of the reflectivity function $r_M(\xi_M,\xi_M')r_A(\xi_A,\xi_A')$.

C is a 4×8 matrix ($\mathbf{W}=\mathbf{CU}$) with the following non-zero elements:

$c_{11}=c_{12}=c_{35}=c_{36}=\frac{1}{2}$; $c_{23}=1/(2\sin\theta_M)$; $c_{33}=-c_{23}$;
$c_{47}=1/(2\sin\theta_A)$; $c_{48}=-c_{47}$.

A is a 6×8 matrix ($\mathbf{Y}=\mathbf{AU}$) with the following non-zero elements:

$a_{11}=(k_I\operatorname{ctg}\theta_M)/2$; $a_{12}=-a_{11}$; $a_{22}=a_{34}=k_I$;
$a_{45}=(k_F\operatorname{ctg}\theta_A)/2$; $a_{46}=-a_{45}$; $a_{55}=a_{67}=k_F$.

B is a 4×6 matrix ($\mathbf{X}=\mathbf{BY}$) with the following non-zero elements:

$b_{11}=\cos\varphi$; $b_{12}=\sin\varphi$; $b_{14}=-\cos(\varphi-2\theta_S)$;
$b_{15}=-\sin(\varphi-2\theta_S)$; $b_{21}=-b_{12}$; $b_{22}=b_{11}$; $b_{24}=-b_{15}$;
$b_{25}=b_{14}$; $b_{33}=1$; $b_{36}=-1$; $b_{41}=\hbar k_I/m$; $b_{44}=-\hbar k_F/m$.

In the above expressions $2\theta_S$ is the scattering angle, θ_M and θ_A are the Bragg angles of the monochromator and analyser crystals, and φ is the angle between $\mathbf{k}_I$ and the X_1 axis of the resolution-function reference frame. To direct the X_1 axis along $\mathbf{Q}_0$ one has to put $\varphi=\mathrm{ATAN2}[-k_F\sin(2\theta_S),k_I-k_F\cos(2\theta_S)]$. All these angles are measured in the trigonometric sense: θ_M from the white-beam direction, θ_S and φ from the direction of $\mathbf{k}_I$, θ_A from $\mathbf{k}_F$. The different configurations of the spectrometer are accounted for automatically by this measuring convention.

The relation (11) expresses the 4×4 covariance matrix $\mathbf{M}^{-1}$ of the conventional spectrometer resolution function through the matrices defined above. When using (11) as such in numerical computations care must be taken to avoid putting $\eta_M=0$ or $\eta_A=0$.

APPENDIX 2

The general case (spatial effects included)

The matrices **F**, **G**, **A** and **B** of Appendix 1 remain unchanged. If there are no Soller collimators, then $\mathbf{G}=0$.

The 13×13 covariance matrix $\mathbf{S}^{-1}=\{\langle v_iv_j\rangle\}$ is cell-diagonal and has the following form: $\mathbf{S}^{-1}=\{\langle y_0^2\rangle,\langle z_0^2\rangle,\mathbf{S}_1^{-1},\mathbf{S}_2^{-1},\mathbf{S}_3^{-1},\langle y_4^2\rangle,\langle z_4^2\rangle\}$, where $\mathbf{S}_i^{-1}$ are the covariance matrices of the distributions $p_i(\mathbf{r}_i)$ describing the shape of the monochromating crystal ($i=1$), sample ($i=2$) and analysing crystal ($i=3$). When the crystals are used in symmetric transmission or reflexion geometry the matrices $\mathbf{S}_1^{-1}$ and $\mathbf{S}_3^{-1}$ are diagonal. The matrix $\mathbf{S}_2^{-1}$ is diagonal for cylindrical samples and for samples disposed symmetrically with respect to the bisector of the scattering angle.

T is a 4×13 matrix ($\mathbf{W}=\mathbf{TV}$) with the following non-zero elements:

$t_{11}=1/(2L_0)$; $t_{13}=\cos\theta_M(1/L_1-1/L_0)/2$;
$t_{14}=\sin\theta_M[1/L_0+1/L_1-2/(\varrho_M\sin\theta_M)]/2$;
$t_{16}=\sin\theta_S/(2L_1)$; $t_{17}=\cos\theta_S/(2L_1)$;
$t_{22}=-1/(2L_0\sin\theta_M)$;
$t_{25}=(1/L_0+1/L_1-2\sin\theta_M/\varrho_M')/(2\sin\theta_M)$;
$t_{28}=-1/(2L_1\sin\theta_M)$; $t_{36}=\sin\theta_S/(2L_2)$;
$t_{37}=-\cos\theta_S/(2L_2)$; $t_{39}=\cos\theta_A(1/L_3-1/L_2)/2$;
$t_{310}=\sin\theta_A[1/L_2+1/L_3-2/(\varrho_A\sin\theta_A)]/2$; $t_{312}=1/(2L_3)$;
$t_{48}=-1/(2L_2\sin\theta_A)$;
$t_{411}=(1/L_2+1/L_3-2\sin\theta_A/\varrho_A')/(2\sin\theta_A)$;
$t_{413}=-1/(2L_3\sin\theta_A)$.

D is a 8×13 matrix ($\mathbf{U}=\mathbf{DV}$) with the following non-zero elements:

$d_{11}=-1/L_0$; $d_{13}=-\cos\theta_M/L_0$; $d_{14}=\sin\theta_M/L_0$;
$d_{22}=d_{11}$; $d_{25}=-d_{11}$; $d_{33}=\cos\theta_M/L_1$; $d_{34}=\sin\theta_M/L_1$;
$d_{36}=\sin\theta_S/L_1$; $d_{37}=\cos\theta_S/L_1$; $d_{45}=-1/L_1$; $d_{48}=-d_{45}$;
$d_{56}=\sin\theta_S/L_2$; $d_{59}=-\cos\theta_A/L_2$; $d_{510}=\sin\theta_A/L_2$;
$d_{68}=-1/L_2$; $d_{611}=-d_{68}$; $d_{79}=\cos\theta_A/L_3$;
$d_{710}=\sin\theta_A/L_3$; $d_{712}=1/L_3$; $d_{811}=-d_{712}$; $d_{813}=d_{712}$.

The 4×4 covariance matrix $\mathbf{M}^{-1}$ of the triple-axis spectrometer resolution function is obtained through the relation (20) with the aid of the matrices defined above.

APPENDIX 3

Simplified case: no Soller collimators, thin crystals and sample

When the thickness of crystals and sample is neglected the x_i and y_i coordinates are no longer independent. The vector **V** of the spatial coordinates has to be modified to $\mathbf{V}=(y_0,y_1,y_2,y_3,y_4,z_0,z_1,z_2,z_3,z_4)$. The covariance matrix $\mathbf{S}^{-1}=\{\langle v_iv_j\rangle\}$ becomes diagonal, with the following elements:

$$\langle y_i^2\rangle=l_i^2\cos^2\chi_i/12;\quad\langle z_i^2\rangle=h_i^2/12$$

where l_i and h_i ($i=0,1,2,3,4$) are the length and the height of the ith thin plate and χ_i is the plate inclination angle with respect to the y_i coordinate axis of Fig. 1 (the neutron source and the detector are likened to thin plates disposed normally to the neutron beams, $\chi_0=\chi_4=0$). The inclination angles χ_1 and χ_3 are zero for crystals in symmetrical reflexion, the angle χ_2 is zero for sample in symmetrical transmission.

The 4×10 matrix **T** has now the following non-zero elements:

$t_{11}=-1/(2L_0)$; $t_{12}=[\sin(\theta_M+\chi_1)/L_0+\sin(\theta_M-\chi_1)/L_1-2\cos\chi_1/\varrho_M]/(2\cos\chi_1)$;
$t_{13}=\cos(\theta_S+\chi_2)/(2L_1\cos\chi_2)$; $t_{26}=-1/(2L_0\sin\theta_M)$;

$t_{27}=(1/L_0+1/L_1-2\sin\theta_M/\varrho'_M)/(2\sin\theta_M)$;
$t_{28}=-1/(2L_1\sin\theta_M)$; $t_{33}=-\cos(\theta_S-\chi_2)/(2L_2\cos\chi_2)$;
$t_{34}=[\sin(\theta_A+\chi_3)/L_2+\sin(\theta_A-\chi_3)/L_3-2\cos\chi_3/\varrho_A]/(2\cos\chi_3)$; $t_{35}=1/(2L_3)$; $t_{48}=-1/(2L_2\sin\theta_A)$;
$t_{49}=(1/L_2+1/L_3-2\sin\theta_A/\varrho'_A)/(2\sin\theta_A)$;
$t_{410}=-1/(2L_3\sin\theta_A)$.

The modified 8×10 matrix **D** of the transformation from spatial to angular variables has the following non-zero elements:

$d_{11}=-1/L_0$; $d_{12}=\sin(\theta_M+\chi_1)/(L_0\cos\chi_1)$;
$d_{22}=\sin(\theta_M-\chi_1)/(L_1\cos\chi_1)$;
$d_{23}=\cos(\theta_S+\chi_2)/(L_1\cos\chi_2)$; $d_{36}=d_{11}$; $d_{37}=-d_{11}$;
$d_{47}=-1/L_1$; $d_{48}=-d_{47}$;
$d_{53}=-\cos(\theta_S-\chi_2)/(L_2\cos\chi_2)$;
$d_{54}=\sin(\theta_A+\chi_3)/(L_2\cos\chi_3)$;
$d_{64}=\sin(\theta_A-\chi_3)/(L_3\cos\chi_3)$; $d_{65}=1/L_3$; $d_{78}=-1/L_2$;
$d_{79}=-d_{78}$; $d_{89}=-d_{65}$; $d_{810}=d_{65}$.

The monochromator unit transmission function $p_M(\mathbf{k}_i)$ obtained by neglecting the correlation with the analyser unit has, in the normal approximation, the expression:

$$p_M(\mathbf{Y})=P_{M0}(2\pi)^{-3/2}\sqrt{\det\mathbf{L}}\exp(-\tfrac{1}{2}\mathbf{Y}^T\mathbf{L}\mathbf{Y})\,. \quad (A3.1)$$

Here $\mathbf{Y}=\mathbf{k}_i-\mathbf{k}_I$ and $\mathbf{L}^{-1}=\{\langle Y_iY_j\rangle\}$. The normalization factor P_{M0} has the expression:

$$P_{M0}=\frac{R_M^{\mathbf{k}}}{4\sin\theta_M}(2\pi)\frac{gg'}{f(\varrho_M)f'(\varrho'_M)} \quad (A3.2)$$

where f, f', g and g' have the following expressions:

$$f(\varrho_M)=(\eta_M^2+t_{11}^2\langle y_0^2\rangle+t_{12}^2\langle y_1^2\rangle+t_{13}^2\langle y_2^2\rangle)^{1/2} \quad (A3.3)$$

$$f'(\varrho'_M)=(\eta_M'^2+t_{26}^2\langle z_0^2\rangle+t_{27}^2\langle z_1^2\rangle+t_{28}^2\langle z_2^2\rangle)^{1/2} \quad (A3.4)$$

$$g=(d_{11}^2d_{22}^2\langle y_0^2\rangle\langle y_1^2\rangle+d_{11}^2d_{23}^2\langle y_0^2\rangle\langle y_2^2\rangle+d_{12}^2d_{23}^2\langle y_1^2\rangle\langle y_2^2\rangle)^{1/2} \quad (A3.5)$$

$$g'=(\langle z_0^2\rangle\langle z_1^2\rangle+\langle z_0^2\rangle\langle z_2^2\rangle+\langle z_1^2\rangle\langle z_2^2\rangle)^{1/2}/(L_0L_1) \quad (A3.6)$$

with the coefficients d_{ij} and t_{ij} given above.

The elements of the covariance matrix of the monochromator unit transmission function have the following expressions:

$$\langle Y_1^2\rangle=\frac{k_I^2\langle\Delta\tau_M^2\rangle}{\tau_M^2}+\frac{k_I^2\operatorname{ctg}^2\theta_M}{4f^2(\varrho_M)}[\eta_M^2d_{11}^2\langle y_0^2\rangle+\eta_M^2(d_{12}-d_{22})^2\langle y_1^2\rangle+\eta_M^2d_{23}^2\langle y_2^2\rangle+d_{11}^2(d_{22}-1/\varrho_M)^2\langle y_0^2\rangle\langle y_1^2\rangle+d_{11}^2d_{23}^2\langle y_0^2\rangle\langle y_2^2\rangle+d_{23}^2(d_{12}-1/\varrho_M)^2\langle y_1^2\rangle\langle y_2^2\rangle] \quad (A3.7)$$

$$\langle Y_1Y_2\rangle=\frac{k_I^2\operatorname{ctg}\theta_M}{4f^2(\varrho_M)}[2\eta_M^2(d_{11}d_{22}\langle y_1^2\rangle-d_{23}^2\langle y_2^2\rangle)+d_{11}^2d_{23}^2\langle y_0^2\rangle\langle y_2^2\rangle-d_{11}^2d_{22}(d_{22}-1/\varrho_M)\langle y_0^2\rangle\langle y_1^2\rangle-d_{23}^2(d_{12}-1/\varrho_M)(d_{12}-2/\varrho_M)\langle y_1^2\rangle\langle y_2^2\rangle] \quad (A3.8)$$

$$\langle Y_2^2\rangle=\frac{k_I^2}{4f^2(\varrho_M)}[4\eta_M^2d_{22}^2\langle y_1^2\rangle+4\eta_M^2d_{23}^2\langle y_2^2\rangle+d_{11}^2d_{22}^2\langle y_0^2\rangle\langle y_1^2\rangle+d_{11}^2d_{23}^2\langle y_0^2\rangle\langle y_2^2\rangle+d_{23}^2(d_{12}-2/\varrho_M)^2\langle y_1^2\rangle\langle y_2^2\rangle] \quad (A3.9)$$

$$\langle Y_3^2\rangle=\frac{k_I^2}{L_1^2f'^2(\varrho'_M)}[\eta_M'^2(\langle z_1^2\rangle+\langle z_2^2\rangle)+t_{26}^2(\langle z_1^2\rangle+\langle z_2^2\rangle)\langle z_0^2\rangle+(t_{26}+1/\varrho'_M)^2\langle z_1^2\rangle\langle z_2^2\rangle]\,. \quad (A3.10)$$

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