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# THE RESOLUTION FUNCTION FOR THE ROTATING-CRYSTAL SPECTROMETER

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# THE RESOLUTION FUNCTION FOR THE ROTATING-CRYSTAL SPECTROMETER

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The resolution function in the $(\vec{Q},\omega)$ space for the rotating-crystal time-of-flight spectrometer is defined. All the instrumental components bringing a contribution to the uncertainties in the measured energy and momentum transfers are taken into account. A detailed analysis of the monochromator unit transmission, including the Doppler effect influence, is presented. An analytic expression is derived for the resolution function in the Gaussian approximation.

## 1. INTRODUCTION

During the last years, the resolution function of the thermal neutron spectrometers used in condensed matter studies has been considered by a number of authors. Its analytical expression for a triple axis neutron spectrometer and for a twin-rotor time-of-flight spectrometer was calculated in refs. /1,2,3/ and in /4/, respectively. For the case of the rotating-crystal spectrometer /5/, a time-of-flight resolution function has been discussed by Furrer/6/. This function depends on the measured cross-section, hence it is not defined exclusively by the instrument.

The present paper contains an analytical treatment of the resolution function in the $(\vec{Q},\omega)$ space for the rotating-crystal

spectrometer. All the sources of the uncertainties in the measured momentum and energy transfers have been considered for a particular channel of the time analyser and a given setting. These sources are: the dimensions and the shape of the monochromator crystal, sample and detector, the Doppler effect, the width of the analyser channel, the collimators angular divergences and the monochromator mosaic spread.

The resolution function is defined in sec.2 and the necessary approximations for obtaining an analytical form are given. In sec.3 the transmission function of the monochromator unit is derived. Unlike the equivalent function calculated in ref. /2/, this function depends on the crystal coordinates and on the time also. This dependence is due to the Doppler effect and to the rotation respectively. The Gaussian expression for the resolution function is given in sec.4 in a form suitable for a simple computer program.

## 2. DEFINITION OF THE RESOLUTION FUNCTION

The layout of a rotating-crystal spectrometer is presented in fig.1. The horizontal and vertical angular divergences of the i-th collimator $C_i$ (i=1,2,3) are $\alpha_i$ and $\beta_i$ respectively. The collimators axes are contained in the horizontal plane. The monochromator crystal, of cylindrical shape with radius $r_o$ and height $z_o$, rotates around a vertical axis contained in a reflecting plane belonging to the most probable mosaic block. Let the coordinate system $(M,\vec{I},\vec{J},\vec{K})$ be connected with the crystal in such a way, that the $\vec{K}$ axis is vertical and the $\vec{I}$ axis is normal to the above - mentioned reflecting plane. Let t=0 be the moment when $\vec{I}$ beco...

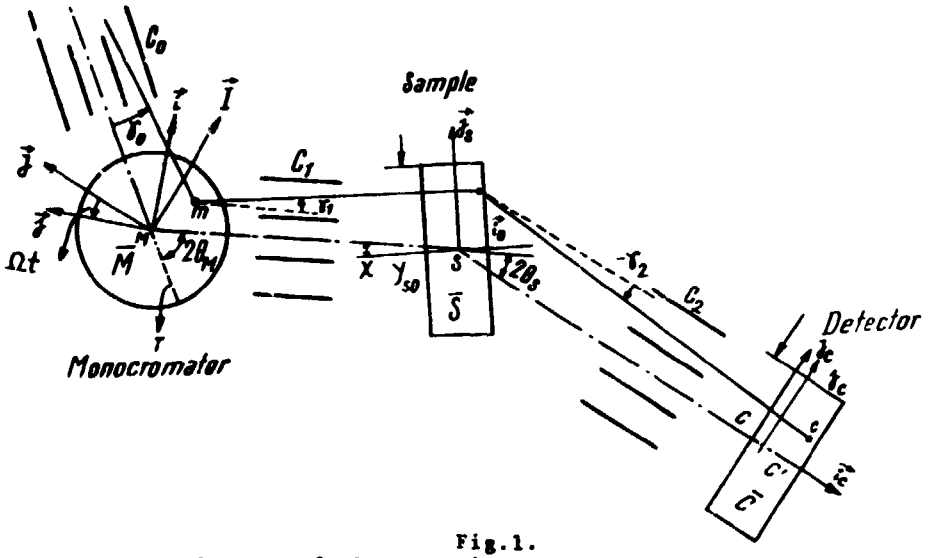


Fig.1.
Layout of the rotating-crystal spectrometer.

external bisectrix of the angle $2\theta_M$ between the axes of the collimators $C_o$ and $C_1$. At t=0 the laboratory coordinate system $(M,\vec{I},\vec{J},\vec{L})$ coincides with $(M,\vec{I},\vec{J},\vec{L})$. The coordinate system for the sample is chosen as in fig.1. The sample is either a rectangular prism of $x_{os},y_{os},z_{os}$ dimensions or a cylinder of $r_{os}$ radius and $z_{os}$ height. The detector (which consists usually of two rows of cylindrical counters of $\rho_o$ radius and a total window of dimensions $y_{oc},z_{oc}$) is considered, for the sake of simplicity, to be a rectangular prism of effective thickness $x_{oc} = \pi\rho_o$. The detector coordinate systems are $(C,\vec{I}_c,\vec{J}_c,\vec{L}_c)$ and $(C',\vec{I}'_c,\vec{J}'_c,\vec{L}'_c)$, the $\vec{I}_c$ and $\vec{I}'_c$ axes being the same, and the segment C'C being defined by the weight center of the absorption function $\langle x_c\rangle$ = C'C. The value of $\langle x_c\rangle$ depends on the mean wavelength corresponding to each time channel. Let us denote MS with $L_I$ and SC with $L_{Fo}$. The segments $L_I$ and $L_F = L_{Fo} + \langle x_c\rangle$ are the mean flight paths of the neutrons

before and after the scattering, respectively.

For a given interplanar distance d of the monochromator, and given angles $2\theta_M$ and $2\theta_S$, in the analyser time channel $T_o$ neutrons will be detected corresponding to the mean scattering process :

$$\vec{Q}_o = \vec{k}_F - \vec{k}_I \qquad (2.1.1)$$

$$\hbar\omega_o = (\hbar^2/2m)(k_I^2 - k_F^2) \qquad (2.1.2)$$

where m is the neutrons mass and

$$k_I = \pi/(d \sin\theta_M) \qquad (2.2.1)$$

$$k_F = L_F k_I / (\hbar k_I T_o/m - L_I) \qquad (2.2.2)$$

The intensity detected in the $T_o$ channel will be :

$$I(T_o) = I(\vec{Q}_o, \omega_o) = \int R(\vec{Q}-\vec{Q}_o, \omega-\omega_o)\, \sigma(\vec{Q},\omega)\, d\vec{Q}\, d\omega \qquad (2.3)$$

where $\sigma(\vec{Q},\omega)$ is the cross section of the sample. $R(\Delta\vec{Q},\Delta\omega)$ is the resolution function of the instrument for a particular time channel /4/. It is defined as the probability of detecting neutrons corresponding to the scattering process associated with the particular point $(\vec{Q}_c+\Delta\vec{Q}, \omega_o+\Delta\omega)$ in the $(\vec{Q},\omega)$ space.

Let us assume that a neutron is reflected at the moment t at the point (x,y,z) with a wave-vector $\vec{k}_I + \Delta\vec{k}_i$, is scattered at $(x_s,y_s,z_s)$ with a wave-vector $\vec{k}_F+\Delta\vec{k}_f$ and absorbed at $(x'_c,y'_c,z'_c)$. The resolution function will be then :

$$R(\Delta\vec{Q},\Delta\omega) = \frac{1}{|\bar{M}||\bar{S}||\bar{C}|} \int_{\bar{M}} dx\, dy \int_{\bar{S}} dx_s\, dy_s \int_{\bar{C}} dx'_c\, dy'_c \int_{-\infty}^{\infty} dt$$

$$\int d(\Delta\vec{k}_i)\, d(\Delta\vec{k}_f)\, P_M(\Delta\vec{k}_i,\vec{r},t)\; T_2(\Delta\vec{k}_f)\; P_c(x'_c,y'_c)\; P_T(\Delta T) \qquad (2.4)$$

$$\delta(\Delta\vec{Q}-\Delta\vec{k}_f+\Delta\vec{k}_i)\; \delta(k_F\Delta k_f - k_f\Delta k_i + (\hbar/m)\Delta\omega)\; \delta(y_s-\varphi_1)\,\delta(y'_c-\varphi_2)$$

The expression (2.4) implies that in a first approximation the resolution function is not affected by the vertical dimensions of the instrumental elements, and that $y_s$ and $y'_c$ are not independent variables. The quantities $|\bar{M}|, |\bar{S}|, |\bar{C}|$ are the areas of the horizontal sections $\bar{M}$, $\bar{S}$, and $\bar{C}$ in the monochromator, sample and detector respectively.

The quantity $\Delta T$ is given by :

$$\Delta T = T - T_o \qquad (2.5.1)$$

where

$$T_o = (m/\hbar)(L_I/k_I + L_F/k_F) \qquad (2.5.2)$$

$T_o$ is the moment of detection of a mean neutron reflected at t=0 at the point M with a wavevector $\vec{k}_I$, scattered at S with a wavevector $\vec{k}_F$ and absorbed in C'. The quantity T is given by

$$T = t + (m/\hbar)(L_i/k_i + L_f/k_f) \qquad (2.5.3)$$

and represents the moment of detection in the same channel of the neutron under consideration in (2.4).

One can write

$$\Delta T = t + (m/h)(\Delta L_i/L_I + \Delta L_f/L_f - L_I\Delta k_i/k_I^2 - L_F\Delta k_f/k_F^2) \tag{2.6}$$

It is easily found that

$$\Delta L_i = L_i - L_I = -\zeta_1 X + \zeta_2 Y + x_s/\cos\chi - \gamma_1 L_I \mathrm{tg}\chi \tag{2.7.1}$$

$$\Delta L_f = L_f - L_F = \xi_1\cos\theta_M X + \xi_1\sin\theta_M Y + \xi_1 L_I\ \gamma_1 - \beta x_s/\cos\chi + x'_c \tag{2.7.2}$$

and also that

$$Y_s = \varphi_1 = (\cos\theta_M/\cos\chi)X + (\sin\theta_M/\cos\chi)Y + \gamma_1 L_I\cos\chi - x_s\mathrm{tg}\chi \tag{2.8.1}$$

$$Y'_c = \varphi_2 = \xi_2\cos\theta_M X + \xi_2\sin\theta_M Y + \gamma_1 L_I\ \xi_2 + x_s\alpha/\cos\chi + \gamma_2 L_F$$

where

$$\zeta_1 = \sin\theta_M + \mathrm{tg}\chi\cos\theta_M \tag{2.9}$$

$$\zeta_2 = \cos\theta_M - \mathrm{tg}\chi\sin\theta_M$$

$$\alpha = \sin 2\theta_s \ ; \quad \beta = \cos 2\theta_s \tag{2.10}$$

$$\xi_1 = \alpha + \beta\mathrm{tg}\chi \ ; \quad \xi_2 = \alpha - \beta\mathrm{tg}\chi \tag{2.11}$$

$\chi$ is the angle between the normal to the sample and the incoming beam ( $\chi = 0$ when the sample is a cylinder). X,Y are the coordinates of a point (x,y) of the monochromator in the laboratory system. The laboratory system $(M,\vec{I},\vec{J},\vec{L})$ is connected with the system $(M,\vec{I},\vec{j},\vec{l})$ by the relations :

$$X = x\cos\Omega t - y\sin\Omega t = x$$
$$Y = y\cos\Omega t + x\sin\Omega t = y \qquad (2.12)$$

Here was taken into account the fact that the instrument transmits only for small $\Omega t$, due to the existence of the collimators $C_o$ and $C_1$. The quantity $\Omega/2\pi$ is the frequency of the monochromator rotation.

The functions under the integral sign in (2.4) are probability functions, with the following meanings : $P_M$ is the transmission of the monochromator unit (collimators $C_o$,$C_1$ and monochromating crystal) $T_2$ - the transmission of the collimator $C_2$, $P_c$ is the probability of absorption in the detector, $P_T$ is the acceptance of the analyser channel. $P_M$ is a convolution between the crystal reflectivity function with the transmission functions of the collimators $C_o$ and $C_1$. These functions have different forms (the crystal reflectivity has a shape given by the mosaic crystal theory, the collimator transmissions are triangular functions, $P_T$ is rectangular with a width $\Delta\tau$, $P_c$ is of the form $\exp(-\mu x_c)$ in the $(0,x_{oc})$ range and zero otherwise). It is reasonable to make use of the Gaussian approximation for each of them, on the grounds that the folding of a large number of functions having arbitrary forms gives a nearly Gaussian.

The Gaussian approximation of the resolution function is obtained by replacing each of the above mentioned functions by a Gaussian of the same dispersion :

$$f_G(x) = \frac{1}{\sqrt{2\pi}\alpha^*} e^{-\frac{1}{2}(x/\alpha^*)^2} \qquad (2.13)$$

where $\langle x \rangle = 0$ was assumed.

For a triangle of half width at half maximum $\alpha$ one has $\alpha^* = \alpha/\sqrt{6}$, and for a rectangle of width $\alpha$, $\alpha^* = \alpha/\sqrt{12}$. In the integrals of the following type :

$$I(\ldots) = \frac{1}{|\bar{D}|} \int_{\bar{D}} du\, dv F(u,v,\ldots) = \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv \psi(u,v)\ F(u,v,\ldots) \tag{2.14.1}$$

where

$$\psi(u,v) = \begin{cases} \dfrac{1}{|\bar{D}|} & \text{for} \quad (u,v) \in D \\ 0 & \text{otherwise} \end{cases}$$

the function $\psi$ has to be replaced by the Gaussian function having the same covariance matrix :

$$\psi_G = \frac{1}{2\pi \alpha_1^* \alpha_2^*}\ e^{-\frac{1}{2}(u^2/\alpha_1^{*2} + v^2/\alpha_2^{*2})} \tag{2.14.2}$$

where $\langle u \rangle = \langle v \rangle = 0$ is assumed, and also $\langle uv \rangle = 0$.

If $\bar{D}$ is the circle of radius $\alpha$, then $\alpha_1^* = \alpha_2^* = \alpha/2$. If $\bar{D}$ is a rectangle of sides $\alpha_1$ and $\alpha_2$, then $\alpha_1^* = \alpha_1/\sqrt{12}$ and $\alpha_2^* = \alpha_2/\sqrt{12}$.

## 3. THE FUNCTIONS $P_M$ AND $P_C$

Let the vertical and horizontal mosaic spread of the crystal be $\eta$. Let be $\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$ the position vector in a

point of the crystal. In the approximation of a weak extinction, after having performed the approximations mentioned in sec.2 for the collimators, for the transmission function of the monochromator unit (for the unity volume of the crystal) one obtains:

$$dP_M = \frac{Q(\vec{r})}{(2\pi)^3 a_o^* a_1^* \beta_o^* \beta_1^*} \exp\left[-\frac{1}{2}\left[\left(\frac{\gamma_o}{a_o^*}\right)^2 + \left(\frac{\delta_o}{\beta_o^*}\right)^2 + \left(\frac{\Delta_h}{\eta}\right)^2 + \left(\frac{\Delta_v}{\eta}\right)^2 + \right.\right.$$

$$\left.\left. + \left(\frac{\gamma_1}{a_1^*}\right)^2 + \left(\frac{\delta_1}{\beta_1^*}\right)^2\right]\right] d\delta_o \qquad (3.1)$$

where $Q(\vec{r})$ is the reflectivity of the unit volume and $a_1^* = a_1/\sqrt{6}$ and $\beta_1^* = \beta_1/\sqrt{6}$ .

By using relations (9,10,11) from the Appendix one obtains :

$$\gamma_o = 2(\Delta k_1/k_I)\,tg\theta_M + \gamma_1 - 4(m/\hbar)\,tg\theta_M \sin^2\theta_M\, \vec{\vec{v\tau}}_p/\tau^2 \qquad (3.2.1)$$

$$\Delta_h = (\Delta k_1/k_I)\,tg\theta_M + \gamma_1 - \omega^* - 2(m/\hbar)\,tg\theta_M\, \vec{\vec{v\tau}}_p/\tau^2 \qquad (3.2.2)$$

$$\Delta_v = (\delta_1 - \delta_o)/(2\sin\theta_M) \qquad (3.2.3)$$

For $\Omega t$ of the order of collimator divergences one can write :

$$\vec{\tau}_p/\tau = \vec{I} + \Omega t\, \vec{J} \qquad (3.3)$$

$$\vec{V} = -\Omega(y + x\Omega t)\, \vec{I} + \Omega(x - y\Omega t)\vec{J} \qquad (3.4)$$

so that .

$$\omega^* = \Omega t \qquad (3.5)$$

$$2(m/\hbar)\vec{v}\vec{\tau}_p/\tau^2 = -2(m/\hbar)(\Omega y/\tau) \qquad (3.6)$$

Putting all these expressions into (3.1) and integrating over $\delta_o$, one obtains :

$$F_M(\Delta\vec{k}_i,\vec{r},t) = P_o \exp\{-\frac{1}{2}\left[\left(\frac{2\Delta k_i/k_I tg\theta_M+\gamma_1+4m\Omega y/(\hbar\tau)tg\theta_M sin^2\theta_M}{\alpha_o^*}\right)^2 + \right.$$

$$\left. + \left(\frac{\Delta k_i/k_I tg\theta_M+\gamma_1+2m\Omega y/(\hbar\tau)tg\theta_M-\Omega t}{\eta}\right)^2 + \left(\frac{\gamma_1}{\alpha_1^*}\right)^2 + \left(\frac{\delta_1}{\beta_1^*}\right)^2 + \frac{\delta_1^2}{\beta_o^{*2}+4\eta^2 sin^2\theta_M}\right]\} \qquad (3.7)$$

where

$$P_o = \frac{Q(\vec{r})\ sin\theta_M}{(2\pi)^{5/2}\eta\alpha_o^*\alpha_1^*\beta_1^*\sqrt{\beta_o^{*2}+4\eta^2 sin^2\theta_M}} \qquad (3.8)$$

It can be shown that for small enough frequencies one has :

$$Q(\vec{r}) \simeq Q(0)\ (1 + \nu\frac{m}{\hbar}\frac{\Omega y}{\tau}) \qquad (3.9)$$

where $\nu$ depends on $\theta_M$. The second term in (3.9) is of the order of $10^{-2}$ and therefore may be neglected.

In a first approximation the absorption function will depend only on $x_c$ :

$$P_C(x_c)\ dx_c = e^{-\mu x_c}(1-e^{-\mu dx_c}) = \mu e^{-\mu x_c} dx_c \qquad (3.1o)$$

The function $\tilde{P}_c(x_c) = x_{oc}^{-1} P_C(x_c)$ appearing in the relation (2.4) becomes, when normalized :

$$\tilde{P}_C(x_c) = \mu e^{-\mu x_c}/(1-e^{-\mu x_{oc}}) \qquad (3.11)$$

The quantity $\mu$ is the absorption coefficient of the detector. It has a weak and linear dependence on the wavelength of the detected neutron :

$$\mu = ck_f^{-1} = ck_P^{-1} = ck_{Po}^{-1} = c(\hbar k_i T_o/m - L_I)/L_{Po} \qquad (3.12)$$

where $c$ is a constant characterizing the absorbant). The quantities $\langle x_c \rangle$ and $\langle x_c^2 \rangle$ have the following expressions :

$$\langle x_c \rangle = \frac{1}{\mu} - x_{oc}/(e^{\mu x_{oc}}-1) \qquad (3.13.1)$$

$$\langle x_c^2 \rangle = (2/\mu)\langle x_c \rangle - x_{oc}^2/(e^{\mu x_{oc}}-1) \qquad (3.13.2)$$

In order to keep the Gaussian approximation one has to put:

$$\tilde{P}_c(x_c) = \frac{1}{\sqrt{2\pi}\varepsilon} \exp\left[-\tfrac{1}{2}(x_c-x_c)^2/\varepsilon^2\right] = \frac{1}{\sqrt{2\pi}\varepsilon} \exp\left[-\tfrac{1}{2}(x_c'/\varepsilon)^2\right] = \tilde{P}_C(x_c') \qquad (3.14.1)$$

where

$$\varepsilon^2 = \langle x_c^2 \rangle - \langle x_c \rangle^2 \qquad (3.14.2)$$

## 4. DERIVATION OF THE RESOLUTION FUNCTION

Within the approximations of sec.2 and . the resolution function has the expression :

$$R(\Delta\vec{Q},\Delta\omega) = R'_o \int d(\Delta\vec{k}_i)\; d(\Delta\vec{k}_f)\,\delta(\Delta\vec{Q}-\Delta\vec{k}_f+\Delta\vec{k}_i)\,\delta(k_F\Delta k_f - k_I\Delta k_i +$$

$$+ m\,\Delta\omega/\hbar)\,\exp\left[-\tfrac{1}{2}(E_1+E_2)\right]\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} du_1\, du_2 du_3\, du_4\, du_5\, \exp(-E_3/2) \tag{4.1}$$

where

$$R'_o = \frac{36\sqrt{2}}{5/2}\,\frac{x_{oc}}{\varepsilon\Delta\tau}\,\frac{P_o}{|\vec{M}||\vec{S}||\vec{C}|} \tag{4.2}$$

(for cylindrical samples $R'_o \pi \Rightarrow R'_o/3$ ), and

$$E_1 = a_7^2 v_3^2 + a_{11}^2 v_4^2 \tag{4.3.1}$$

$$E_2 = a_{13}^2\,\delta_1^2 + a_{14}^2\,\delta_2^2 \tag{4.3.2}$$

$$E_3 = \sum_{i,j=1}^{5} M_{ij}u_i u_j + 2\sum_{i=1}^{5} c_i u_i + \sum_{i=1}^{5} d_i^2 = U'MU + 2C'U + D'D \tag{4.3.3}$$

$$C = K\,D\;; \qquad D = J\,V \tag{4.4}$$

The quantities $a_i$ (i=1,?,...,32) are given in table I, and the matrices M,K,J in tables II and III. E is the unity matrix, and the vectors U and V are :

$$U = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix} \equiv \begin{pmatrix} t \\ x \\ y \\ x_s \\ x'_c \end{pmatrix} \qquad V = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} \equiv \begin{pmatrix} \Delta k_i \\ \Delta k_f \\ \gamma_1 \\ \gamma_2 \end{pmatrix} \tag{4.5}$$

Making use of the translation :

$$U = W - N^{-1}C \tag{4.6}$$

one obtains for $E_3$ :

$$E_3 = W'NW - C'N^{-1}C + D'ED = W'NW + F_4 \tag{4.7}$$

and the last five integrals in (4.1) may be written as (see ref.7):

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} du_1 \dots du_5 \exp(-E_3/2) = \exp(-E_4/2) \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dw_1 \dots dw_5$$

$$\exp\left(-\frac{1}{2}\sum_{i,j=1}^{5} N_{ij}v_i v_j\right) = (2\pi)^{5/2}\exp(-E_4/2)/|N|^{1/2} \tag{4.8}$$

where $|N|$ is the determinant of the matrix N .

By using (4.4) one gets for $E_4$ :

$$E_4 = D'(E-K'N^{-1}K)D = V'FV \tag{4.9}$$

where

$$F = J'(E-K'N^{-1}K)J \tag{4.10}$$

Now, one has to rewrite the elements $F_{33}$ and $F_{44}$ of the matrix F with the aid of $E_1$ from (4.3):

$$F_{33}(\text{new}) = F_{33}(\text{old}) + a_7^2$$
$$F_{44}(\text{new}) = F_{44}(\text{old}) + a_{11}^2 \qquad (4.11)$$

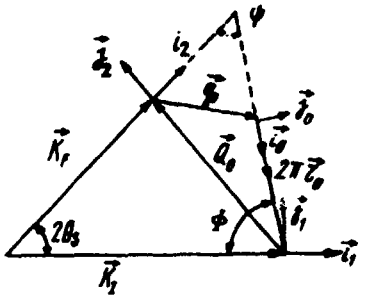


Fig.2.
Geometry of the scattering process in the reciprocal space.

It remains to carry out the integrals over $\Delta\vec{k}_i$ and $\Delta\vec{k}_f$. According to fig.2, one has :

$$\Delta\vec{k}_i = \Delta k_i\vec{I}_1 + k_I\gamma_1\vec{J}_1 + k_I\delta_1\vec{I}_1 = (b\Delta k_i - ak_I\gamma_1)\vec{I}_o + (a\Delta k_i + bk_I\gamma_1)\vec{J}_o + k_I\delta_1\vec{I}_o \qquad (4.12.1)$$

$$\Delta\vec{k}_f = \Delta k_f\vec{I}_2 + k_F\gamma_2\vec{J}_2 + k_F\delta_2\vec{I}_2 = (-B\Delta k_f - Ak_F\gamma_2)\vec{I}_o + (A\Delta k_f - Bk_F\gamma_2)\vec{J}_o + k_F\delta_2\vec{I}_o \qquad (4.12.2)$$

$$\Delta\vec{Q} = \Delta Q_x\vec{I}_o + \Delta Q_y\vec{J}_o + \Delta Q_z\vec{I}_o \qquad (4.12.3)$$

where $a = \sin\phi$; $b = \cos\phi$ ; $A = \sin\psi$ ; $B = \cos\psi$ (4.13)

By taking into account that

$$d(\Delta\vec{k}_i)\,d(\Delta\vec{k}_f) = k_I^2k_F^2\,d(\Delta k_i)\,d(\Delta k_f)\,d\gamma_1 d\gamma_2 d\delta_1 d\delta_2 = k_I^2k_F^2 dv_1 dv_2 dv_3 dv_4 d\delta_1 d\delta_2 \qquad (4.14)$$

and by setting :

$$\Delta Q_x = X_1; \quad \Delta Q_y = X_2 \; ; \; \Delta\omega = X_4 \text{ and } \Delta k_1 = v_1 = X_3 \qquad (4.15)$$

one obtains for the resolution function :

$$R(\Delta\vec{Q},\Delta\omega) = \frac{(2\pi)^{5/2} R'_o}{|N|^{1/2}} \frac{k_I}{k_F} \int_{-\infty}^{\infty} d\delta_1 \int_{-\infty}^{\infty} d\delta_2 e^{-E_2/2} \, \delta(\delta_2 - \delta_1 - \Delta Q_z/k_F)$$

$$\int_{-\infty}^{\infty} .. \int_{-\infty}^{\infty} dv_1 dv_2 dv_3 dv_4 \left[\prod_{i=2}^{4} \delta(v_i - \sum_{j=1}^{4} I_{ij} X_j)\right] \exp(-\tfrac{1}{2} \sum_{i,j=1}^{4} F_{ij} v_i v_j) \qquad (4.16)$$

where $\lambda = k_I/k_F$ and :

$$I = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & \lambda & -m/(\hbar k_F) \\ B/(\alpha k_I) & -A/(\alpha k_I) & (\lambda-\beta)/(\alpha k_I) & -m/(\hbar\alpha k_I k_F) \\ -b/(\alpha k_F) & -A/(\alpha k_F) & (\lambda\beta-1)/k_F & -m\beta/(\hbar\alpha k_F^2) \end{pmatrix} \qquad (4.17)$$

The integral over $\delta_1$ and $\delta_2$ from (4.16) becomes :

$$I_1 = (2\pi/(k_F^2 a_{13}^2 + k_I^2 a_{14}^2))^{1/2} k_F \exp - \frac{1}{2} \frac{a_{13}^2 a_{14}^2}{k_F^2 a_{13}^2 + k_I^2 a_{14}^2} (\Delta Q_z)^2 \qquad (4.18)$$

and the integrals over $v_1, v_2, v_3, v_4$

$$I_2 = \int_{-\infty}^{\infty} dX_3 \exp(-\frac{1}{2} \sum_{i,j=1}^{4} s_{ij}X_iX_j) \qquad (4.19)$$

where :

$$S = I'FI \qquad (4.20)$$

By putting :

$$M_{ij} = S_{ij} - S_{3i}S_{3j}/S_{33} \qquad (i,j=1,2,3,4) \qquad (4.21)$$

one may write for the integrals $I_2$ :

$$I_2 = (2\pi/S_{33})^{1/2} \exp(-\frac{1}{2} \sum_{i,j=1}^{4} M_{ij}X_iX_j) \qquad (4.22)$$

In this last expression the indices i,j=3 are only formal, as from (4.21) it may be seen that $M_{i3}=M_{3j}=0$ for any i and j.

Finally, if one rewrites :

$$\Delta Q_z = X_3 \quad \text{and} \quad M_{33} = a_{13}^2a_{14}^2/(k_F^2a_{13}^2 + k_I^2a_{14}^2) \qquad (4.23)$$

one obtains the resolution function in the form :

$$R(X_1,X_2,X_3,X_4) = R_o \exp(-\frac{1}{2} \sum_{i,j=1}^{4} M_{ij}X_iX_j) \qquad (4.24)$$

where

$$R_o = R'_o \frac{(2\pi)^{7/2}}{a_{13}a_{14}} k_I \left( \frac{M_{33}}{|N| s_{33}} \right)^{1/2} \qquad (4.25)$$

It is a Gaussian function in the quadridirensional space $(\vec{Q},\omega)$. As in ref./2/, the elements $M_{3i}=M_{i3}$ $(i\neq 3)$ are zero, so that the resolution in $Q_z$ and the resolution in $Q_x, Q_y, \omega$ are independent each of another.

Although (4.24) is an approximation for the resolution function, it accurately gives the center of gravity and the variance of the real function. However, due to the approximation given by (3.14), the most probable value is not given exactly, though it is to be expected that the difference will be small.

Finally, let us mention that from (4.24) one may define a resolution function depending on the time of flight, $R_\sigma(\Delta T)$, in the conditions which are discussed in ref./6/. Generally, this function depends on the scattering cross-section $\sigma$, except for the case of a weak dependence of $\sigma$ on $\vec{Q}$.

Table I

The expressions of the coefficients $a_i$. For cylindrical samples the expressions are given in brackets <...> .

$a_1 = 2\sqrt{6}\ tg\theta_M/(\alpha_o k_I)$ ; $a_2 = tg\theta_M/(\eta k_I)$; $a_3 = -m\sqrt{12}\ L_I/(\hbar\Delta\tau k_I^2)$

$a_4 = -m\sqrt{12}\ L_F/(\hbar\Delta\tau k_F^2)$; $a_5 = \sqrt{6}/\alpha_o$ ; $a_6 = 1/\eta$ ; $a_7 = \sqrt{6}/\alpha_1$ ;

$a_8 = m\sqrt{12}\ L_I(\xi_1/k_F - tg\chi/k_I)/(\hbar\Delta\tau)$; $< m\sqrt{12}\ L_I\xi_1/(\hbar\Delta\tau k_F)>$ ;

$a_9 = \sqrt{12}\ L_I cos\chi/y_{os}$ ; $<2L_I/r_{os}>$ ; $a_{10} = \sqrt{12}\ L_I\xi_2/y_{oc}$; $a_{11} = \sqrt{6}/\alpha_2$;

$a_{12} = \sqrt{12}\ L_F/y_{oc}$; $a_{13} = \sqrt{6}(\beta_1^{-2} + (\beta_o^2 + 24\eta^2 sin^2\theta_M)^{-1})^{1/2}$; $a_{14} = \sqrt{6}/\beta_2$;

$a_{15} = -\Omega/\eta$ ; $a_{16} = \sqrt{12}/\Delta\tau$; $a_{17} = m\sqrt{12}(\xi_1 cos\theta_M/k_F - \zeta_1/k_I)/(\hbar\Delta\tau)$ ;

$a_{18} = 2/r_o$ ; $a_{19} = \sqrt{12}\ cos\theta_M/(y_{os} cos\chi)$; $<2cos\theta_M/r_{os}>$ ;

$a_{20} = \sqrt{12}\xi_2 cos\theta_M/y_{oc}$; $a_{21} = 4m\sqrt{6}\ \Omega tg\theta_M sin^2\theta_M/(\hbar\alpha_o\tau)$ ;

$a_{22} = 2m\Omega tg\theta_M/(\hbar\tau)$; $a_{23} = m\sqrt{12}(\xi_1 sin\theta_M/k_F + \zeta_2/k_I)/(\hbar\Delta\tau)$ ;

$a_{24} = 2/r_o$ ; $a_{25} = \sqrt{12}\ sin\theta_M/(y_{os} cos\chi)$; $<2sin\theta_M/r_{os}>$ ;

$a_{26} = \sqrt{12}\xi_2 sin\theta_M/y_{oc}$; $a_{27} = -m\sqrt{12}(\beta/k_F - 1/k_I)/(\hbar\Delta\tau cos\chi)$ ;

$< -m\sqrt{12}(\beta/k_F - 1/k_I)/(\hbar\Delta\tau)>$ ; $a_{28} = \sqrt{12}/x_{os}$; $<2/r_{os}>$ ;

$a_{29} = -\sqrt{12}\ tg\chi/y_{os}$ ; $<0>$ ; $a_{30} = \sqrt{12}\alpha/(y_{oc} cos\chi)$; $<\sqrt{12}\alpha/y_{oc}>$ ;

$a_{31} = m\sqrt{12}/(\hbar\Delta\tau k_F)$; $a_{32} = 1/\tau'$.

## Table II

The symmetrical matrix $N_{ij}$ $(i,j=1,2,\ldots,5)$ $(N_{ij}=N_{ji})$

$N_{11} = a_{15}^2+a_{16}^2$; $N_{12} = a_{16}a_{17}$; $N_{13}= a_{15}a_{22}+a_{16}a_{23}$; $N_{14}= a_{16}a_{27}$;

$N_{15} = a_{16}a_{31}$; $N_{22}= a_{17}^2a_{18}^2a_{19}^2a_{20}^2$; $N_{23}= a_{17}a_{23}+a_{19}a_{25}+a_{20}a_{26}$;

$N_{24} = a_{17}a_{27}+a_{19}a_{29}+a_{20}a_{30}$; $N_{25} = a_{17}a_{31}$;

$N_{33} = a_{21}^2+a_{22}^2+a_{23}^2+a_{24}^2+a_{25}^2+a_{26}^2$; $N_{34} = a_{23}a_{27}+a_{25}a_{29}+a_{26}a_{30}$;

$N_{35} = a_{23}a_{31}$; $N_{44}= a_{27}^2+a_{28}^2+a_{29}^2+a_{30}^2$; $N_{45}=a_{27}a_{31}$; $N_{55}=a_{31}^2+a_{32}^2$

## Table III

The matrices K(5,5) and J(5,4)

$$K = \begin{pmatrix} 0 & a_{15} & a_{16} & 0 & 0 \\ 0 & 0 & a_{17} & a_{19} & a_{20} \\ a_{21} & a_{22} & a_{23} & a_{25} & a_{26} \\ 0 & 0 & a_{27} & a_{29} & a_{30} \\ 0 & 0 & a_{31} & 0 & 0 \end{pmatrix} \qquad J = \begin{pmatrix} a_1 & 0 & a_5 & 0 \\ a_2 & 0 & a_6 & 0 \\ a_3 & a_4 & a_8 & 0 \\ 0 & 0 & a_9 & 0 \\ 0 & 0 & 0 & a_{12} \end{pmatrix}$$

## APPENDIX

## CHANGE OF ANGULAR DIVERGENCES AND THE ENERGY RESOLUTION AT REFLECTION FROM ROTATING CRYSTALS

It is well known (see for instance ref./8/) that the Bragg law is modified in the case of a moving crystal. For a perfect crystal, small enough, moving with a velocity $\vec{v}$, the momentum and energy conservation laws in a reflection process are (in the laboratory system) :

$$\vec{k}_i = \vec{k}_o + \vec{\tau} \qquad (A.1.1)$$

$$k_i^2 = k_o^2 + (2m/\hbar)\vec{v}\,\vec{\tau} \qquad (A.1.2)$$

where $\vec{\tau}$ is the reciprocal lattice vector, $\vec{k}_o$ and $\vec{k}_i$ are the wave vectors of the neutron before and after reflection. If one denotes the angles before and after reflection by $\theta_{mo}$ and $\theta_{mi}$ respectively (in the laboratory system), the expressions (A.1)are equivalent with :

$$\tau = 2k_o \sin\theta_{mo} + (2m/\hbar)\,\frac{\vec{v}\vec{\tau}}{\tau} = 2k_i \sin\theta_{mi} - (2m/\hbar)\,\frac{\vec{v}\vec{\tau}}{\tau} \qquad (A.2)$$

For given $\theta_{mo}$ one obtains :

$$k_o = \frac{\tau}{(2\sin\theta_{mo})}\left(1 - 2\frac{m}{\hbar}\,\frac{\vec{v}\vec{\tau}}{\tau^2}\right) \qquad (A.3)$$

and in the approximation $(2m/\hbar)\ \frac{\vec{v}\vec{\tau}}{\tau^2} << 1$ (A.4)

one obtains :

$$k_i = (1-2\frac{m}{\hbar}\frac{\vec{v}\vec{\tau}}{\tau^2}\cos 2\theta_{mo})\tau/(2\sin\theta_{mo}) \tag{A.5}$$

$$\sin\theta_{mi} = \sin\theta_{mo}(1+4\frac{m}{\hbar}\frac{\vec{v}\vec{\tau}}{\tau^2}\cos^2\theta_{mo}) \tag{A.6}$$

which is equivalent with

$$\theta_{mi} = \theta_{mo} + 2\frac{m}{\hbar}\frac{\vec{v}\vec{\tau}}{\tau^2}\sin 2\theta_{mo} \tag{A.6'}$$

Let us consider now the real crystal in the layout of fig.1. A neutron which passes the $C_o$ collimator along its axis, and is reflected in the point $\vec{r}=0$ at the momentum t=0 on the most probable mosaic block, will have after reflection a wave vector $k_I$ and a direction parallel to the axis of the collimator $C_1$. A neutron having the direction $(\gamma_o,\delta_o)$, reflected at a moment t in a point $\vec{r}$ on a certain mosaic block $\vec{\tau}(\Delta_h,\Delta_v)$, will have after reflection a wave vector $(k_i,\gamma_1,\delta_1)$. Here $\Delta_h = \vec{\tau}\vec{j}/\tau$ and $\Delta_v = \vec{\tau}\vec{i}/\tau$ . Our purpose is to calculate $\gamma_1$, $\delta_1$ and $k_i$. Taking into account fig.3 one can write :

$$\theta_{mo} = \theta_M + \Delta_h + \omega^* - \gamma_o \tag{A.7.1}$$

$$\theta_{mi} = \theta_M - \Delta_h - \omega^* + \gamma_1 \tag{A.7.2}$$

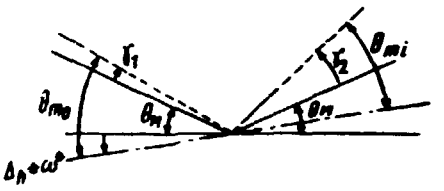


Fig.3.
Geometry of the reflection process in the monochromating crystal in real space.

Here $\omega^*$ is the angle between $\vec{\tau}_p$ and the $\vec{I}$ axis. For small values of $\omega^*$ one has :

$$\omega^* = \vec{\tau}_p \vec{I}/\tau \qquad (A.8)$$

By substracting the relations (A.7) and using (A.6') one obtains :

$$\gamma_1 = -\gamma_o + 2(\Delta_h+\omega^*) + 2\frac{m}{\hbar}\frac{\vec{v}\vec{\tau}}{\tau^2}\sin 2\theta_M \qquad (A.9)$$

The last term in (A.9) is the contribution of the Doppler effect. This effect does not change the vertical divergence (in a first approximation), therefore :

$$\delta_1 = -\delta_o + 2\Delta_v \sin\theta_M \qquad (A.10)$$

From the relation :

$$\tau = 2k_I \sin\theta_M = 2k_i \sin\theta_{mi} - 2\frac{m}{\hbar}\frac{\vec{v}\vec{\tau}}{\tau} \qquad (A.11)$$

it follows immediately :

$$\Delta k_i/k_I = (\Delta_h + \omega^* - \gamma_1)\mathrm{ctg}\theta_M + 2\frac{m}{\hbar}\frac{\vec{v}\vec{\tau}}{\tau^2} \qquad (A.12)$$

In the relations (A.9) and (A.11) $\vec{\tau}$ may be replaced by $\vec{\tau}_p$, because only the first-order terms are retained.

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