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On the Resolution of Slow-Neutron Spectrometers. II. The Resolution Function for Time-of-Flight Diffractometry

BY A. D. STOICA

Institute for Atomic Physics, Bucharest, P. O. Box 35, Romania

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The normal approximation to the resolution function defined in the scattering-vector space is calculated for a time-of-flight (TOF) diffractometer. The application to powder and single-crystal diffractometry is discussed. The conditions of time focusing are derived in a simple way. The quasielastic scattering case is also considered.

Introduction

The conventional neutron-diffraction technique for structure analysis makes use of crystal diffractometers at steady reactors. A time-of-flight (TOF) version of the diffraction technique has also been developed during recent years, mostly at pulsed neutron sources (Buras & Leciejewicz, 1963, 1964; Buras, Leciejewicz, Nitc, Sosnowska, Sosnowski & Shapiro, 1964; Buras, Mikke, Lebech & Leciejewicz, 1965; Reichelt & Rodgers, 1966; Steichele & Arnold, 1973). In this version a pulsed polychromatic beam impinges on the sample and the time of arrival at the detector of the neutrons scattered at fixed angle is measured. Various aspects of the TOF method (intensity, focusing effects, resolution) have been treated in several papers (Buras, 1963; Buras & Holas, 1968; Holas, 1968*a*, *b*).

In the case of powder diffractometry a one-dimensional time-of-flight resolution function may be defined. For single-crystal samples, however, one needs a resolution function in the three-dimensional **Q** space, similar to the one defined for conventional diffraction by Cooper & Nathans (1968). To our knowledge, no calculations have been so far reported on this function for TOF diffraction. It is the aim of this paper to calculate and to discuss it.

The diffractometer resolution function $R(\mathbf{Q}-\mathbf{Q}_0)$ is defined generally through the relation:

$$I(\mathbf{Q}_0)=\int R(\mathbf{Q}-\mathbf{Q}_0)\sigma(\mathbf{Q})\mathrm{d}\mathbf{Q} \qquad (1)$$

where $I(\mathbf{Q}_0)$ is the measured weighted mean value of the elastic cross section $\sigma(\mathbf{Q})=(\mathrm{d}\sigma/\mathrm{d}\Omega)_{\mathrm{el}}$, $\mathbf{Q}=\mathbf{k}_i-\mathbf{k}_f$, $\mathbf{Q}_0=\mathbf{k}_{i0}-\mathbf{k}_{f0}$. Here $\mathbf{k}_i$ and $\mathbf{k}_f$ are the wave vectors of the incident and scattered neutrons, and $\mathbf{k}_{i0}$ and $\mathbf{k}_{f0}$ the corresponding mean values.

An accurate general method of calculating resolution functions has been described in the preceding paper (Stoica, 1975). The tensors of any-order moments of the three-dimensional resolution function $R(\mathbf{Q}-\mathbf{Q}_0)$ can be calculated if one knows (1) the matrix relating the components of the vector $\mathbf{Q}-\mathbf{Q}_0$ with the original variables of the problem (the 'original parameters') and (2) the tensors of the same order of the original-parameter probability distribution moments.

The resolution function for elastic scattering is calculated in § 1. The calculation procedure makes use of two transformations: one from the original variables (spatial and temporal coordinates) to the intermediate reciprocal coordinates in the wave-vector space, and subsequently one from the intermediate coordinates to the natural variables of the resolution function. This procedure makes it possible to account for the spatial configuration of the TOF diffraction set-up and for the related effects of time focusing. These focusing effects are discussed in § 2. In § 3 the quasielastic scattering case is considered.

1. The resolution function in the normal approximation

A schematic representation of a TOF diffraction experiment geometry is shown in Fig. 1. The case of a pulsed reactor is considered. The original variables characterizing the scattering process are: (1) the coordinates of the neutron emission point from the moderator, $\mathbf{r}_0$: (2) the moment of emission t_0; (3) the coordinates of the point where the scattering takes place, $\mathbf{r}_1$; (4) the coordinates of the detection point $\mathbf{r}_2$; and, finally, (5) the moment of detection t_2. All these variables are deviations from the corresponding mean values. To calculate the resolution function in the normal approximation one has to know the matrix of their second-order probability moments. The structure of this matrix is given in Table 1. The elements marked by asterisks are zero if no Soller collimators are used.

To calculate the covariance matrix of the resolution function it is convenient to introduce a set of intermediate parameters: $\varepsilon=\Delta k_i/k_{i0},\gamma_i,\delta_i,\gamma_f,\delta_f$, the same as for the conventional crystal diffractometer. Here $\Delta k_i=k_i-k_{i0}$; γ_i,γ_f and δ_i,δ_f are the angular deviations from the most probable directions in the horizontal (scattering) plane and vertical plane respectively. In the linear approximation these intermediate parameters are connected with the original ones by a matrix $\mathbf{T}_1$ whose elements are defined by the relations given in Appendix 1. The covariance matrix of the intermediateparameter probability distribution is obtained immediately as $\mathbf{T}_1\mathbf{E}_2\mathbf{T}_1'$, where $\mathbf{E}_2$ is the matrix given in Table 1. Explicitly, one obtains:

$$\begin{aligned}
\langle\varepsilon^2\rangle &= T_0^{-2}(\langle t_0^2\rangle+\langle t_2^2\rangle)+L_0^{-2}(\langle x_0^2\rangle \\
&\qquad +4\sin^2\theta_s\langle y_1^2\rangle+\langle x_2^2\rangle) \\
\langle\varepsilon\gamma_i\rangle &= L_1^{-1}L_0^{-1}(\langle x_0y_0\rangle+2\sin\theta_s\langle y_0y_1\rangle \\
&\quad -2\sin^2\theta_s\langle x_1y_1\rangle-2\sin\theta_s\cos\theta_s\langle y_1^2\rangle) \\
\langle\varepsilon\gamma_f\rangle &= L_2^{-1}L_0^{-1}(2\sin\theta_s\cos\theta_s\langle y_1^2\rangle-2\sin^2\theta_s\langle x_1y_1\rangle \\
&\qquad +\langle x_2y_2\rangle-2\sin\theta_s\langle y_1y_2\rangle) \\
\langle\gamma_i^2\rangle &= L_1^{-2}(\langle y_0^2\rangle-2\sin\theta_s\langle y_0x_1\rangle-2\cos\theta_s\langle y_0y_1\rangle \\
&\quad +\sin^2\theta_s\langle x_1^2\rangle+2\sin\theta_s\cos\theta_s\langle x_1y_1\rangle \\
&\quad +\cos^2\theta_s\langle y_1^2\rangle) \\
\langle\gamma_f^2\rangle &= L_2^{-2}(\sin^2\theta_s\langle x_1^2\rangle-2\sin\theta_s\cos\theta_s\langle x_1y_1\rangle \\
&\quad +\cos^2\theta_s\langle y_1^2\rangle+2\sin\theta_s\langle x_1y_2\rangle-2\cos\theta_s\langle y_1y_2\rangle \\
&\quad +\langle y_2^2\rangle) \\
\langle\gamma_i\gamma_f\rangle &= L_1^{-1}L_2^{-1}(\sin^2\theta_s\langle x_1^2\rangle-\cos^2\theta_s\langle y_1^2\rangle \\
&\quad -\sin\theta_s\,\langle y_0x_1\rangle+\sin\theta_s\langle x_1y_2\rangle+\cos\theta_s\langle y_0y_1\rangle \\
&\quad +\cos\theta_s\,\langle y_1y_2\rangle \\
\langle\delta_i^2\rangle &= L_1^{-2}(\langle z_0^2\rangle+\langle z_1^2\rangle-2\langle z_0z_1\rangle) \\
\langle\delta_f^2\rangle &= L_2^{-2}(\langle z_1^2\rangle+\langle z_2^2\rangle-2\langle z_1z_2\rangle) \\
\langle\delta_i\delta_f\rangle &= L_1^{-1}L_2^{-1}(\langle z_0z_1\rangle-\langle z_1^2\rangle+\langle z_1z_2\rangle)\,. \qquad (2)
\end{aligned}$$

To obtain the covariance matrix of the resolution function in the $\mathbf{X}=\mathbf{Q}-\mathbf{Q}_0$ space one has to know the matrix of the linearized relation between X_i and the

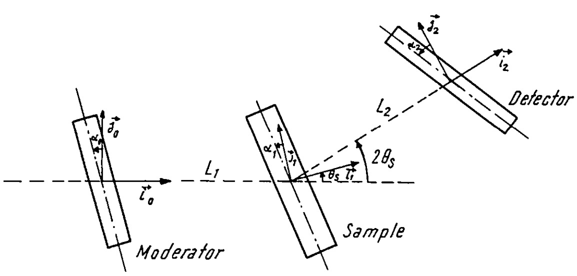

Fig. 1. The geometry of a TOF diffraction arrangement at a pulsed reactor. L_1 is the distance from moderator to sample, L_2 is the distance from sample to detector, $L_0=L_1+L_2$. The coordinate systems used in the computations are shown.

intermediate parameters. This matrix is defined by the relations given in Appendix 2. For the covariance matrix elements one gets then:

$$\begin{aligned}
\langle X_1^2\rangle &= 4k_{i0}^2\sin^2\theta_s\langle\varepsilon^2\rangle-4k_{i0}^2\sin\theta_s\cos\theta_s(\langle\varepsilon\gamma_i\rangle \\
&\quad -\langle\varepsilon\gamma_f\rangle)+k_{i0}^2\cos^2\theta_s(\langle\gamma_i^2\rangle+\langle\gamma_f^2\rangle-2\langle\gamma_i\gamma_f\rangle) \\
\langle X_2^2\rangle &= k_{i0}^2\sin^2\theta_s(\langle\gamma_i^2\rangle+\langle\gamma_f^2\rangle+2\langle\gamma_i\gamma_f\rangle) \\
\langle X_3^2\rangle &= k_{i0}^2(\langle\delta_i^2\rangle+\langle\delta_f^2\rangle+\langle\delta_i\delta_f\rangle) \\
\langle X_1X_2\rangle &= 2k_{i0}^2\sin^2\theta_s(\langle\varepsilon\gamma_i\rangle+\langle\varepsilon\gamma_f\rangle) \\
&\quad -k_{i0}^2\sin\theta_s\cos\theta_s(\langle\gamma_i^2\rangle-\langle\gamma_f^2\rangle)\,. \qquad (3)
\end{aligned}$$

The resolution function in the normal approximation is given by the expression:

$$R(\mathbf{X})=R_0(2\pi)^{-3/2}|\{M_{ij}\}|^{1/2}\exp\left(-\tfrac{1}{2}\sum_{i,j,=1}^{3}M_{ij}X_iX_j\right) \qquad (4)$$

where the resolution matrix $\{M_{ij}\}$ is the inverse of the covariance matrix $\{\langle X_iX_j\rangle\}$.

In a TOF diffraction experiment the diffraction pattern is obtained as a time-of-flight spectrum. It is of interest to calculate the widths of the Bragg peaks appearing in such a spectrum. The time dispersion of these peaks can be calculated easily with the aid of (4). For a single-crystal sample with mosaic spread η the following expression is obtained for the time dispersion $\langle\Delta\tau^2\rangle$ of the peak centred around the time T_0 and corresponding to a reciprocal-lattice vector $2\pi\boldsymbol{\tau}=\mathbf{Q}_0$:

$$\langle\Delta\tau^2\rangle=(T_0/Q_0)^2\left(\langle X_1^2\rangle-\frac{\langle X_1X_2\rangle^2}{\langle X_2^2\rangle+Q_0^2\eta^2}\right)\,. \qquad (5)$$

From this general expression, the particular cases of ideal single crystals and powder samples are obtained by putting $\eta=0$ and $\eta=\infty$ respectively.

2. Focusing effects in TOF diffractometry

The TOF diffraction pattern represents a scan along X_1 in the reciprocal lattice of the sample crystal. It is equivalent to the $\theta:2\theta$ scan in conventional diffraction.

Because of the angular distribution of the mosaic blocks, the Bragg scattering for a given reciprocal-lattice vector $\boldsymbol{\tau}$ is restricted to $\mathbf{Q}-\mathbf{Q}_0$ contained in surface normal to $\mathbf{Q}_0$, *i.e.* normal to the direction of the scan. Focusing effects may therefore occur when the major

Table 1. *The structure of the covariance matrix of the original parameters of the problem*

$$\mathbf{E}_2=\begin{bmatrix}
\langle t_0^2\rangle & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \langle t_2^2\rangle & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \langle x_0^2\rangle & \langle x_0y_0\rangle & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \langle x_0y_0\rangle & \langle y_0^2\rangle & 0 & \langle x_1y_0\rangle^* & \langle y_0y_1\rangle^* & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \langle z_0^2\rangle & 0 & 0 & \langle z_0z_1\rangle^* & 0 & 0 & 0 \\
0 & 0 & 0 & \langle x_1y_0\rangle^* & 0 & \langle x_1^2\rangle & \langle x_1y_1\rangle & 0 & 0 & \langle x_1y_2\rangle^* & 0 \\
0 & 0 & 0 & \langle y_0y_1\rangle^* & 0 & \langle x_1y_1\rangle & \langle y_1^2\rangle & 0 & 0 & \langle y_1y_2\rangle^* & 0 \\
0 & 0 & 0 & 0 & \langle z_0z_1\rangle^* & 0 & 0 & \langle z_1^2\rangle & 0 & 0 & \langle z_1z_2\rangle^* \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \langle x_2^2\rangle & \langle x_2y_2\rangle & 0 \\
0 & 0 & 0 & 0 & 0 & \langle x_1y_2\rangle^* & \langle y_1y_2\rangle^* & 0 & \langle x_2y_2\rangle & \langle y_2^2\rangle & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \langle z_1z_2\rangle^* & 0 & 0 & \langle z_2^2\rangle
\end{bmatrix}.$$

axis of the resolution ellipse in the scattering plane is also normal to X_1. These effects are analogous to those occurring when dispersion surfaces are measured with triple-axis spectrometers.

The orientation of the resolution ellipsoid in reciprocal space is sensitive to the shape of the moderator, the sample and the detector. To describe this effect, we shall replace the actual shapes by ellipsoids having the same second-order moments of the coordinates in real space. Let M_n and m_n $(n=0,1,2)$ be the dispersions along the two axes of the real-space ellipsoids which are contained in the scattering plane, and let α_n be the angle between the major axis and the y_n coordinate axis (see Fig. 1). The corresponding elements of the matrix shown in Table 1 then have the following expressions:

$$\begin{aligned}\langle x_n^2\rangle &= \cos^2\alpha_n m_n + \sin^2\alpha_n M_n\\ \langle y_n^2\rangle &= \sin^2\alpha_n m_n + \cos^2\alpha_n M_n\\ \langle x_n y_n\rangle &= \sin\alpha_n \cos\alpha_n (m_n - M_n)\,. \qquad (6)\end{aligned}$$

When one of the M_n becomes very large, the major axis of the resolution ellipse in the X_1, X_2 plane tends to become orientated along a certain asymptotic direction. This direction can easily be found by neglecting in the matrix of Table 1 all the elements which do not contain that M_n. For the angle β_n between the asymptotic $(M_n \to \infty)$ direction and the X_1 axis one obtains through (2) and (3) the following expressions:

$$\begin{aligned}&\operatorname{ctg}\beta_0 = -\operatorname{ctg}\theta_s - 2(L_1/L_0)\operatorname{tg}\alpha_0\\ &\operatorname{ctg}\beta_1 =\\ &\frac{(4/L_0)\operatorname{tg}\theta_s + (1/L_1+1/L_2)\operatorname{ctg}\theta_s - (1/L_1-1/L_2)\operatorname{tg}\alpha_1}{(1/L_1-1/L_2)-(1/L_1+1/L_2)\operatorname{tg}\theta_s\operatorname{tg}\alpha_1}\\ &\operatorname{ctg}\beta_2 = \operatorname{ctg}\theta_s - 2(L_2/L_0)\operatorname{tg}\alpha_2\,. \qquad (7)\end{aligned}$$

The focusing conditions correspond to $\beta_n = \pi/2$:

$$\begin{aligned}&\operatorname{tg}\alpha_0 = -(\tfrac{1}{2})(1+L_2/L_1)\operatorname{ctg}\theta_s\\ &\operatorname{tg}\alpha_1 = -(L_1/L_2/L_1)^{-1}4\operatorname{tg}\theta_s + (2+L_1/L_2\\ &\quad + L_2/L_1)\operatorname{ctg}\theta_s\\ &\operatorname{tg}\alpha_2 = (\tfrac{1}{2})(1+L_1/L_2)\operatorname{ctg}\theta_s\,. \qquad (8)\end{aligned}$$

The conditions minimize simultaneously $\langle X_1^2\rangle$ and $\langle X_1X_2\rangle^2$. For this reason they coincide with the conditions obtained by Holas (1968*b*) for the minimization of the time dispersion of Bragg peaks for powders.

3. Quasielastic scattering case

These resolution function defined in $\{\mathbf{Q}\}$ space has the advantage of being useful for different types of elastic cross section. Moreover, it also make it possible to treat the case of quasielastic scattering.

In considering the quasielastic-scattering case, care must be taken to account for the differences between conventional and TOF measurements at fixed angle without energy analysis. Because in TOF diffraction measurements neither the incident nor the final energy of the neutron is fixed, the measured quantity at fixed angle is not $d\sigma/d\Omega$ as in the case of a crystal diffractometer. In fact, one can define a modified $(d\sigma/d\Omega)_{\mathrm{TOF}}$ which is obtained by integrating the scattering law $S(\mathbf{Q},\omega)$ along a certain curve in $\{\mathbf{Q},\omega\}$ space. This curve does not coincide with the curve implied in the definition of $d\sigma/d\Omega$.

Considering the case of small energy transfers (quasielastic scattering), one has:

$$\Delta k_f = \Delta k_i - \frac{m}{\hbar k_{i0}}\,\omega$$

$$\Delta k_i = \Delta k_{i0} + \frac{m}{\hbar k_{i0}}\,\frac{L_2}{L_1+L_2}\,\omega$$

where Δk_{i0} is the deviation of k_i from k_{i0} for purely elastic scattering.

The deviation $\mathbf{X}$ of the wave-vector transfer from the mean value will now include a contribution $\mathbf{X}_\omega$ due to the inelasticity of the scattering:

$$\begin{aligned}&X_1 = X_{10} + X_{1\omega} = X_{10} + \frac{m}{\hbar k_{i0}}\,\frac{L_2-L_1}{L_2+L_1}\sin\theta_s\omega\\ &X_2 = X_{20} + X_{2\omega} = X_{20} + \frac{m}{\hbar k_{i0}}\cos\theta_s\omega\\ &X_3 = X_{30}\,. \qquad (9)\end{aligned}$$

The expressions for X_{10}, X_{20}, X_{30} are those given in Appendix 2 for purely elastic scattering.

The measured intensity of scattered neutrons at fixed angle will be:

$$I(\mathbf{Q}_0) = \int R(\mathbf{X}_0)\,(d\sigma/d\Omega)_{\mathrm{TOF}}d\mathbf{X}_0 \qquad (10)$$

where

$$(d\sigma/d\Omega)_{\mathrm{TOF}} \propto \int S(\mathbf{Q}+\mathbf{X}_\omega,\omega)d\omega$$

$$\mathbf{X}_\omega = \left(\frac{m}{\hbar k_{i0}}\,\frac{L_2-L_1}{L_2+L_1}\,\xi\sin\theta_s\,,\ \frac{\hbar k_{i0}}{m}\,\xi\cos\theta_s\,,0\right). \qquad (11)$$

The conventional two-axis measurement case may be obtained by putting $L_2=0$:

$$\mathbf{X}_\omega = \left(-\frac{m}{\hbar k_{i0}}\,\xi\sin\theta_s, \frac{m}{\hbar k_{i0}}\,\xi\cos\theta_s\,,0\right).$$

It is seen that $\mathbf{X}_\omega$ is normal to $\mathbf{Q}_0$ if $L_1=L_2$. This means that in (11) one effectively integrates the scattering law at constant Q. This is important (Carpenter & Sutton, 1972) since the measurement then gives directly the static structure factor $\Gamma(\mathbf{Q}) = \hbar\int S(\mathbf{Q},\omega)d\omega$, provided that the scattering is indeed quasielastic and that $S(\mathbf{Q},\omega)$ has a weak dependence on the orientation of $\mathbf{Q}$.

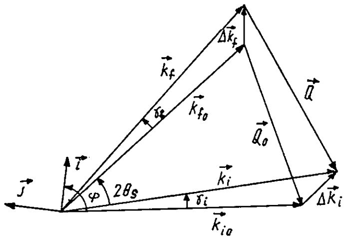

Fig. 2. The scattering diagram for the elastic scattering case.

One should pay attention to the following circumstance: the integral (10) may also be put in the form

$$I(Q_0) \propto \int R(\mathbf{X}-\mathbf{X}_\omega)S(\mathbf{Q}_0+\mathbf{X},\omega)\mathrm{d}\mathbf{X}\mathrm{d}\omega \,. \qquad (12)$$

The function $R^*(\mathbf{X},\omega)=R(\mathbf{X}-\mathbf{X}_\omega)$ in this relation does not have the properties required for a resolution function in the $\{\mathbf{Q},\omega\}$ space, because its covariance matrix is singular and therefore $R^*(\mathbf{X},\omega)$ is not zero at all points at infinity.

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APPENDIX 1

By using the notations from Fig. 1 and by taking into account that $k_i=(m/\hbar)\,(L/T)$ and $k_{i0}=(m/\hbar)\,(L_0/T_0)$, one obtains in a first approximation $\varepsilon\equiv\Delta k_i/k_{i0}=(\Delta L/L_0)-(\Delta T/T_0)$. In the small-angle approximation one obtains then:

$$\varepsilon=\frac{t_0-t_2}{T_0}+\frac{\mathbf{i}_0(\mathbf{r}_1-\mathbf{r}_0)+\mathbf{i}_2(\mathbf{r}_2-\mathbf{r}_1)}{L_1+L_2}$$

$$=\frac{t_0-t_2}{T_0}+\frac{-x_0-2\sin\theta_s y_1+x_2}{L_1+L_2}$$

$$\gamma_i=(\mathbf{r}_1\mathbf{j}_0-\mathbf{r}_0\mathbf{j}_0)/L_1=(-y_0+\sin\theta_s x_1+\cos\theta_s y_1)/L_1$$

$$\delta_i=(\mathbf{r}_1\mathbf{k}_0-\mathbf{r}_0\mathbf{k}_0)/L_1=(-z_0+z_1)/L_1$$

$$\gamma_f=(\mathbf{r}_2\mathbf{j}_2-\mathbf{r}_1\mathbf{j}_2)/L_2=(\sin\theta_s x_1-\cos\theta_s y_1+y_2)L_2$$

$$\delta_f=(\mathbf{r}_2\mathbf{k}_2-\mathbf{r}_1\mathbf{k}_2)/L_2=(-z_1+z_2)/L_2\,.$$

APPENDIX 2

The most probable scattering vector is $\mathbf{Q}_0=\mathbf{k}_{i0}-\mathbf{k}_{f0}$ with $k_{i0}=k_{f0}$. The coordinate system is chosen as in Fig. 2. Then

$$Q_0=R'(\varphi)\begin{pmatrix}k_{i0}\\0\\0\end{pmatrix}-R'(\varphi-2\theta_s)\begin{pmatrix}k_{i0}\\0\\0\end{pmatrix}$$

where $R'(\varphi)$ is the transpose of the rotation matrix around the axis z by an angle φ. It results that:

$$\mathbf{Q}_0=[\cos\varphi-\cos(\varphi-2\theta_s)]k_{i0}\mathbf{i}$$
$$-[\sin\varphi-\sin(\varphi-2\theta_s)]k_{i0}\mathbf{j}\,.$$

Let the coordinate axis x be directed along $\mathbf{Q}_0$. This means $\varphi=\theta_s-(\pi/2)$ sign $\theta_s\equiv\theta_s-(\pi/2)\xi$. By using the notation from Fig. 2 one obtains in the small-angle approximation:

$$X_1=2\xi k_{i0}\sin\theta_s+\xi k_{i0}\cos\theta_s(-\gamma_i+\gamma_f)$$

$$X_2=\xi k_{i0}\sin\theta_s(\gamma_i+\gamma_f)$$

$$X_3=k_{i0}(\delta_i-\delta_f)\,.$$

The sign of θ_s has no influence on the even-order moments of the resolution function, but determines the sign of the odd-order moments. Therefore changing the sense of θ_s changes the sign of the asymmetrical part of the resolution function in $\{\mathbf{Q}\}$ space.

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