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On the Resolution of Slow-Neutron Spectrometers.
I. A General Method to Calculate Resolution Functions

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Starting from a general definition of the resolution function one gets a rigorous method of calculating the shape of this function. The tensors of the probability moments of the parameters controlled in the measuring device are used in the computation. The application to neutron spectrometry is discussed.

Introduction

The experimental data in neutron spectrometry usually require a special treatment for the purpose of removing the contribution of the instrument. An important step forward in this field was the introduction of the resolution function concept. The multidimensional resolution function was first calculated for triple-axis spectrometers (Cooper & Nathans, 1967) and for crystal diffractometers (Cooper & Nathans, 1968). Later on, the resolution-function technique was extended also to the time-of-flight neutron spectrometry (Komura & Cooper, 1970; Furrer, 1971; Popa, 1974).

To calculate the resolution functions one generally begins with a detailed analysis of each spectrometer element, aiming at establishing its influence on the detected scattering event. Then integrations over a certain number of variables are performed successively. To simplify the integration one usually accepts the Gaussian approximation for the probability distributions involved, so that only the normal approximation to the resolution function is actually obtained. The computation method is cumbersome and does not reveal the general structure of the result.

In this paper an alternative approach to the resolution-function problem is presented. Formulae are given for computing the resolution-function moments of any order by using the probability moments of the original variables of the problem. The resolution function itself is built from its moments with the aid of an expansion. There results a simple prescription for calculating the resolution function in the normal approximation (by using second-order moments) with easy access to higher-order approximations (by including higher-order moments). § 1 describes the method for the general case, without restrictions specific to neutron spectrometry. In § 2 the method is applied to the case of double- and triple-axis neutron crystal spectrometers. Other applications will be described in subsequent papers.

1. The resolution function. General relations

To define the resolution function in a general manner, let us consider an abstract experiment consisting in the measurement of a certain physical quantity A which depends on a set of parameters ξ_i $(i=1,2,\ldots,n)$. These parameters, the natural variables of A, generally do not coincide with the parameters actually controlled in the experiment, whose number may be quite large in complex cases. Let us define the *original parameters* η_i $(i=1,2,\ldots,m;\ m\geq n)$ as the set of controlled parameters whose distribution function is known *a priori* or can be evaluated empirically.

The resolution function $R(\mathbf{X})$ is defined as the probability distribution of ξ_i assuming the values $\xi_i=\bar{\xi}_i+X_i$ when the quantity A is measured. Generally A is a random variable, so that the process of measurement gives the mean value:

$$\begin{aligned}\mu(A|\bar{\xi}_1,\bar{\xi}_2,\ldots,\bar{\xi}_n)&=\int A\mathrm{d}F(A,\xi_1,\xi_2,\ldots,\xi_n)\\&=\int A\mathrm{d}F(A|\xi_1,\xi_2,\ldots,\xi_n)R(\mathbf{X})\mathrm{d}\mathbf{X}\\&=\int M(A|\xi_1,\xi_2,\ldots,\xi_n)R(\mathbf{X})\mathrm{d}\mathbf{X}\,.\end{aligned}\tag{1}$$

Here $F(A,\xi_1,\xi_2,\ldots,\xi_n)$ and $F(A|\xi_1,\xi_2,\ldots,\xi_n)$ are the distribution functions of the events $(A,\xi_1,\xi_2,\ldots,\xi_n)$ and (A given $\xi_1,\xi_2,\ldots,\xi_n$) respectively, and $M(A|\xi_1,\xi_2,\ldots,\xi_n)$ is the conditional expectation of the random variable A. The aim of the experiment is to determine the regression of A on $\xi_1,\xi_2,\ldots,\xi_n$. To achieve this one has to know the resolution function $R(\mathbf{X})$. The results of physical interest can be obtained either by deconvolution from the experimental values of $\mu(A|\bar{\xi}_1,\bar{\xi}_2,\ldots,\bar{\xi}_n)$ or by convoluting theoretical models with the resolution function and comparing with experimental data.

To compute the resolution function two assumptions will be made in the following: (1) the original parameters $\eta_1,\ldots,\eta_m$ are independent; and (2) the functional relations between the variables of the resolution function ξ_i and the original parameters η_j can be linearized:

$$X_i=\beta_i^jY_j\,,\quad Y_j=\eta_j-\bar{\eta}_j\quad(j=1,2,\ldots,m)\,.$$

It can be shown then (Appendix 1) that the pth-order moments of the resolution function are connected with the corresponding probability moments of the original parameters through the relation:

$$\mathbf{E}X_{i_1}X_{i_2}\ldots X_{i_p}=\beta^{j1}_{i1}\beta^{j2}_{i2}\ldots\beta^{jp}_{ip}\mathbf{E}Y_{j1}Y_{j2}\ldots Y_{jp}\,. \tag{2}$$

This theorem can be extended to sample moments. Moreover, the resolution-function moments, if any, are correctly estimated by the sample moments. There exists no general method of fitting distributions when sample moments are known. In the one-dimensional case the analytical method of Pearson can be used. The normal approximation belongs to this class of fittings.

In the multidimensional case the above formalism gives a simple prescription for computing the resolution function in the normal approximation:

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

where the resolution matrix $\{M_{ij}\}$ is the inverse of the covariance matrix $\{\mathbf{E}X_iX_j\}$ (Miller, 1964).

In matrix notation ($\mathbf{X}=\mathbf{BY}$, $\mathbf{E}_2=\{\mathbf{E}Y_iY_j\}$) one has therefore the following relation for the determination of the resolution matrix:

$$\mathbf{M}^{-1}=\mathbf{BE}_2\mathbf{B}' \tag{4}$$

where $\mathbf{B}'$ is the transpose of $\mathbf{B}$.

The quadratic form $\sum M_{ij}X_iX_j$ must be positive definite. By means of a unique orthogonal transformation it can be reduced to the canonical form $\sum Z_i^2/\alpha_i^2$. If the resolution function is not much different from a normal distribution, it is convenient to use the expansion:

$$\begin{aligned}R(\mathbf{X})=&R_0(2\pi)^{-n/2}|\{M_{ij}\}|^{1/2}\\ &\times\exp\left(-\tfrac{1}{2}\sum_{i=1}^{n}\frac{Z_i^2}{\alpha_i^2}\right)\Bigg\{\sum_{m1,\ldots,mn}A_{m1\cdots mn}\\ &\times H_{m1}\left(\frac{Z_1}{\sqrt{2}\alpha_1}\right)\ldots H_{mn}\left(\frac{Z_{nn}}{\sqrt{2}\alpha_n}\right)\Bigg\}\end{aligned} \tag{5}$$

where $H_m(u)$ are the normalized Hermite polynomials. The coefficients of this expansion can be determined by adjusting the theoretical moments to the sample moments. The following relation is obtained in this way:

$$\begin{aligned}A_{m1\ldots mn}=&\pi^{n/2}\sum_{j1,\ldots,jn}2^{-(j_1+\ldots+j_n)/2}\frac{C^{j1}_{m1}\ldots C^{jn}_{mn}}{(\alpha_1)^{j1}\ldots(\alpha_n)^{jn}}\\ &\mathbf{E}Z_1^{j1}\ldots Z_n^{jn}\end{aligned} \tag{6}$$

where C^j_m is the coefficient in front of u^j in the normalized Hermite polynomial $H_m(u)$.

2. The resolution function of crystal spectrometers

The measured quantity in neutron spectrometry is the scattering cross section. The original parameters in the experiment are the magnitudes and orientations of the incident and scattered neutron wave vectors $\mathbf{k}_i$ and $\mathbf{k}_f$.

The case of a triple-axis spectrometer will be considered first. In this case the resolution function is defined in $\{\mathbf{Q},\omega\}$ space (Cooper & Nathans, 1967). We shall denote by X_i the coordinates in that space ($X_1=Q_x-Q_{x0}$, $X_2=Q_y-Q_{y0}$, $X_3=Q_z-Q_{z0}$, $X_4=\omega-\omega_0$, the axis X_3 being normal to the scattering plane) and by Y_j the original parameters ($Y_1=\Delta k_i$, $Y_2=k_{i0}\gamma_i$, $Y_3=k_{i0}\delta_i$, $Y_4=\Delta k_f$, $Y_5=k_{f0}\gamma_f$, $Y_6=k_{f0}\delta_f$, where Δk_i and Δk_f are the deviations of the wave-vector moduli from their mean values k_{i0} and k_{f0}, γ_i,γ_f and δ_i,δ_f the angular deviations from the most probable directions in the horizontal and vertical planes respectively, the scattering plane being the horizontal one).

The linearized relationship between $\mathbf{X}$ and $\mathbf{Y}$ (see Grabcev, 1973) has the form $\mathbf{X}=\mathbf{BY}$ with the following matrix $\mathbf{B}$:

$$\mathbf{B}=\begin{pmatrix}\cos\varphi & \sin\varphi & 0 & -\cos(\varphi-2\theta_s) & -\sin(\varphi-2\theta_s) & 0\\ -\sin\varphi & \cos\varphi & 0 & \sin(\varphi-2\theta_s) & -\cos(\varphi-2\theta_s) & 0\\ 0 & 0 & 1 & 0 & 0 & -1\\ \dfrac{\hbar k_{i0}}{m} & 0 & 0 & -\dfrac{\hbar k_{f0}}{m} & 0 & 0\end{pmatrix}. \tag{7}$$

Here $2\theta_s$ is the scattering angle and φ is the angle between $\mathbf{k}_{i0}$ and the X_1 axis.

As the monochromator and analyser units are independent, the tensor $\mathbf{T}_p$ of the pth probability moments of the original parameters has the form:

$$\mathbf{T}_p=\begin{cases}\mathbf{E}_p(Y_1,Y_2,Y_3) & \text{for combinations containing } Y_1, Y_2, Y_3 \text{ only}\\ \mathbf{E}_p(Y_4,Y_5,Y_6) & \text{for combinations contaning } Y_4, Y_5, Y_6 \text{ only}\\ 0 & \text{for mixed combinations.}\end{cases}$$

Here $\mathbf{E}_p(Y_1,Y_2,Y_3)$ and $\mathbf{E}_p(Y_4,Y_5,Y_6)$ are the tensors of the pth probability moments of the original parameters controlled in the monochromator and analyser units respectively. The procedure of experimental determination of the original parameter distribution will be described in a separate paper.

According to the method described in the previous section, the tensors of the pth-order moments of the resolution function are given by the relation (2). For the particular case of the second-order moments the corresponding matrix (the covariance matrix) is given in Appendix 2. By inverting it one obtains the resolution matrix $\{M_{ij}\}$ of the normal approximation to the resolution function.

If the inelastic scattering cross section does not depend on the orientation of $\mathbf{Q}$ (isotropic samples), then it is enough to define a two-dimensional resolution function $R(\Delta Q,\Delta\omega)$. Its covariance-matrix elements are also given in Appendix 2.

In the neutron-diffraction case the measured quantity is the elastic cross section. The resolution function is defined in $\mathbf{Q}$ space (Cooper & Nathans, 1968). The original parameters are Y_1, Y_2, Y_3 and $Y_4=k_{i0}\gamma_f$, $Y_5=k_{i0}\delta_f$. The tensors $\mathbf{T}_p$ and the matrix $\mathbf{B}$ should be modified in the following way:

$$\mathbf{T}_p=\begin{cases}\mathbf{E}_p(Y_1,Y_2,Y_3) & \text{for combinations containing } Y_1, Y_2, Y_3 \text{ only}\\ \mathbf{E}_p(Y_4,Y_5) & \text{for combinations containing } Y_4, Y_5 \text{ only}\\ 0 & \text{for mixed combinations},\end{cases}$$

$$\mathbf{B}=\begin{pmatrix}2\xi\sin\theta_s & -\xi\cos\theta_s & 0 & \xi\cos\theta_s & 0\\ 0 & \xi\sin\theta_s & 0 & \xi\sin\theta_s & 0\\ 0 & 0 & 1 & 0 & -1\end{pmatrix}. \qquad (7a)$$

The coordinate axis X_1 was directed along $\mathbf{Q}_0$, *i.e.* $\varphi=\theta_s-(\pi/2)\operatorname{sign}\theta_s$, $\xi\equiv\operatorname{sign}\theta_s$ (Grabcev, 1974).

The covariance matrix for this case is given in Appendix 2. Here again one may define a one-dimensional resolution function $R(\Delta Q)$ if the elastic scattering does not depend on the orientation of $\mathbf{Q}$. To construct the Gaussian approximation of this function one should use the dispersion $\langle\Delta Q^2\rangle$ given in Appendix 2.

3. Discussion

To calculate the resolution function in the normal approximation one can start from the explicit expressions of the transmission functions of the monochromator and analyser units (see, for instance, Dorner, 1972). The second-order probability moments of the transmission functions $p_i(\mathbf{k}_i)$ and $p_f(\mathbf{k}_f)$ are obtained by inverting their associated matrices. With the aid of the matrix $\mathbf{B}$ given by (7) one obtains then through (4) and (3) the resolution function normalized to $R_0=V_iV_f\equiv\int p_i(\mathbf{k}_i)\mathrm{d}\mathbf{k}_i\int p_f(\mathbf{k}_f)\mathrm{d}\mathbf{k}_f$ (Dorner, 1972). The results obtained in this way are equivalent to those derived earlier (Cooper & Nathans, 1967; Bjerrum-Møller & Nielsen, 1970; Werner & Pynn, 1971; Quittner, 1971; Grabcev, 1973), up to the choice of the X_1 coordinate axis and to some possible minor mistakes.

The method proposed in this paper has the computational advantage of using matrix language for constructing the normal approximation to the resolution function. It also makes it possible to go beyond the normal approximation in a simple way. Moreover, it makes it possible to use more refined theoretical models (including spatial effects and non-Gaussian shape of the reflectivity curves) for the transmission functions $p_i(\mathbf{k}_i)$ and $p_f(\mathbf{k}_f)$, and also to use experimental determinations for the moments of these functions.

APPENDIX 1

Let us consider a vector space ζ_n and a basis in this space $(\mathbf{j}_1,\ldots,\mathbf{j}_n)$. Let $F(y_1,\ldots,y_n)$ be a distribution function defined in this space. For the pth-order probability moments we shall use the notation:

$$\mathbf{E}y_{k1}y_{k2}\ldots y_{k_p}=\int y_{k1}y_{k2}\ldots y_{k_p}\mathrm{d}F(\mathbf{Y}_n)$$
$$=\int y_{k1}y_{k2}\ldots y_{k_p}P(\mathbf{Y}_n)\mathrm{d}\mathbf{Y}_n\,.$$

Theorem I: *The multitude of pth-order probability moments forms a pth order tensor*

Let us consider the linear transformation $y'_k=\tau^h_ky_h$ (or, in matrix transcription, $\mathbf{Y}'_n=\mathbf{T}\mathbf{Y}_n$). From the normalization condition $\int\mathrm{d}F(\mathbf{Y}'_n)=\int\mathrm{d}F(\mathbf{Y}_n)=1$ it follows that $P(\mathbf{Y}'_n)=(\det\mathbf{T})^{-1}P(\mathbf{Y}_n[\mathbf{Y}'_n])$. Then:

$$\mathbf{E}y'_{k1}y'_{k2}\ldots y'_{k_p}=\int y'_{k1}y'_{k2}\ldots y'_{k_p}\mathrm{d}F(\mathbf{Y}'_n)$$
$$=(\det\mathbf{T})^{-1}\tau^{h1}_{k1}\tau^{h2}_{k2}\ldots\tau^{hp}_{kp}\int y_{h1}y_{h2}\ldots y_{h_p}P(\mathbf{Y}_n)\left|\frac{\partial\mathbf{Y}'_n}{\partial\mathbf{Y}_n}\right|\mathrm{d}\mathbf{Y}_n$$
$$=\tau^{h1}_{k1}\tau^{h2}_{k2}\ldots\tau^{hp}_{kp}\mathbf{E}y_{h1}y_{h2}\ldots y_{h_p}\,.$$

Lemma: Let ζ_m be a subspace of the space ζ_n, in which $(\mathbf{j}_1,\mathbf{j}_2,\ldots,\mathbf{j}_m)$ is a basis. We shall define the following distribution function: $F(\mathbf{Y}_m)=\int F(\mathbf{Y}_n)\mathrm{d}\mathbf{Y}_{n-m}$, where $\mathrm{d}\mathbf{Y}_{n-m}=\mathrm{d}y_{m+1}\mathrm{d}y_{m+2}\ldots\mathrm{d}y_n$. *The tensor of the pth-order moments associated with the distribution function* $F(\mathbf{Y}_m)$ *is a subtensor of the pth-order tensor associated with the distribution function* $F(\mathbf{Y}_n)$. Indeed, one has:

$$\mathbf{E}'y_{k1}y_{k2}\ldots y_{k_p}=\int y_{k1}y_{k2}\ldots y_{k_p}F(\mathbf{Y}_m)\mathrm{d}\mathbf{Y}_m$$
$$=\int y_{k1}y_{k2}\ldots y_{k_p}F(\mathbf{Y}_n)\mathrm{d}\mathbf{Y}_m\mathrm{d}\mathbf{Y}_{n-m}$$
$$=\mathbf{E}y_{k1}y_{k2}\ldots y_{k_p}\,,$$

where it was taken into account that $k_\mu\le m$.

Theorem II: Consider the linearly independent linear forms $z_i=\alpha^j_iy_j$ such that $i\le m$, where m may take any value from 1 to n. *The tensor of the pth-order moments associated with the distribution function of the quantities* z_i *is given by the expression*

$$\mathbf{E}z_{k1}z_{k2}\ldots z_{k_p}=\alpha^{h1}_{k1}\alpha^{h2}_{k2}\ldots\alpha^{hp}_{kp}\mathbf{E}y_{h1}y_{h2}\ldots y_{h_p}\,.$$

Let us consider in ζ_n the vector $\mathbf{Z}'_n=\{\mathbf{Z}_m,\mathbf{Y}_{n-m}\}$. One has $z'_i=\beta^j_iy_j$, where $\beta^j_i=\alpha^j_i$ for $i\le m$ and $\beta^j_i=\delta^j_i$ for $m<i\le n$. On account of the tensor properties and of the above lemma one obtains the desired result:

$$\mathbf{E}z_{k1}z_{k2}\ldots z_{k_p}=\mathbf{E}z'_{k1}z'_{k2}\ldots z'_{k_p}$$
$$=\beta^{h1}_{k1}\beta^{h2}_{k2}\ldots\beta^{hp}_{kp}\mathbf{E}y_{h1}y_{h2}\ldots y_{h_p}$$
$$=\alpha^{h1}_{k1}\alpha^{h2}_{k2}\ldots\alpha^{hp}_{kp}\mathbf{E}y_{h_1}y_{h2}\ldots y_{h_p}\,.$$

APPENDIX 2

The covariance matrices of the original-parameter probability distributions for the triple-axis spectrometer case have the following structure:

$$\mathbf{E}_2(Y_1,Y_2,Y_3)=\begin{pmatrix}\langle\Delta k_i^2\rangle & k_{i0}\langle\Delta k_i\gamma_i\rangle & 0\\ k_{i0}\langle\Delta k_i\gamma_i\rangle & k_{i0}^2\langle\gamma_i^2\rangle & 0\\ 0 & 0 & k_{i0}^2\langle\delta_i^2\rangle\end{pmatrix}$$

$$\mathbf{E}_2(Y_4,Y_5,Y_6)=\begin{pmatrix}\langle\Delta k_f^2\rangle & k_{f0}\langle\Delta k_f\gamma_f\rangle & 0\\ k_{f0}\langle\Delta k_f\gamma_f\rangle & k_{f0}^2\langle\gamma_f^2\rangle & 0\\ 0 & 0 & k_{f0}^2\langle\delta_f^2\rangle\end{pmatrix}.$$

Here the tacit assumption was made that no correlation exists between Δk_i and δ_i, and between Δk_f and δ_f respectively. This is justified by the fact that, to a first approximation, the angular deviations in the vertical plane do not influence the condition of Bragg reflexion.

The matrix product (4) gives the following explicit expressions for the elements of the covariance matrix of the triple-axis spectrometer resolution function:

$$\begin{aligned}\langle X_1^2\rangle=&\cos^2\varphi\langle\Delta k_i^2\rangle-2k_{i0}\sin\varphi\cos\varphi\langle\Delta k_i\gamma_i\rangle\\&+k_{i0}^2\sin^2\varphi\langle\gamma_i^2\rangle+\cos^2\varphi'\langle\Delta k_f^2\rangle\\&-2k_{f0}\sin\varphi'\cos\varphi'\langle\Delta k_f\gamma_f\rangle+k_{f0}^2\sin^2\varphi'\langle\gamma_f^2\rangle\end{aligned}$$

$$\begin{aligned}\langle X_2^2\rangle=&\sin^2\varphi\langle\Delta k_i^2\rangle+2k_{i0}\sin\varphi\cos\varphi\langle\Delta k_i\gamma_i\rangle\\&+k_{i0}^2\cos^2\varphi\langle\gamma_i^2\rangle+\sin^2\varphi'\langle\Delta k_f^2\rangle\\&-2k_{f0}\sin\varphi'\cos\varphi'\langle\Delta k_f\gamma_f\rangle+k_{f0}^2\cos^2\varphi'\langle\gamma_f^2\rangle\end{aligned}$$

$$\langle X_3^2\rangle=k_{i0}^2\langle\delta_i^2\rangle+k_{f0}^2\langle\delta_f^2\rangle$$

$$\langle X_4^2\rangle=(\hbar/m)^2k_{i0}^2\langle\Delta k_i^2\rangle+(\hbar/m)^2k_{f0}^2\langle\Delta k_f^2\rangle$$

$$\begin{aligned}\langle X_1X_2\rangle=&\sin\varphi\cos\varphi\langle\Delta k_i^2\rangle\\&+k_{i0}(\cos^2\varphi-\sin^2\varphi)\langle\Delta k_i\gamma_i\rangle-k_{i0}^2\sin\varphi\cos\varphi\langle\gamma_i^2\rangle\\&+\sin\varphi'\cos\varphi'\langle\Delta k_f^2\rangle-k_{f0}\langle\Delta k_f\gamma_f\rangle\\&+k_{f0}^2\sin\varphi'\cos\varphi'\langle\gamma_f^2\rangle\end{aligned}$$

$$\begin{aligned}\langle X_1X_4\rangle=&(\hbar/m)k_{i0}\cos\varphi\langle\Delta k_i^2\rangle-(\hbar/m)k_{i0}^2\sin\varphi\langle\Delta k_i\gamma_i\rangle\\&+(\hbar/m)k_{f0}\cos\varphi'\langle\Delta k_f^2\rangle\\&-(\hbar/m)k_{f0}^2\sin\varphi'\langle\Delta k_f\gamma_f\rangle\end{aligned}$$

$$\begin{aligned}\langle X_2X_4\rangle=&-(\hbar/m)k_{i0}\sin\varphi\langle\Delta k_i^2\rangle\\&+(\hbar/m)k_{i0}^2\cos\varphi\langle\Delta k_i\gamma_i\rangle\\&-(\hbar/m)k_{f0}\sin\varphi'\langle\Delta k_f^2\rangle\\&-(\hbar/m)k_{f0}^2\cos\varphi'\langle\Delta k_f\gamma_f\rangle\end{aligned}$$

$$\langle X_1X_3\rangle=\langle X_2X_3\rangle=\langle X_3X_4\rangle=0\,.$$

Here $\varphi'=\varphi-2\theta_s$.

If the scattering does not depend on the direction of $\mathbf{Q}$, then the expression (7) of the matrix $\mathbf{B}$ reduces to its first and last lines, provided the coordinate axis X_1 is directed along $\mathbf{Q}_0$. In this case it is enough to know the two-dimensional resolution function $R(\Delta Q,\Delta\omega)$. The elements of its covariance matrix are:

$$\begin{aligned}\langle\Delta Q^2\rangle&=\langle X_1^2\rangle\\\langle\Delta\omega^2\rangle&=\langle X_4^2\rangle\\\langle\Delta Q\Delta\omega\rangle&=\langle X_1X_4\rangle\end{aligned}$$

where

$$\varphi=-\xi\left|\operatorname{atan}\left(\frac{-k_{f0}\sin 2\theta_s}{k_{i0}-k_{f0}\cos 2\theta_s}\right)\right|.$$

For the diffractometer the covariance matrix is obtained in a similar way. It has the following elements:

$$\begin{aligned}\langle X_1^2\rangle=&4k_{i0}^2\sin^2\theta_s\langle\varepsilon^2\rangle-4k_{i0}^2\sin\theta_s\cos\theta_s\langle\varepsilon\gamma_i\rangle\\&+k_{i0}^2\sin^2\theta_s(\langle\gamma_i^2\rangle+\langle\gamma_f^2\rangle)\end{aligned}$$

$$\langle X_2^2\rangle=k_{i0}^2\sin^2\theta_s(\langle\gamma_i^2\rangle+\langle\gamma_f^2\rangle)$$

$$\langle X_3^2\rangle=k_{i0}^2(\langle\delta_i^2\rangle+\langle\delta_f^2\rangle)$$

$$\begin{aligned}\langle X_1X_2\rangle=&2k_{i0}^2\sin^2\theta_s\langle\varepsilon\gamma_i\rangle\\&-k_{i0}^2\sin\theta_s\cos\theta_s(\langle\gamma_i^2\rangle-\langle\gamma_f^2\rangle)\end{aligned}$$

$$\langle X_1X_3\rangle=\langle X_2X_3\rangle=0\,.$$

Here $\varepsilon=\Delta k_i/k_{i0}$.

If the elastic scattering cross section does not depend on the direction of $\mathbf{Q}$ one can define a one-dimensional resolution function with the dispersion $\langle\Delta Q^2\rangle=\langle X_1^2\rangle$.

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