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IMPROVEMENTS IN RESOLUTION CALCULATION FOR TRIPLE AXIS AND TIME-OF-FLIGHT

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ABSTRACT

In the calculation of the resolution function for a neutron spectrometer the scattering probabilities for the various components (moderator, monochromator, sample, etc.) are usually described separately by Gaussian functions. We will show how to extend the resolution calculation to non-Gaussian (e.g. asymmetric) probability functions. In addition, we present a refinement of the formalism by including the mutual dependencies between the probability functions of different components. These improvements can be applied both on triple-axis and time-of-flight instruments. As an example the procedure will be discussed on the resolution function of a diffractometer at a pulsed source (ROTAX-Diff. at ISIS). In particular we will focus on the treatment of the asymmetric time distribution of the methane moderator, leading to asymmetric peak shapes in the measured spectra.

1.) Introduction

Browsing through publications concerning resolution calculation of neutron spectrometers it is common sense that all probability distributions are approximated by Gaussian functions. In most cases this approximation is quite sufficient if not accurate. In some cases, however, it is not appropriate at all. The well defined edges of diaphragms or detector channels or the sample itself are examples of rectangular distributions, poorly approximated by Gaussian functions. Further we must deal with asymmetric functions like the temporal distributions of the incoming neutrons on a pulsed source arising from the properties of the moderator. A correct treatment of the asymmetry is crucial in the time-of-flight analysis of the measured peaks. In this paper we will present some ideas how to use non-Gaussian functions in the resolution function so that the calculation can still be carried out analytically. These calculations are mainly based on the use of the error-function erf(x) and Gaussian expansion. The latter has been used successfully for the description of Lorentzians in an analytical 4d-convolution [1].
Further we will show a refinement in the algorithm of resolution calculation. All probability distributions (Gaussian or non-Gaussian) will be expressed in terms of the basic coordinates in space and time of the various components of the spectrometer. In the process of integration over these variables all

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mutual dependencies between different distributions (i.e. different probability functions contain the same variable) are automatically included.
As a first step we have carried out this algorithm for ROTAX-Diff. [2,3], a diffractometer at the pulsed source ISIS, including the asymmetric pulse shape of the moderator. The principles of this calculation can be well demonstrated on this comparatively simple example. A comparison with experimental results as well as more complicated calculations for the ROTAX-spectrometer and triple-axis instruments including focusing techniques are in progress.

2.) Non-Gaussian distributions

For this subject we will demonstrate the analytic treatment of non-Gaussian functions in the resolution calculation. Two different methods will be discussed: Gaussian expansion and the use of the error-function erf(x). As examples we have chosen rectangular distributions and, as an asymmetric case, the moderator time structure on a pulsed source. In addition, a Gaussian expansion for $\exp(-x^4)$-terms is shown as well.

a) Rectangular distributions

For the definition of these function we use the unit-step function $\theta(x)$:

$$\theta(x) := \begin{cases} 1, x \geq 0 \\ 0, x < 0 \end{cases} \tag{1}$$

A rectangular distribution *w(x)* is then created by:

$$w(x) := \theta(x+1) - \theta(x-1) \tag{2}$$

Many components can be described by this function, like the shape of sample or analyser or detector channels. A rectangular sample with the dimensions *a* and *b* then reads:

$$p_S(x,y) = w(2x/a) \cdot w(2y/b) \tag{3}$$

i) Use of erf(x)

For further mathematical treatment it is much more convenient not to use this discontinuous function but to deal with the continuous error-function:

$$w\left(\frac{x}{a}\right) = \frac{1}{2} \lim_{\varepsilon \to 0} \left[\operatorname{erf}\left(\frac{x+a}{\varepsilon}\right) - \operatorname{erf}\left(\frac{x-a}{\varepsilon}\right) \right] \tag{4}$$

Products of these functions can be expressed as sums:

$$\lim_{\varepsilon\to 0}\left[\operatorname{erf}\left(\frac{x-a_1}{\varepsilon}\right)\cdot\operatorname{erf}\left(\frac{x-a_2}{\varepsilon}\right)\right]=\lim_{\varepsilon\to 0}\left[\operatorname{erf}\left(\frac{x-a_1}{\varepsilon}\right)-\operatorname{erf}\left(\frac{x-a_2}{\varepsilon}\right)\right]\cdot\operatorname{erf}\left(\frac{a_1-a_2}{\varepsilon}\right)+1 \qquad (5)$$

Together with Gaussian distributions we end up with single products of these two kinds of functions. Therefore we have to deal with integrals of the following type, easily solved analytically:

$$\int_{-\infty}^{\infty}\exp\left(-a^2x^2\right)\cdot\operatorname{erf}\left(b\pm x\right)dx=\frac{\sqrt{\pi}}{a}\cdot\operatorname{erf}\left(\frac{ab}{\sqrt{a^2+1}}\right) \qquad (6)$$

ii) Gaussian expansion

With this method we approximately describe an (almost) arbitrary function by a sum of Gaussians. Fitting parameters can be height, width and centre of the Gaussians. In most cases restrictions will be made on the parameters to simplify the fitting procedure. For a function like $p_S(x,y)$ we use equidistant 2-dimensional Gaussians of the same height. This restriction drastically simplifies the calculation of the parameters with little loss of accuracy. Fig.1 shows a plot of a rectangular structure approximated by 3x10 Gaussians.

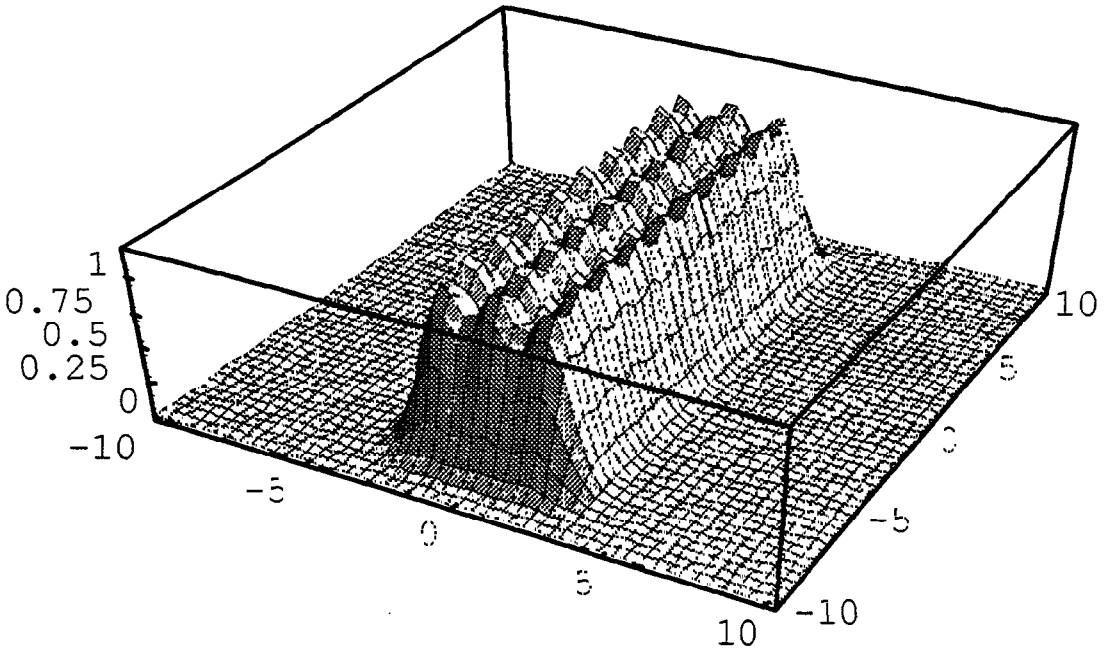

*Fig1: Gaussian expansion for a 2-dim. rectangular distribution with 3*10 peaks*

The equation for this approximation reads

$$w(2x/a)\cdot w(2y/b)\approx A\cdot\sum_{i=1}^{m}\exp\left[-\mu_1^2\cdot\left(x-x_i\right)^2\right]\cdot\sum_{j=1}^{n}\exp\left[-\mu_2^2\cdot\left(y-y_j\right)^2\right] \qquad (7)$$

with

$$x_i = x_0 + i \cdot \Delta x; \quad y_j = y_0 + j \cdot \Delta y \tag{8}$$

From symmetry considerations the final number of parameters can be further reduced to five. They can be determined in general, only depending on n and m, by non-linear least-square methods.

b) Moderator Time Structure

For a mathematical model of these type of functions we follow the guidelines given in [4]. For the methane moderator at the spallation source ISIS we end up with the following equation:

$$\begin{aligned} p_M(\Delta t_M) = &\left[2\tau_1 R + 2\tau_2(1-R)\right]^{-1} \cdot \left[R \cdot \exp\left(\kappa_1^2 - \Delta t_M / \tau_1\right) \cdot \operatorname{erfc}\left(\kappa_1 - \Delta t_M / \sigma\right) + \right. \\ &\left. (1-R) \cdot \exp\left(\kappa_2^2 - \Delta t_M / \tau_2\right) \cdot \operatorname{erfc}\left(\kappa_2 - \Delta t_M / \sigma\right)\right]; \\ \kappa_{1,2} &= \sigma / 2\tau_{1,2}; \\ R(\lambda) &= \frac{1}{2} \operatorname{erfc}\left(\frac{c}{\lambda_0} - \frac{c}{\lambda}\right) \end{aligned} \tag{9}$$

with
$\tau_1 = 32.0$ μsec; $\tau_2 = 2.5$ μsec /Å; $\sigma = 1.5$ μsec/Å; $c = 3.4$ Å; $\lambda_0 = 2.45$ Å
and the complementary error-function
erfc(x) = 1 - erf(x) .

The time structure $p_M(\Delta t_M)$ is given normalised so that the integration over Δt_M will yield 1.

i) Use of erf(x)

Since the function $p_M(\Delta t_M)$, defined by eq.9, is already given in terms of Gaussians and error-functions it can be directly used in the resolution calculation. We get integrals like eq.6 and the calculation is straight forward.

ii) Gaussian expansion

Despite the nice mathematical description we have got in eq.9 we have to consider that this is the result of theoretical predictions and the parameters are based on Monte-Carlo-Simulations. Therefore, the real time structure may look a little different due to circumstances in the set-up of the moderator which are not included in the calculations. Considering a case where the function would just be determined experimentally by a series of data-points the Gaussian expansion will deliver a very accurate and easy way to handle those functions in the resolution calculations.

$$p_M(\Delta t_M) \approx \sum_{j=1}^{n} c_j \cdot \exp\left[-a_j^2 \cdot \left(x - b_j\right)^2\right] \tag{10}$$

Fig.2 shows the result of a 7-peak Gaussian expansion for eq.9 and neutron energy of 50 meV. It demonstrates that a small number of Gaussians is already sufficient to describe a function like eq.9 with

high accuracy. It should be mentioned that this particular function just serves as an example, the expansion will work equally well throughout a wide range of functions.

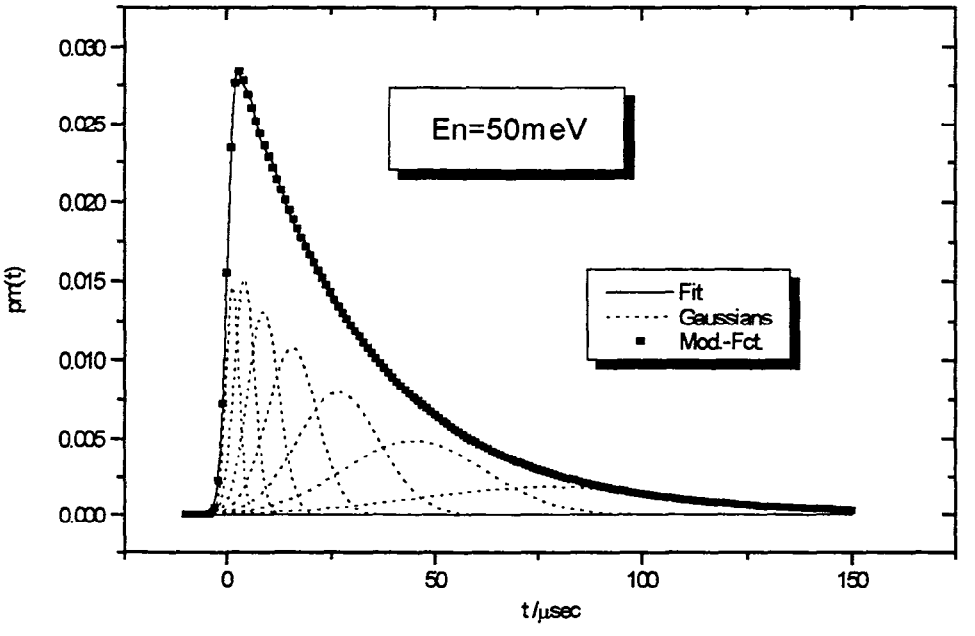

Fig.2: 7-peak Gaussian expansion of a moderator time structure

c) Expansion for exp(-x⁴)- terms

The function exp(-x⁴) shall be a final example for a non-Gaussian distribution. Why this function? We will mention two cases:

i) Quadratic Terms:
If the linearisation which is usually carried out for all variables in the resolution calculation is not sufficient quadratic terms may be used in addition. Putting them into Gaussian distributions will result in exp(-x⁴)-terms.

ii) Dispersion Relations
For the general use of quadratic terms from a dispersion relation in the convolution with the resolution function we need to deal with q⁴-terms in the exponentials. Also in this case the following expansion shows an analytic way to do the calculation with sufficient accuracy.

$$\exp\left(-x^4\right) \approx c_1 \cdot \exp\left[-a_1 \cdot (x+b)^2\right] + c_2 \cdot \exp\left(-a_2 \cdot x^2\right) + c_1 \cdot \exp\left[-a_1 \cdot (x-b)^2\right] \qquad (11)$$

with
$a_1 = 5.6064$; $a_2 = 2.7981$; $b = 0.66432$; $c_1 = 0.55693$; $c_2 = 0.91027$;

A plot is shown in Fig.3. We will use this expansion for a generalisation of the 4d-convolution in [1]. Calculations are in progress.

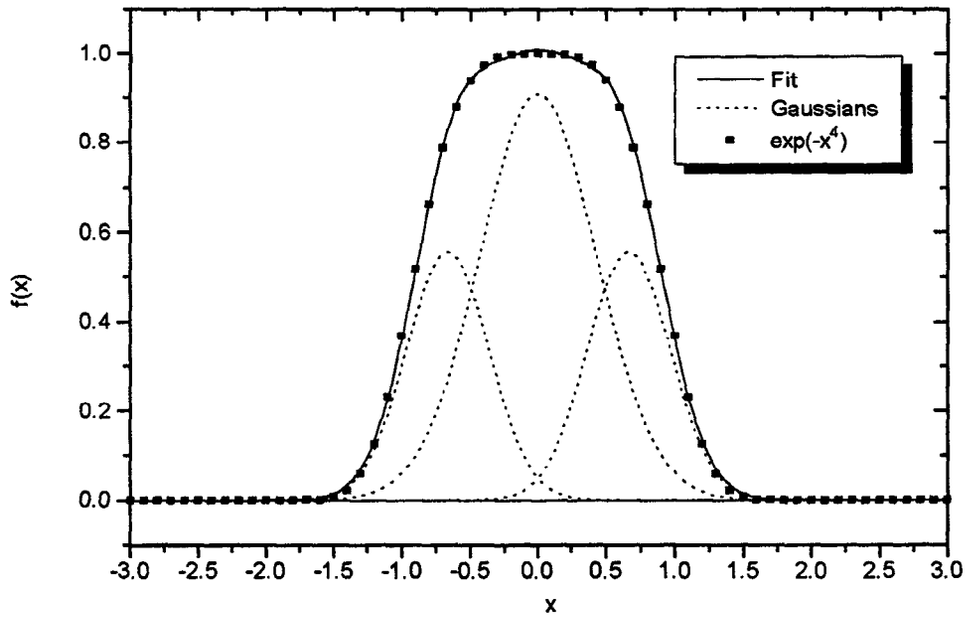

Fig.3: 3-peak Gaussian expansion for the function exp(-x⁴)

3) Refined resolution formalism

The principle of the refinement is the use of the basic coordinates in space and (if applicable) in time for all components so that all misfits and their probability distributions are expressed in terms of the coordinates of sample, analyser, detector, etc. Integrations are then performed on these variables and therefore *simultanuously* on all distributions which are depending on them. This includes automatically all dependencies between distributions treated separately otherwise. Two short examples shall be given:

i) Time-of-flight:

Let us assume an angular misfit γ_i of incoming neutrons at the sample. It is clear that neutrons with $\gamma_i>0$ will preferably arrive at one side of the sample and vice versa (cf. fig.4a). Thus the misfit of the secondary length ΔL_f (and the corresponding time-of-flight) is directly related to γ_i because both are functions of the sample coordinates x_S and y_S. Two separate distributions for γ_i and ΔL_f will not take in account this mutual dependency. In the refined formalism the integration coordinates will not be γ_i and ΔL_f but the coordinates x_S and y_S instead.

ii) Triple-axis:

For this instrument we consider a focusing analyser. Depending on the angular misfit of the incoming neutrons they will find a mosaic spread centred on different values η_0 (cf. fig.4b). Therefore η_0 is directly connected to the coordinate y_A. Assuming a Gaussian distribution of width σ for the mosaic spread η this fact can easily be expressed by a probability function for η depending on y_A .

$$p(\eta) = \exp\left[-\left(\eta - \eta_0(y_A)\right)^2 / \sigma^2\right] \tag{12}$$

Again, the mutual dependencies between mosaic spread and angular misfit are included in the refined formalism by using the basic coordinates. In addition, this kind of treatment provides a straight forward way to include focusing techniques at triple-axis machines into the resolution calculation .

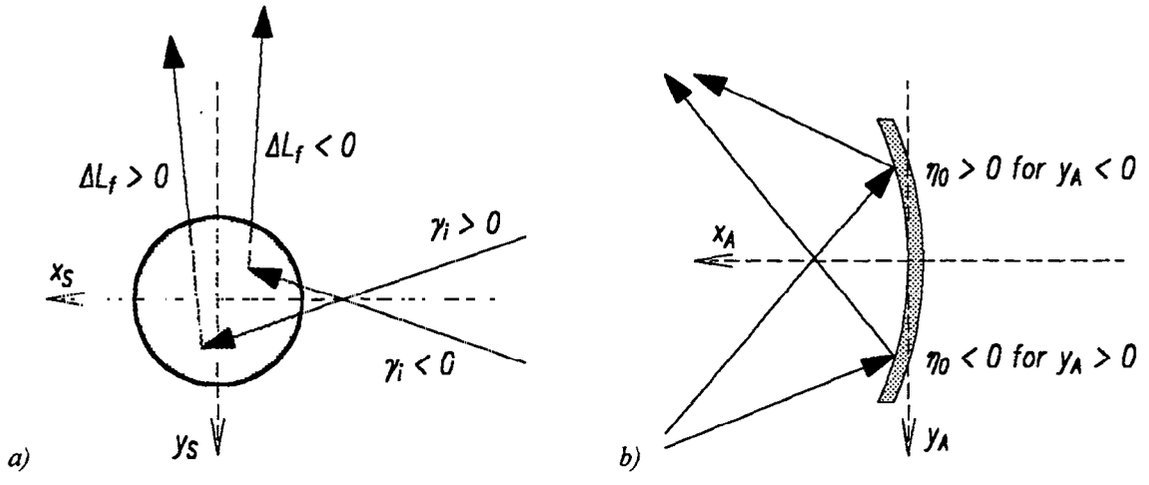

Fig.4: Schematic diagrams of misfit combinations for time-of flight and triple-axis machines

4) Resolution function of ROTAX-Diff.

Using the formalism described above we have calculated the resolution function of ROTAX-Diff., i.e. the diffraction mode of the ROTAX spectrometer installed at ISIS [2,3]. Fig.5 shows the set-up with the relevant variables and coordinate systems.

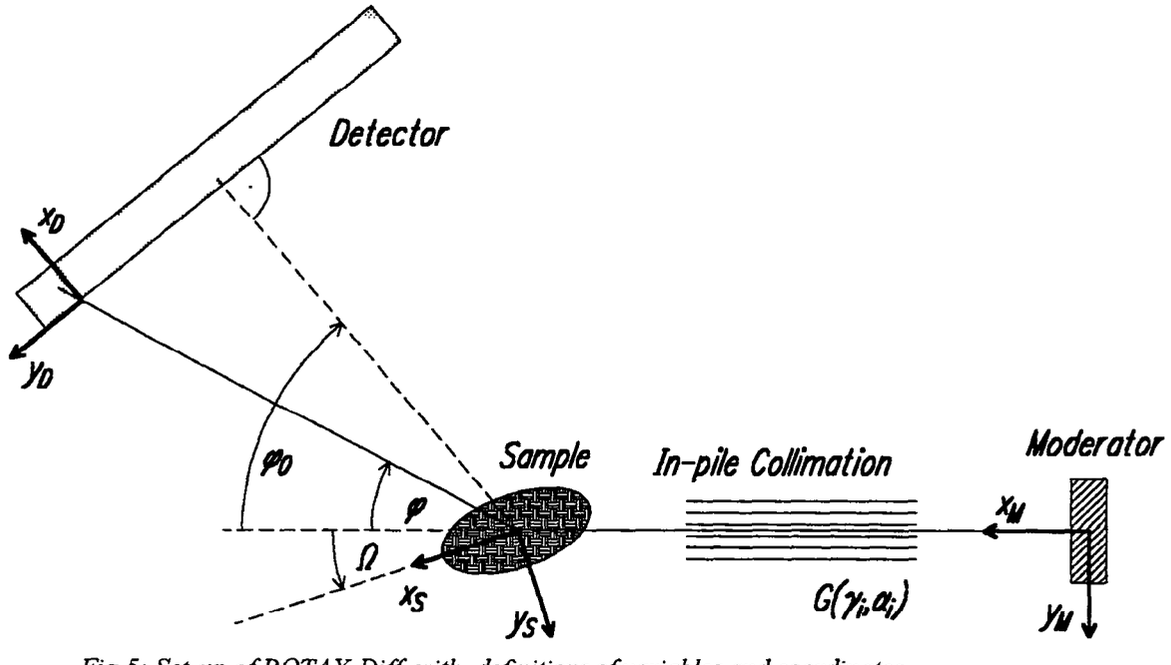

Fig.5: Set-up of ROTAX-Diff. with definitions of variables and coordinates

So far we have used the Gaussian approximation for all probability distributions except the time structure of the moderator. It is very important to include this asymmetric function since it leads to correspondingly asymmetric peaks in the measured spectra as well. Further improvements beyond the Gaussian approximations will be made where the experimental data show that improvements are necessary. Tests are planned for the near future.
The calculation includes the in-pile collimation (α_i), size of moderator (b_M), sample (a_S, b_S) and detector channel (a_D, b_D) as well as the moderator time structure $p_M(\Delta t_M)$ and the time width of the detector channels (τ_D). The resolution function is then given by

$$\begin{aligned} p(\Delta d) = \int & \delta\left(\Delta d + d_0 \cdot \Delta k / k_0 + \Delta\theta \cdot d_0 \cdot \cot\theta\right) \\ & \cdot \delta\left(\gamma_i - \left(x_S \cdot \sin\Omega + y_S \cdot \cos\Omega - y_M\right) / L_i\right) \\ & \cdot \mathrm{G}(\gamma_i, \alpha_i) \cdot \mathrm{G}(y_M, b_M) \cdot \mathrm{G}(x_S, a_S) \cdot \mathrm{G}(y_S, b_S) \cdot \mathrm{G}(x_D, a_D) \cdot \mathrm{G}(y_D, b_D) \cdot \mathrm{G}(\Delta t_D, \tau_D) \\ & \cdot p_M(\Delta t_M)\, dy_M\, dx_S\, dy_S\, dx_D\, dy_D\, d\Delta t_D\, d\Delta t_M \\ = & \frac{t_0 \cdot V_M}{\sqrt{\pi} \cdot \tau_D \cdot d_0 \cdot Y_M} \cdot \int \exp\left[-\frac{V_M^2}{Y_M^2} \cdot \left(\frac{\Delta d}{d_0} - \frac{\Delta t_M}{t_0} \right)^2 \right] \cdot p_M(\Delta t_M)\, d\Delta t_M \end{aligned} \tag{13}$$

with

$$\mathrm{G}(x,a) := \exp(-x^2 / a^2) \tag{14}$$

and the time structure of the moderator as defined in eq.9. For the calculation all coordinates are transformed into the sample coordinate system. The corresponding equations and definitions of all misfits and abbreviations can be found in the appendix. The final integration is carried out according to eq.6.

5) Conclusion

In this paper we have introduced some ideas to improve the resolution calculation with mathematical methods to go beyond the Gaussian approximation but still keep the calculation analytical. Both the error-function and Gaussian expansion are the keys to perform this task. Further, we have shown a refined formalism to achieve a more accurate description of the dependencies for the probability distributions among each other. The formalism works for both Gaussian and non-Gaussian distributions. As an example it has been used for a time-of-flight diffractometer fully including the asymmetric time structure of the moderator. For the future we plan to present complete calculations for triple-axis machines including flux enhancement techniques like focusing devices and, on the time-of-flight sector, the resolution function for the ROTAX-spectrometer with its non-uniformly spinning analyser which will really emphasize these new techniques in resolution calculation.

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Appendix

Basic equations, definitions and abbreviations for the resolution calculation (eq.13):

Detector coordinates in sample coordinates:

$$\begin{pmatrix} x_{D(\hat{S})} \\ y_{D(\hat{S})} \end{pmatrix} = L_f \cdot \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} + \begin{pmatrix} \cos\varphi_0 & -\sin\varphi_0 \\ \sin\varphi_0 & \cos\varphi_0 \end{pmatrix} \begin{pmatrix} x_D \\ y_D \end{pmatrix} \tag{15}$$

Moderator coordinates in sample coordinates:

$$\begin{pmatrix} x_{M(\hat{S})} \\ y_{M(\hat{S})} \end{pmatrix} = -L_i \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} x_M \\ y_M \end{pmatrix} \tag{16}$$

Sample axis rotation:

$$\begin{pmatrix} x_{\hat{S}} \\ y_{\hat{S}} \end{pmatrix} = \begin{pmatrix} \cos\Omega & -\sin\Omega \\ \sin\Omega & \cos\Omega \end{pmatrix} \begin{pmatrix} x_S \\ y_S \end{pmatrix} \tag{17}$$

Deviations in lengths and angles:

$$\Delta L_i = x_S \cdot \cos\Omega - y_S \cdot \sin\Omega - x_M \tag{18}$$

$$\Delta L_f = -x_S \cdot \cos(\Omega - \varphi) + y_S \cdot \sin(\Omega - \varphi) - x_D \cdot \cos(\varphi_0 - \varphi) - y_D \cdot \sin(\varphi_0 - \varphi) \tag{19}$$

$$\begin{aligned} \Delta\varphi = {} & \frac{1}{L_f} \cdot \left[-x_S \cdot \sin(\Omega - \varphi) - y_S \cdot \cos(\Omega - \varphi) + x_D \cdot \sin(\varphi_0 - \varphi) + y_D \cdot \cos(\varphi_0 - \varphi) \right] \\ & + \frac{1}{L_i} \cdot \left[-x_S \cdot \sin\Omega - y_S \cdot \cos\Omega + y_M \right] \end{aligned} \tag{20}$$

$$\gamma_i = \frac{1}{L_i} \cdot \left(x_S \cdot \sin\Omega + y_S \cdot \cos\Omega - y_M \right) \tag{21}$$

Deviations in wave vector and d-spacing:

$$\frac{\Delta d}{d_0} = -\frac{\Delta k}{k_0} - \Delta\theta \cdot \cot\theta \tag{22}$$

$$\frac{\Delta k}{k_0}=\frac{1}{L_0}\cdot\left[2x_S\cdot\sin\theta\cdot\sin(\theta-\Omega)-2y_S\cdot\sin\theta\cdot\cos(\theta-\Omega)-x_M\right.$$
$$\left.+x_D\cdot\cos(\varphi_0-\varphi)-y_D\cdot\sin(\varphi_0-\varphi)\right]-\frac{\Delta t_D+\Delta t_M}{t_0} \tag{23}$$

Abbreviations:

$$L_0=L_i+L_f;\quad t_0=\frac{mL_0}{\hbar k_0};\quad \theta=\frac{\varphi}{2};\quad d_0=\frac{k_0}{\pi\cdot\sin\theta} \tag{24}$$

$$V_M^2=\left(A_i^2V_S^2+B_M^2\hat{V}_S^2\right)\cdot V_D^2$$
$$Y_M^2=B_M^2Y_S^2+\left(K_0^2K'^2+A_i^2Y_D^2\right)\cdot V_S^2+\left(A_i\overline{K}_c-A_{ic}K_0K'\right)^2\cdot A_S^2+\left(A_i\overline{K}_s-A_{is}K_0K'\right)^2\cdot B_S^2$$
$$Y_S^2=\left(Y_D^2+V_D^2\right)\cdot\hat{V}_S^2-V_D^2\overline{V}_S^2/V_S^2$$
$$V_S^2=A_S^2B_S^2$$
$$\hat{V}_S^2=A_{ic}^2A_S^2+A_{is}^2B_S^2+V_S^2$$
$$\overline{V}_S^2=A_{is}B_S^2\overline{K}_s+A_{ic}A_S^2\overline{K}_c$$
$$V_D^2=A_D^2B_D^2$$
$$Y_D^2=V_D^2+A_D^2\hat{K}_c^2+B_D^2\hat{K}_s^2$$
$$A_M=1/a_M$$
$$B_M=1/b_M$$
$$A_S=1/a_S$$
$$B_S=1/b_S$$
$$A_D=1/a_D$$
$$B_D=1/b_D$$
$$A_i=1/a_i$$
$$A_{is}=A_i\cdot\sin\Omega$$
$$A_{ic}=A_i\cdot\cos\Omega$$
$$\hat{K}_s=K\cdot\sin(\varphi_0-\varphi)+\cos(\varphi_0-\varphi)$$
$$\hat{K}_c=K\cdot\cos(\varphi_0-\varphi)-\sin(\varphi_0-\varphi)$$
$$\overline{K}_s=K\cdot\sin(\Omega-\varphi)+\cos(\Omega-\varphi)+K'\cdot\sin\Omega-\cos\Omega$$
$$\overline{K}_c=K\cdot\cos(\Omega-\varphi)-\sin(\Omega-\varphi)+K'\cdot\cos\Omega+\sin\Omega$$
$$K=\frac{\cot\theta}{2v}$$
$$K'=\frac{\cot\theta}{2(1-v)}$$
$$v=\frac{L_f}{L_i}$$