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Resolution matching between energy and momentum in position-sensitive detector on chopper spectrometer

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Abstract

We derived analytical expressions of energy (E) and momentum (Q) resolutions on a chopper spectrometer, including timing and geometrical parameters, such as a pulse width at a moderator, an opening time of a chopper, spectrometer lengths, sizes of a moderator, of a sample and of a position-sensitive detector (PSD) and pixel sizes in a PSD. For a long linear PSD, resolutions change for pixels dependently on their positions inside the PSD, because of the change in the flight path lengths. Controlling the pixel sizes can reduce such nonuniformity in resolutions. However, in order to diminish the nonuniformity in both of the E and Q resolutions simultaneously, the PSD length was found to be limited.

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Keywords: PSD; Chopper spectrometer; Pulsed neutron; HRC; J-PARC

A chopper spectrometer is useful to study dynamics of many materials such as magnetic systems, strong correlated electrons systems, liquid, amorphous and living organisms. The reason is that the scattering function $S(Q,E)$ over a wide range of (Q,E) space (10^{-3}–10^{1} Å^{-1} and 10^{-2}–10^{3} meV even at the present time of writing) is efficiently given by many position-sensitive detectors (PSDs), compared to an inverted geometry spectrometer and a triple axis spectrometer. A PSD is linear rod shaped, is ~m long and is divided into pixels. However, the instrumental resolution at the endmost pixel is not the same as that at the central pixel, because the neutron flight path length from a sample to the end is different from that from the sample to the center. Such an unequal resolution makes it difficult to obtain a uniform quality of $S(Q,E)$.

Varying pixel sizes in a PSD can reduce such a resolution difference. Since the longer flight path gives the higher instrumental resolution, a pixel size at the end should be larger than that at the center qualitatively. In the present paper, we calculate E and Q resolutions on a chopper spectrometer and the ratios of the resolutions at the end to those at the center. The calculations include timing and geometrical parameters, such as a pulse width at a moderator, an opening time of a chopper, spectrometer lengths, sizes of a moderator, of a sample and of a PSD and pixel sizes in a PSD.

Figs. 1(a) and (b) show finite timing and geometrical parameters of a chopper spectrometer in the calculations. L_1, L_2 and L_3 are distances between the centers of the moderator and the sample, those of the sample and the PSD and those of the chopper and the sample, respectively. $\langle\phi_h\rangle$ and $\langle\phi_v\rangle$ mean the horizontal and vertical scattering angles. t_m, t_{ch}, (x_m, y_m), (x_s, y_s, z_s) and (x_d, y_d, z_d) indicate deviations of the time at the moderator, the time at the chopper, the positions on the moderator, in the sample and in the pixel between the most probable neutrons and the other neutrons, respectively. The positions of the slightly rogue neutrons are represented by $\boldsymbol{r}_m = (x_m, y_m, 0), \boldsymbol{r}_s = (x_s, y_s, L_1 + z_s)$ and $\boldsymbol{r}_d = ((L_2 + z_d)\sin\langle\phi_h\rangle + x_d\cos\langle\phi_h\rangle, L_2\tan\langle\phi_v\rangle + y_d, (L_2 + z_d)\cos\langle\phi_h\rangle - x_d\sin\langle\phi_h\rangle + L_1)$.

An energy transfer resolution $\delta E/\langle E_i\rangle$ is derived below. The incident and final velocities of the most probable

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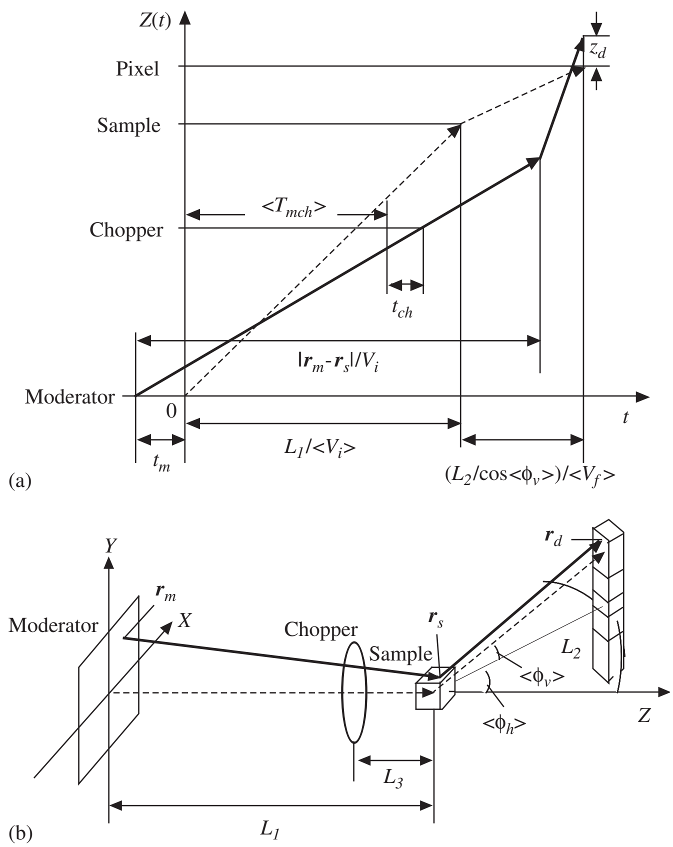

Fig. 1. Timing (a) and geometrical (b) parameters used for the present calculations of instrumental resolutions. Broken arrows and thick solid arrows indicate most probable neutrons and the other neutrons, respectively. All the neutrons are detected at the same pixel and time. The PSD is divided into 5 pixels as an example. The center of the PSD is located on the scattering plane and the PSD is mounted to be perpendicular to the scattering plane. The PSD length is expressed by $2L_2\tan\langle\phi_\mathrm{v}\rangle$.

neutrons and the other neutrons are described by

$$\langle V_\mathrm{i}\rangle = \frac{L_1 - L_3}{\langle T_\mathrm{mch}\rangle}, \quad \langle V_\mathrm{f}\rangle = \alpha\langle V_\mathrm{i}\rangle,$$

$$V_\mathrm{i} = \frac{\frac{L_1-L_3}{L_1+z_\mathrm{s}}|\boldsymbol{r}_\mathrm{m} - \boldsymbol{r}_\mathrm{s}|}{\langle T_\mathrm{mch}\rangle + t_\mathrm{ch} + t_\mathrm{m}},$$

$$V_\mathrm{f} = \frac{|\boldsymbol{r}_\mathrm{d} - \boldsymbol{r}_\mathrm{s}|}{\left(\frac{L_1}{\langle V_\mathrm{i}\rangle} + \frac{L_2/\cos\langle\phi_\mathrm{v}\rangle}{\langle V_\mathrm{f}\rangle}\right) - \left(\frac{|\boldsymbol{r}_\mathrm{m}-\boldsymbol{r}_\mathrm{s}|}{V_\mathrm{i}} - t_\mathrm{m}\right)},$$

where $\langle T_\mathrm{mch}\rangle$ is a time that the most probable neutrons spend from the moderator to the chopper. Both for elastic scattering ($\alpha = 1$) and inelastic scattering ($\alpha \neq 1$), the ratio of a deviation of energy transfer (δe) to the incident energy ($\langle E_\mathrm{i}\rangle$) is described by

$$\frac{\delta e}{\langle E_\mathrm{i}\rangle} = \frac{(V_\mathrm{f}^2 - V_\mathrm{i}^2) - (\langle V_\mathrm{f}\rangle^2 - \langle V_\mathrm{i}\rangle^2)}{\langle V_\mathrm{i}\rangle^2}.$$

Hereafter, we assume that t_m, t_ch, x_m, y_m, x_s, y_s, z_s, x_d, y_d and z_d (p_j, $j = 1-10$) are normally distributed with full-widths at half-maximum (FWHMs) of δt_m, δt_ch, δx_m, δy_m, δx_s, δy_s, δz_s, δx_d, δy_d and δz_d (δp_j, $j = 1-10$), respectively. δt_m and δt_ch indicate the pulse width at the moderator and the opening time of the chopper. The other FWHMs are calculated by $(\delta x_\mathrm{m}, \delta y_\mathrm{m}, \delta x_\mathrm{s}, \delta y_\mathrm{s}, \delta z_\mathrm{s}, \delta x_\mathrm{d}, \delta y_\mathrm{d}, \delta z_\mathrm{d}) = c\times(X_\mathrm{m}, Y_\mathrm{m}, X_\mathrm{s}, Y_\mathrm{s}, Z_\mathrm{s}, X_\mathrm{d}, Y_\mathrm{d}, Z_\mathrm{d})$, where $X_\mathrm{m}\times Y_\mathrm{m}$ is the moderator area, $X_\mathrm{s}\times Y_\mathrm{s}\times Z_\mathrm{s}$ is the sample volume, X_d is the PSD width, Y_d is the pixel size, Z_d is the PSD depth and c is the factor to transform these parameters to the FWHMs. Using the above equations, one can obtain

$$\begin{aligned}
\left(\frac{\delta E}{\langle E_\mathrm{i}\rangle}\right)^2 &= \sum_{j=1}^{10}\left\{\frac{\partial(\delta e/\langle E_\mathrm{i}\rangle)}{\partial p_j}\delta p_j\right\}^2 \\
&= \left(1 + \alpha^3\frac{L_3\cos\langle\phi_\mathrm{v}\rangle}{L_2}\right)^2\left(\frac{2\delta t_\mathrm{m}}{\langle T_\mathrm{mch}\rangle}\right)^2 \\
&\quad + \left(1 + \alpha^3\frac{L_1\cos\langle\phi_\mathrm{v}\rangle}{L_2}\right)^2\left(\frac{2\delta t_\mathrm{ch}}{\langle T_\mathrm{mch}\rangle}\right)^2 \\
&\quad + (\alpha^2\cos^2\langle\phi_\mathrm{v}\rangle\sin\langle\phi_\mathrm{h}\rangle)^2\left(\frac{2\delta x_\mathrm{s}}{L_2}\right)^2 \\
&\quad + (\alpha^2\sin\langle\phi_\mathrm{v}\rangle\cos\langle\phi_\mathrm{v}\rangle)^2\left(\frac{2\sqrt{\delta y_\mathrm{s}^2 + \delta y_\mathrm{d}^2}}{L_2}\right)^2 \\
&\quad + (\alpha^2\cos\langle\phi_\mathrm{v}\rangle(\alpha - \cos\langle\phi_\mathrm{h}\rangle\cos\langle\phi_\mathrm{v}\rangle))^2\left(\frac{2\delta z_\mathrm{s}}{L_2}\right)^2 \\
&\quad + (\alpha^2\cos^2\langle\phi_\mathrm{v}\rangle)^2\left(\frac{2\delta z_\mathrm{d}}{L_2}\right)^2. \qquad (1)
\end{aligned}$$

The first and second terms are the same as Eq. (8.15) in the Windsor's text [1]. The other terms are introduced by the finite sizes of moderator, sample and detector. The value of $\delta E/\langle E_\mathrm{i}\rangle$ is independent of x_m, y_m and x_d within the first order approximation.

A deviation of the scattering angle is represented by

$$\delta\varphi = \phi - \langle\phi\rangle,$$
$$\langle\phi\rangle = \arccos[\cos\langle\phi_\mathrm{v}\rangle\cos\langle\phi_\mathrm{h}\rangle],$$
$$\phi = \arccos\left[\frac{(\boldsymbol{r}_\mathrm{s} - \boldsymbol{r}_\mathrm{m})\cdot(\boldsymbol{r}_\mathrm{d} - \boldsymbol{r}_\mathrm{s})}{|\boldsymbol{r}_\mathrm{s} - \boldsymbol{r}_\mathrm{m}||\boldsymbol{r}_\mathrm{d} - \boldsymbol{r}_\mathrm{s}|}\right].$$

Therefore,

$$\begin{aligned}
(\delta\phi)^2 &= \sum_{j=1}^{10}\left\{\frac{\partial(\delta\varphi)}{\partial p_j}\delta p_j\right\}^2 \\
&= \left(\frac{\sin\langle\phi_\mathrm{h}\rangle}{2\sqrt{\sin^2\langle\phi_\mathrm{h}\rangle + \tan^2\langle\phi_\mathrm{v}\rangle}}\frac{2\delta x_\mathrm{m}}{L_1}\right)^2 \\
&\quad + \left(\frac{\tan\langle\phi_\mathrm{v}\rangle}{2\sqrt{\sin^2\langle\phi_\mathrm{h}\rangle + \tan^2\langle\phi_\mathrm{v}\rangle}}\right)^2\left(\frac{2\sqrt{\delta y_\mathrm{m}^2 + \delta y_\mathrm{s}^2}}{L_1}\right)^2 \\
&\quad + \left(\frac{(L_2/L_1 + \cos\langle\phi_\mathrm{h}\rangle\cos^2\langle\phi_\mathrm{v}\rangle)\sin\langle\phi_\mathrm{h}\rangle}{2\sqrt{\sin^2\langle\phi_\mathrm{h}\rangle + \tan^2\langle\phi_\mathrm{v}\rangle}}\frac{2\delta x_\mathrm{s}}{L_2}\right)^2
\end{aligned}$$