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Resolution considerations for polarized triple-axis spectrometry

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It is well known that the cross-sections for triple-axis polarized beam spectroscopy depend on the relative orientation of the neutron polarization $\hat{\boldsymbol{P}}$ and the momentum transfer $\boldsymbol{Q}$. This orientational dependence of the cross-sections can give rise to large resolution effects when the direction of $\boldsymbol{Q}$ varies substantially over the resolution function, which is often the case with polarized beam measurements because relaxed resolution is frequently employed to compensate for reduced intensities. This is also true when measurements are made at small wave vectors, as is necessary for amorphous materials. We find that the positions of excitations can be shifted significantly, and the intensities can deviate by a factor of two or more from the ideal case.

The polarized beam triple-axis technique is known to be a very powerful method for identifying the origin of both magnetic cross-sections and nuclear cross-sections [1]. For example, with the incident neutron polarization $\hat{\boldsymbol{P}}$ parallel to the momentum transfer $\boldsymbol{Q}$, $\hat{\boldsymbol{P}} \| \boldsymbol{Q}$, ferromagnetic spin waves can only be observed for spin-flip scattering, and in fact for the $(-\ +)$ configuration the spin waves can only be observed for neutron energy loss scattering, while for the $(+\ -)$ configuration spin waves can only be observed in neutron energy gain. For $\hat{\boldsymbol{P}} \perp \boldsymbol{Q}$, on the other hand, the $(+\ -)$ and $(-\ +)$ cross-sections are equal in strength for energy gain and energy loss, and $\frac{1}{4}$ the intensity of the $\hat{\boldsymbol{P}} \| \boldsymbol{Q}$ situation. Such selection rules are often utilized to separate and identify cross-sections. However, when the relative orientation of $\hat{\boldsymbol{P}}$ and $\boldsymbol{Q}$ vary substantially over the extent of the instrumental resolution function, substantial distortions of the expected scattering intensities can occur, in addition to the usual resolution effects applicable to unpolarized neutron scattering. Convolutions of the resolution function with the appropriate polarized beam cross-sections have been carried out for a number of cases, and compared with experimental data. The corrections are largest in cases when the resolution is very coarse, as would be expected, but coarse resolution is often employed with polarized beam measurements to compensate for the reduction in instrumental intensity. The resolution effects are also large when measurements are made at small wave vectors, as is necessary for amorphous materials, and this is the case of particular interest here. We find that the positions of excitations can be shifted significantly, and the intensities can deviate by a factor of two or more from the ideal case.

The angular dependence of the polarized neutron cross-section for spin wave creation (minus sign) and destruction (plus sign) is given by [2, 3]:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega^2} \propto 1 + (\hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{M}})^2 \mp 2(\hat{\boldsymbol{P}} \cdot \hat{\boldsymbol{Q}})(\hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{M}}) , \tag{1}$$

where $\hat{\boldsymbol{Q}}$, $\hat{\boldsymbol{M}}$, and $\hat{\boldsymbol{P}}$ are unit vectors in the directions of the neutron momentum transfer $\boldsymbol{Q}$, the magnetization direction $\boldsymbol{M}$, and the incident neutron polarization $\hat{\boldsymbol{P}}$. Consider first the horizontal field configuration, with $\hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{M}} \cong 1$ and $\hat{\boldsymbol{P}} \cdot \hat{\boldsymbol{Q}} \cong \pm 1$. Equation (1) reduces to $2 \pm 2P$, so that for spin wave creation we have a maximum value of 4 with $P = -1$ ($(-\ +)$ configuration) and 0 for $P = +1$ ($(+\ -)$ configuration). For spin wave destruction we have 4 for $P = +1$ [$(+\ -)$] and 0 for $P = -1$ [$(-\ +)$]. This corresponds to the familiar conservation of spin angular momentum; a spin wave can be created in this geometry only if the incident neutron moment is antiparallel to the magnetization, and can be destroyed only if the moment is parallel. On the other hand, for the vertical field configuration we have $\hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{M}} \cong 0$ and $\hat{\boldsymbol{P}} \cdot \hat{\boldsymbol{Q}} \cong 0$, and the cross-section for energy gain and energy loss is unity and independent of $\hat{\boldsymbol{P}}$. Hence for either the $(-\ +)$ or $(+\ -)$ configurations we will see equal intensities of spin waves in energy gain and energy loss.

If the instrumental resolution allows the direction of $\boldsymbol{Q}$ to deviate substantially from $\hat{\boldsymbol{M}}$, then we must take this angular variation into account when convoluting the resolution with the appropriate cross-section. In the horizontal configuration $\hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{M}} \equiv \cos\theta$, and eq. (1) becomes

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega^2} \propto 1 + \cos^2\theta[1 \mp 2P] , \tag{2}$$

so that we obtain $1 + 3\cos^2\theta$ for $(-\ +)$ and $(+\ -)$ in energy loss and energy gain, respectively, and $1 - \cos^2\theta$ for $(+\ -)$ and $(-\ +)$ in loss and gain. In the vertical field configuration we have

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega^2} \propto 1 + \sin^2\phi[1 \mp 2P] , \tag{3}$$

where we have defined $\phi = \pi/2 + \theta$. Then we obtain $1 + 3\sin^2\phi$ for (− +) and (+ −) in energy loss and energy gain, respectively, and $1 - \sin^2\phi$ for (+ −) and (− +) in loss and gain.

These angular variations are quite important for the case of amorphous systems, in which the spin waves are only well defined around the (0 0 0) reciprocal lattice position. Here $\boldsymbol{Q} = \boldsymbol{q}$ and the direction can vary substantially over the resolution volume, with the dominant variation coming from the coarse vertical resolution. To illustrate the nature of the effects we chose the particular case of a ferromagnet, with dispersion relation $E_{sw} = Dq^2$. Typical experimental parameters for these types of measurements are E_i = 14.8 meV, and collimation (FWHM) of 10′-10′-10′-20′. We took a convenient value of $D = 70$ meV Å^2. The kinematical details of these types of scans are given elsewhere [4].

Figure 1 shows the convolution of the polarized spin wave cross-sections with the instrumental resolution function [5] for the vertical field situation, $\hat{\boldsymbol{P}} \perp \boldsymbol{Q}$, and (− +) spin-flip scattering. The vertical resolution in this case was chosen to be 0.1 Å^{-1}. For $q = 0.05$ Å^{-1} the ratio of the energy loss ($E > 0$) to energy gain ($E < 0$) peak is 2.1, while the ideal ratio is 0.9, and is given by the $k_f^3 \cot\theta_A$ resolution factor for the analyzer [5] (and a very small contribution from the detailed balance factor). With increasing q we see that the ratio becomes closer to the ideal, and for q = 0.1 Å^{-1} the ratio has decreased to 1.2.

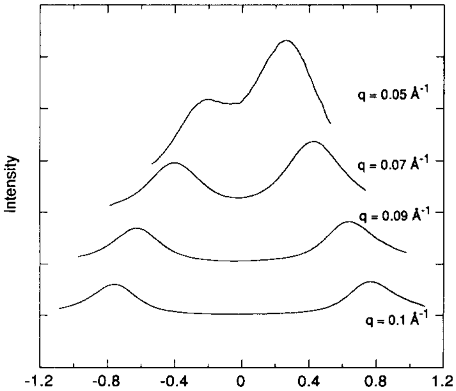

Fig. 1. Spin-flip (spin wave) scattering as a function of q. The ideal ratio of energy loss to energy gain is ~0.9, while the effect of the vertical resolution ($Q_z = 0.1$ Å^{-1}) is to make this ratio greater than unity. The instrumental distortion of the intensity of the peaks is seen to decrease with increasing q, as the effect of the vertical resolution becomes less important.

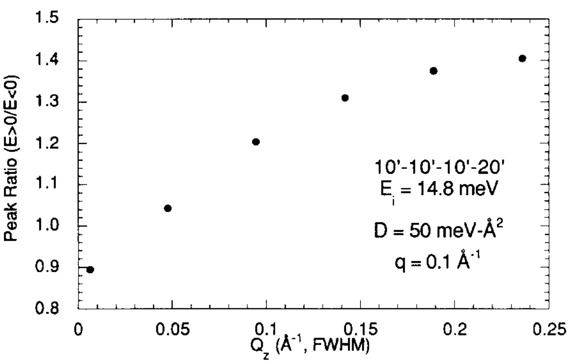

Fig. 2. Ratio of the energy loss to energy gain intensities as a function of the component of vertical resolution. The ideal ratio is 0.89, given by the $k_f^3 \cot\theta_A$ factor.

The effect of the vertical resolution is shown in fig. 2, where the ratio of the energy loss to energy gain peak at $q = 0.1$ Å^{-1} is plotted as a function of the vertical component of the resolution. For tight vertical resolution we get the ideal ratio given by $k_f^3 \cot\theta_A$, and then this ratio rapidly increases with increasing Q_z. The observed peak positions also start out at the ideal value given by Dq^2, and then shift by 20% to larger energy transfer over the same range of Q_z. These calculations are in 'semi-quantitative' agreement with our recent measurements on the amorphous $Fe_{86}B_{14}$ system [6], while for complete agreement we must include the energy-dependent reflectivity of the analyzer crystal, which has not been accurately measured yet.

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