Absolute cross-section normalization of magnetic neutron scattering data

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We discuss various methods to obtain the resolution volume for neutron scattering experiments, in order to perform absolute normalization on inelastic magnetic neutron scattering data. Examples from previous experiments are given. We also try to provide clear definitions of a number of physical quantities which are commonly used to describe neutron magnetic scattering results, including the dynamic spin correlation function and the imaginary part of the dynamic susceptibility. Formulas that can be used for general purposes are provided and the advantages of the different normalization processes are discussed.
I. INTRODUCTION

Magnetic neutron scattering is a powerful technique for studying the magnetic structure and spin dynamics of various material systems. Sometimes obtaining only relative scattering intensities is sufficient. Increasingly it is necessary to convert the magnetic scattering intensities to absolute units, i.e., in terms of magnet moments ($\mu_B$) or spin ($S$) per site. The principle of this normalization process has been described previously [1–3]. Here we describe practical details of the normalization process and discuss potential problems. In addition, closely related yet different physical quantities, such as the dynamic spin correlation function $S(Q, \omega)$ and the imaginary part of the dynamic susceptibility $\chi''(Q, \omega)$ are used to describe magnetic neutron scattering intensities. It is important to clarify the definition of and conversion between these quantities. These are the main purposes of this paper.

The neutron scattering intensity measured at the detector can be written as a convolution of the differential scattering cross-section $d^2\sigma/d\Omega dE$, which depends on the sample itself, and the instrument resolution function $R(Q_0, E_0, Q, E)$, which is mainly determined by parameters related to the instrument set-up [4]:

$$I(Q, E) = \int \frac{d^2\sigma}{d\Omega dE} R(Q_0, E_0, Q, E) dQ_0 dE_0,$$

where $Q$ and $E$ are the wave-vector and energy transfer. In practice, it is customary to divide the detector counts by the monitor counts, the latter being inversely proportional to the incident neutron wave-vector $k_i$. Therefore the modified neutron scattering intensity becomes:

$$\tilde{I}(Q, E) = k_i \int \frac{d^2\sigma}{d\Omega dE} R(Q_0, E_0, Q, E) dQ_0 dE_0.$$

This is typically the case for measurements done on triple-axis spectrometers [5] (TAS). For measurements done on time-of-flight spectrometers where $k_i$-independent monitors are sometimes used, there are usually data reduction options for users to choose, so that the end data are presented in a format where the end data are presented in a format where $k_i$ and $k_f$ are properly taken care of. This subtle difference will be discussed again when we describe the resolution volume determination in details below.

Here we only discuss the case of scattering with unpolarized neutrons. For coherent magnetic scattering from a system with a single species of magnetic atom [5],

$$d^2\sigma = \frac{N k_f}{\hbar} \rho^2 e^{-2W} \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \bar{Q}_\alpha \bar{Q}_\beta) S^{\alpha\beta}(Q, \omega).$$

The parameters used in Eq. 5 are explained below:

$N$ is the total number of unit cells, $p = (\frac{\gamma_0 p}{2}) g f(Q)$, and $\gamma_0 = 0.2695 \times 10^{-12}$ cm, $f(Q)$ is the magnetic form factor. $k_f$ and $k_i$ are final and incident neutron wave-vectors. $e^{-2W}$ is the Debye-Waller factor. $\alpha, \beta$ denote the Cartesian Coordinates $x, y,$ and $z$, and $Q_\alpha, Q_\beta$ are the projections of the unit wave-vector $Q$ on the Cartesian axes.

$$S^{\alpha\beta}(Q, \omega) = \frac{1}{2\pi} \int dt e^{-i\omega t} \sum_{l} \int dQ e^{iQ \cdot r_l} \left( S^{\alpha}_{0}(0) S^{\beta}_{1}(t) \right),$$

is the dynamic spin correlation function, which is typically what one would eventually want to determine. $S^{\alpha\beta}(Q, \omega)$ satisfies a simple sum rule when integrated over a Brillouin zone:

$$\int_{BZ} dQ S^{\alpha\beta}(Q, \omega) dQ dE = \frac{1}{3} S(S + 1) \delta_{\alpha\beta}.$$

It is also related to the imaginary part of the dynamic susceptibility $\chi''(Q, \omega)$ via the fluctuation-dissipation theorem [6]:

$$\chi^{\alpha\beta''}(Q, \omega) = g^2 \mu^2 B_0 \pi \left( 1 - e^{-\hbar \omega/k_B T} \right) S^{\alpha\beta}(Q, \omega).$$

Note that the prefactors we have included in this definition are necessary in order that $\chi''$ is consistent with the bulk susceptibility, as we will show later.

We then make a necessary approximation to “decouple” the instrument resolution and the scattering response function.

$$\tilde{I}(Q, E) \approx \frac{N}{\hbar} \rho^2 e^{-2W} \tilde{S}(Q, \omega) k_f R_0(Q, E),$$
where \( R_0(Q, E) = \int R(Q_0, E_0, Q, E) dQ_0 dE_0 \) is the resolution volume, which should only be instrument dependent, and will later be referred to as \( R_0 \). \( \tilde{S}(Q, \omega) = \sum_{\alpha, \beta} (\delta_{\alpha, \beta} - \hat{Q}_\alpha \hat{Q}_\beta) S^{\alpha \beta}(Q, \omega) \) is the modified dynamic spin correlation function, taking into account that our scattering measurements are only sensitive to spin (fluctuations) along directions perpendicular to the wave-vector transfers. In the common case of isotropic spin excitations, as in a paramagnetic phase, \( S^{xx}(Q, \omega) = S^{yy}(Q, \omega) = S^{zz}(Q, \omega) \), thus

\[
\tilde{S}(Q, \omega) = 2S^{zz},
\]  

The approximation in Eq. 7 is acceptable if \( \tilde{S}(Q, \omega) \) is relatively smooth in the region of interest. When the real \( \tilde{S}(Q, \omega) \) has sharp features relative to the resolution volume, usually the accurate non-distorted \( \tilde{S}(Q, \omega) \) will only be obtainable through a deconvolution process, which is beyond the scope of this paper. Nevertheless, this approximation is always valid if one is interested in the total spectral weight, i.e. \( Q \) and energy integral of \( S(Q, \omega) \).

After putting all the numbers together, one can ultimately write down:

\[
\tilde{S}(Q, \omega) = \frac{13.77 \text{(barn}^{-1}) I(Q, E)}{g^2 |f(Q)|^2 e^{-2W} N k_f R_0},
\]  

where 1 barn = \( 10^{-24} \text{cm}^2 \) is the unit for neutron scattering cross-section. We will see in later discussions that the denominator has the units of energy divided by cross-section (typically \( \text{barn}^{-1}\cdot\text{meV} \) or \( \text{barn}^{-1}\cdot\text{eV} \)), thus \( \tilde{S}(Q, \omega) \) here has a unit of \( \text{meV}^{-1} \) or \( \text{eV}^{-1} \). Alternatively, if one wants to express the results as squared magnetic moment per site, in units of \( \mu_B^2 \cdot \text{meV}^{-1} \) or \( \mu_B^2 \cdot \text{eV}^{-1} \), the appropriate formula is

\[
\tilde{M}(Q, \omega) = g^2 \mu_B^2 \tilde{S}(Q, \omega) = \frac{13.77 \text{(barn}^{-1}) \mu_B^2 |f(Q)|^2 e^{-2W} N k_f R_0}{|f(Q)|^2 e^{-2W} N k_f R_0},
\]  

which only differs by a factor of \( g^2 \mu_B^2 \) compared to \( \tilde{S}(Q, \omega) \). It is worthwhile to mention that in many literature people use expressions such as \( I(Q, \omega) \), or simply \( S(Q, \omega) \) when plotting magnetic neutron scattering results. In most cases, unless explicitly noted, they actually correspond to either \( \tilde{S}(Q, \omega) \) or \( \tilde{M}(Q, \omega) \) that we discussed above.

Sometimes it may be preferable to write the magnetic neutron scattering results in a form directly related to bulk susceptibility measurements. For such a purpose, the imaginary part of the dynamic susceptibility \( \chi^{\alpha \beta'}(Q, \omega) \) is often used, which can be converted from \( S^{\alpha \beta}(Q, \omega) \) using Eq. 6. This quantity is related to the bulk susceptibility through the Kramers-Kronig transformation:

\[
\chi^{\alpha \beta'}(Q, 0) = \frac{1}{\pi} \int d\omega \frac{1}{\omega} \chi^{\alpha \beta'}(Q, \omega),
\]  

For the typical case of paramagnetic scattering from non-interacting spins, the bulk susceptibility

\[
\chi = \frac{g^2 \mu_B^2}{3k_BT} S(S + 1) = \chi^{\alpha \alpha'}(0, 0).
\]  

Using Eq. 4 one can verify that the definition of \( \chi^{\alpha \beta} \) in Eq. 6 satisfies Eq. 12. Using Eqs. 8, 6 and 9 we have:

\[
\chi^{zz'}(Q, \omega) = \chi^{zz'} = \frac{\pi}{2} \mu_B^2 \left( 1 - e^{-\hbar \omega/k_BT} \right) \frac{13.77 \text{(barn}^{-1}) I(Q, E)}{|f(Q)|^2 e^{-2W} N k_f R_0}.
\]  

In the case of anisotropic spin excitations, to avoid confusion it would make more sense to use the different components of \( \chi^{\alpha \beta'} \) explicitly rather than the general form \( \chi^{zz'} \).

The Landé-\( g \) factor, the magnetic form factor \( f(Q) \), and the Debye-Waller factor \( e^{-2W} \) are sample dependent and can be estimated. For example \( g \approx 2, e^{-2W} \approx 1 \) for small \( Q \) where \( f(Q) \) is large. And the magnetic form factor \( f(Q) \) can be looked up in tables [7]. Therefore, in order to determine the absolute magnitude of \( \tilde{S}(Q, \omega) \) from the measured intensity \( I(Q, E) \), one needs to know the resolution volume \( R_0 \). In general, to obtain the resolution volume one could use the following references: (i) nuclear Bragg peaks; (ii) sample incoherent elastic scattering; (iii) standard sample (e.g. vanadium) incoherent elastic scattering, and (iv) sample phonon scattering. For single crystal samples, extinction in Bragg scattering can often significantly affect the absolute Bragg intensities, and a good understanding of the instrument resolution is required, so (i) is less commonly used nowadays. In this report, we will discuss some examples in our neutron scattering experiments where the magnetic scattering is normalized using (ii) or (iv), providing formulas that one will be able to easily adapt to other measurements. We also briefly discuss the case (iii).
II. EXPERIMENT

The experiments we discuss here include measurements on two different material systems. The first system is a Fe-based superconductor FeTe$_{1-x}$Se$_x$, the so-called “11” compound. Measurements on the “11” single crystal samples discussed here were all performed on the BT7 and SPINS triple-axis-spectrometers at the NIST center for neutron research (NCNR) (see Ref. 8 for more details). We used horizontal beam collimations of Guide-open-S-05’-240’ (S represents “sample”) for the inelastic scattering measurements on SPINS with fixed final energy of 5 meV and a cooled Be filter after the sample to reduce higher-order neutrons. At BT7, we used beam collimations of open-50’-S-50’-240’ with fixed final energy of 14.7 meV and two pyrolytic graphite filters after the sample. The second system is the multiferroic BiFeO$_3$. Neutron inelastic scattering experiments on the BiFeO$_3$ single crystal were performed on the ARCS time-of-flight spectrometer at the Spallation Neutron Source (SNS) at Oak Ridge National laboratory (see Ref. 9). The data discussed here are those using a 40 meV neutron incident energy. All the data are described in reciprocal lattice units (r.l.u.) of $(a^*, b^*, c^*) = (2\pi/a, 2\pi/b, 2\pi/c)$.

III. RESULTS AND DISCUSSION

A. Normalization with sample incoherent elastic scattering

This is one of the most straight-forward methods in doing absolute calibration. Since the cross-section for incoherent elastic scattering is quite simple:

$$\frac{d\sigma}{d\Omega}\bigg|_{\text{inc}} = \frac{N}{4\pi} \sum_j \sigma_{j,\text{inc}}^e e^{-2W_j},$$

the summation is performed over all atoms in the unit cell, where $\sigma_j$ is the incoherent neutron scattering cross-section of the $j$th atom. Based on Eq. 2, the energy integrated incoherent elastic scattering intensity

$$\int \tilde{I}(Q, E) dE = \frac{N}{4\pi} \sum_j \sigma_{j,\text{inc}}^e e^{-2W_j} k_i R_0$$

can be obtained by doing an energy scan through $h\omega = 0$ at a wave-vector transfer $Q$ far away from any magnetic/nuclear Bragg peaks. For elastic scattering, $k_i = k_f$, therefore we have

$$N k_f R_0 = 4\pi \int \tilde{I}(Q, E) dE \sum_j \sigma_{j,\text{inc}}^e e^{-2W_j}.$$  

Now we use data from two samples as examples. The integrated incoherent elastic scattering intensities, the sum of the incoherent scattering cross-sections, and the resolution volumes are given in Table I. If we neglect the variation of the Debye-Waller factor (assuming $e^{-2W} \sim 1$), knowing $N k_f R_0$, we can then use Eq. 9 or Eq. 10 to convert magnetic scattering into absolute units.

Figures 1(c) and (d) show magnetic scattering measured at $h\omega = 2$ meV, for $Q$ along the [110] direction across (0.5,0.5,0) from both samples 1 and 2. The measurements are performed on two similar samples with different weights, and on two different instruments (SPINS vs. BT7). Before the proper normalization, intensities per minute [Fig. 1(c)] for the two measurements are obviously not comparable. Yet the results shown in units of $\mu^2 f_{\text{inc}}^{-1}$ after normalization suggest that the two scans have very similar absolute intensities, as they should.

The procedure described above is one of our standard procedures for normalizing magnetic scattering intensities using sample incoherent elastic scattering. There are, of course, a few issues that need to be discussed. First, the procedure described above was for triple-axis measurements using a fixed-E$_f$ mode, where $k_f$ would be a constant for all energy and wave-vector transfers. If a constant-E$_i$ mode is used, $k_f$ would vary for different energy transfers. The volume $N k_f R_0$ can still be obtained with the

| Sample       | $\int \tilde{I}(Q, E) dE$ (meV) | $\sum_j \sigma_{j,\text{inc}}^e$ (barn) | $N k_f R_0$ (meV-barn$^{-1}$) |
|--------------|--------------------------------|--------------------------------------|-------------------------------|
| FeTe$_{0.7}$Se$_{0.3}$ | 91.0/6780000 = $1.34 \times 10^{-3}$ | 0.4 + 0.7 $\times 0.09 + 0.3 \times 0.32 = 0.559$ | 3.02 $\times 10^{-3}$ |
| FeTe$_{0.55}$Se$_{0.45}$ | 1128.8/1400000 = $8.03 \times 10^{-3}$ | 0.4 + 0.55 $\times 0.09 + 0.45 \times 0.32 = 0.594$ | 1.70 $\times 10^{-3}$ |

TABLE I. Parameters for the two FeTe$_{1-x}$Se$_x$ samples. The integrated intensities listed in the table are obtained from fits to the data sets shown in Fig. 1(a) and (b), and have already been divided by monitor counts.
FIG. 1. (a) and (b): Incoherent elastic energy scans through $\hbar \omega = 0$ taken from single crystals of FeTe$_{0.70}$Se$_{0.30}$ (red) and FeTe$_{0.55}$Se$_{0.45}$ (blue), measured at $Q = (1.3, 0.3, 0)$, with monitor counts being $6.78 \times 10^5$ per minute, and $1.4 \times 10^5$ per minute, performed on SPINS and BT7, respectively. (c): Constant energy scans for magnetic scattering at $\hbar \omega = 2$ meV, going along the transverse direction across $Q = (0.5, 0.5, 0)$. The intensities have been plotted as per minute. (d): Constant energy scans for magnetic scattering at $\hbar \omega = 2$ meV. The intensities have been normalized to absolute units.
same methods. However, when using Eqs.9 or 10 one will need to use the correct $k_f$ for the measured energy transfer, not the $k_f$ for the incoherent elastic scattering measurements (which is the same as $k_i$). The situation is simpler for measurements performed on time-of-flight instruments, where the factors $k_i$ and $k_j$ have already been taken care of in properly reduced data sets available to users. One can use the same methods to obtain the resolution volume $Nf_0 = Nk_fR_0$, which can later be used in Eqs.9 or 10 in place of $Nk_fR_0$, without having to worry about the change of $k_f$.

Secondly, the number $N$ used here is the number of unit cells. Therefore the results correspond to squared moment/spin per formula unit. If there are more than one magnetic ions in a formula unit, the results need to be scaled properly to obtain squared moment/spin per site if that is desired.

The advantage of using sample incoherent elastic scattering is of course its simplicity. It is usually fast to perform an incoherent elastic scan, and no sample changing is required. However, for samples with relatively small incoherent scattering cross-sections, incoherent elastic scattering coming from sample holders and sample environments can have a large contribution. Therefore with this method it is common that one could over-estimate the resolution volume, and under-estimate the real magnitude of magnetic scattering intensities.

\section*{B. Normalization with standard sample incoherent elastic scattering}

Because vanadium has a large incoherent scattering cross-section, it is often used as a standard sample for normalization purposes. The principle is the same as described in the previous section. Nevertheless, in order to use a vanadium sample for normalization, one needs to know the number of unit cells in both the measured sample and the vanadium standard sample $(N_{\text{sample}} = N_{\text{vanadium}})$. A standard procedure would then be to carry out an incoherent elastic scan using the vanadium standard sample under the same instrumental set-up; and use the energy integrated intensity and Eq. 16 to obtain $N_{\text{vanadium}}k_fR_0$. Knowing the weight of the vanadium sample and measured sample, one can then obtain $N_{\text{sample}}k_fR_0$.

The large incoherent scattering cross-section from vanadium makes incoherent elastic background from the sample environment less of an issue in the normalization process, thus providing a significant advantage over the method using sample incoherent scattering. Standard vanadium normalization runs can be readily performed without any detailed knowledge of the sample itself. This is another advantage of using vanadium normalization over sample phonon normalization (see next subsection); while for phonon normalization, one needs to have some basic knowledge of the sample phonon spectra to know where the measured energy transfer, not $\omega(q)$. For acoustic phonons at small $q = Q - G$ values, $S(Q, \omega)$ can be approximated to:

$$S(Q, \omega) = \frac{n_q}{\omega(q)} |F_N(G)|^2 \frac{|Q \cdot \xi|^2}{2M} e^{-2W} \delta(\omega - \omega(q)).$$

Here $G$ is the Bragg wave-vector near which the phonon is being measured. $n_q = \frac{1}{1-e^{-\omega(q)/k_B T}}$ is the Bose factor, $F_N(G)$ is the acoustic phonon structure factor which is the same as the Bragg structure factor at $G$. $\xi$ is the unit vector along the phonon polarization direction, and $|Q \cdot \xi|^2$ gives the “polarization factor”. $M = \sum_j m_j$ is the summation of the atomic mass in the unit cell.

Phonon measurements can typically be performed as constant-Q or constant-E scans. For a constant-Q scan, the energy integrated phonon intensity can be written as:

$$\int I(Q, \xi)dE = \frac{n_q}{\omega(q)} \frac{\hbar Q^2}{2m M} \cos^2 \beta |F_N(G)|^2 e^{-2W} Nk_f R_0.$$  

Here $m$ is the mass of neutron. Rewriting $S(Q, \omega)$ in this format makes it easier to put numbers in. One will not have to write atomic weights in units of kg or g, but can rather use the inverse atomic numbers in place of $M$. $\frac{\hbar Q^2}{2m}$ is then the neutron energy.
TABLE II. Parameters for longitudinal phonon measurements on BiFeO₃. The first two rows are results from constant-E cuts near 
\( G = (3,0,0) \) and \( (1,1,0) \) [see Fig. 3(a) and (b)]; and the last row are results from a constant-\( Q \) cut [see Fig. 3(c)] at \( Q = (1.3,0,0) \). For all measurements, \( T = 300 \, K \), \( \frac{m}{\hbar^2} = \frac{1}{317} \), \( \cos^2 \beta = 1.0 \).

| \( Q \) (r.l.u.) | \( h\omega \) (meV) | \( d\omega/dq \) (meV/Å⁻¹) | \( n_q \) | \( \frac{hQ^2}{2m} \) (meV) | \( \int \hat{I}(Q,E)dq \) (Å⁻¹) | \( |F_N(G)|^2 \) (barn) | \( N\tilde{R}_0 \) (meV barn⁻¹) |
|----------------|----------------|----------------|-------|----------------|----------------|----------------|----------------|
| (3,0,0)        | 5.0            | 20.85          | 5.69  | 46.95          | 0.00198         | 868.2          | 2.78 \times 10⁻⁴ |
| (1,1,0)        | 4.0            | 18.37          | 6.98  | 10.43          | 0.00124         | 1653.11        | 2.37 \times 10⁻⁴ |
| (1.3,0,0)      | 6.92           | 4.26           | 8.82  | 0.00538        |                 | 651.1          | 3.0 \times 10⁻⁴ |

at wave-vector \( Q \) which is practically just \( 2.0717Q^2 \) in units of meV where \( Q \) should have units of Å⁻¹. \( \beta \) is the angle between \( Q \) and \( \xi \).

An alternative approach is to perform constant-E scans where the \( Q \)-integrated phonon energy can be obtained:

\[
\int \hat{I}(Q,E)dq = \frac{1}{d\omega/dq \omega(q)} \frac{n_q}{2m} \frac{(hQ)^2}{M} \cdot \cos^2 \beta |F_N(G)|^2 e^{-2W} Nk_f R_0. \tag{20}
\]

Here \( d\omega/dq \) is the phonon velocity at the measured energy/wave-vector. The unit used for \( q \) should be the same in the intensity integral and phonon velocity on both sides of the equation so that they can cancel out.

We use examples from our measurements of BiFeO₃ single crystals on the time-of-flight spectrometer ARCS at SNS as an example to show how one can obtain the resolution volume \( N\tilde{R}_0 \) with phonons. In Table II the numbers are given for longitudinal phonons measured near (110), (300), and (100) Bragg peaks. We also assume that the Debye-Waller factor \( e^{-2W} \) is close to 1. As discussed previously, the time-of-flight data have already been treated so that the factors \( k_i \) and \( k_f \) are removed, and we use \( N\tilde{R}_0 \) instead of \( Nk_f R_0 \).

The resolution volume \( N\tilde{R}_0 \) from the three phonon profiles shown in Table II and Fig. 3 are consistent within expected error bars. After obtaining \( N\tilde{R}_0 \), we can use Eqs. [9] and [10] to normalize magnetic scattering intensities [9]. Assuming \( g = 2 \), we were able to calculate the integrated spectral weight and a spin per site of \( S \sim 2.1 \) per Fe, which is in good agreement with the theoretical expectation of \( S = 5/2 \) for Fe³⁺.

The advantage of using phonon scattering for normalization is that by avoiding the use of elastic scattering, there is less background contribution in the normalization process. Nevertheless, other factors such as phonon anharmonicity, variation of the Debye-Waller factor and uncertainties in the structure factor \( |F_N(G)|^2 \) can still lead to systematic errors. It is reasonable to expect a systematic error in the range of \( \sim 20\% \) in these normalization processes.

IV. SUMMARY

In this paper, we have discussed various methods for performing absolute normalization of magnetic inelastic neutron scattering data. The resolution volume can be obtained using Eqs. [16] [19] or [20] depending on the reference chosen for the normalization. Data-sets from previous experiments are given as examples for the normalization process. The modified dynamic spin correlation function \( S'(Q,\omega) \), or the imaginary part of the dynamic susceptibility \( \chi''(Q,\omega) \), have been clearly defined in the paper; and these quantities can then be obtained using Eq. [9] [10] or [13]. The formulas described here are for general purposes and independent of instrument configurations. We hope they can serve as easy-to-use references for future inelastic neutron scattering measurements.

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FIG. 2. (a) and (b): Constant-Energy cuts through $\hbar \omega = 5$ and 4 meV near $Q = (3, 0, 0)$ and $(1, 1, 0)$ along the longitudinal direction. Here the phonon intensities include phonons on both sides (short-$Q$ and long-$Q$) of the Bragg peaks, and are fitted with double-Gaussians. The $q$-integrated intensities listed in Table II use half of the double-Gaussian areas. The sample is a BiFeO$_3$ single crystal, measured on ARCS at SNS. (c) A constant-$Q$ cut taken at $Q = (1.3, 0, 0)$.
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