RESOLUTION EFFECTS FOR SYSTEMS WITH STRONG DISPERSION

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The effects of instrumental resolution are considered for systems where the dispersion relations vary rapidly with wave vector q. In such cases the observed profile of scattering in a "scan" is determined primarily by the wave vector resolution of the instrument rather than the more customary situation where the energy resolution is most important. We show that when the energy transfer varies substantially during the course of a constant-q measurement the observed scattering can be strongly distorted from that expected. To demonstrate these effects explicitly, calculations of the low temperature spin-wave lineshapes and integrated intensities in iron are presented for the case of a triple-axis spectrometer operated in both constant-q and constant-E modes, but the general results are also applicable to time-of-flight and constant-Q spectrometers.

Recently considerable debate and discussion has ensued over the proper inelastic neutron scattering scan to use in determining the scattering function $S(q, E)$ in systems where the energy dependence of the scattering is a strong function of the wave vector (i.e. highly dispersive systems). Many years ago Brockhouse et al. [1] demonstrated that for triple-axis spectrometers the constant-q technique with variable incident energy offers a number of advantages to the experimenter. If the scattering is normalized with a "$1/v$" detector in the incident beam then $S(q, E)$ is obtained directly in the raw data in cases where the instrumental resolution function is small in comparison to the distribution of scattering of interest, while if the opposite is true (e.g. for sharp excitations) then the correct excitation energies and integrated intensities can be readily obtained. Of course there are a number of conditions which must be fulfilled in order to obtain reliable data in this way. For example, with sharp excitations the dispersion relation should be approximately linear over the region of (q, E) that the resolution samples and the resolution function should not vary appreciably over

the course of a "scan". In strongly dispersive systems, however, these conditions are not satisfied very well, and hence experimentalists have resorted to other techniques such as constant-E scans to obtain the dispersion relations of interest. In the present paper we report detailed calculations of the low temperature spin-wave lineshapes and integrated intensities for a system with moderate dispersion, iron. We compare directly the numerical results obtained in constant-q with those obtained with the constant-E technique to explicitly show where reliable results can be obtained. The results for other systems of interest, such as one-dimensional conductors, weak itinerant magnets, and other 3d magnetic systems, will be presented elsewhere.

The intensity at any (q_0, E_0) can be obtained by performing the four-dimensional convolution of the resolution function [2] with the scattering cross section $S(q, E)$:

$$I(q_0, E_0) = \int \int \int \int S(q, E)$$
$$\times R(q - q_0, E - E_0)\, dE\, dq. \quad (1)$$

A scan then consists of a sequence of observations

of $I(\boldsymbol{q}_0, E_0)$. The advantage of a triple-axis spectrometer is that the momentum and energy transfer can be varied in any combination desired, whereas for time-of-flight and constant-Q spectrometers this flexibility is greatly reduced. For the scattering function we assume an isotropic spin-wave dispersion relation of the form

$$E_{\rm sw} = D|\boldsymbol{q}|^2 , \tag{2}$$

where we take $D = 280$ meV-Å^2 appropriate for iron at low (room) temperature [3]. For the calculations we also assume the spin waves have no intrinsic linewidths, and the temperature factor is set to unity ($T = 0$ K). Thus ideally the integrated intensity at each $\boldsymbol{q}$ is the same. The numerical results were obtained using the convolution technique of Haywood [4].

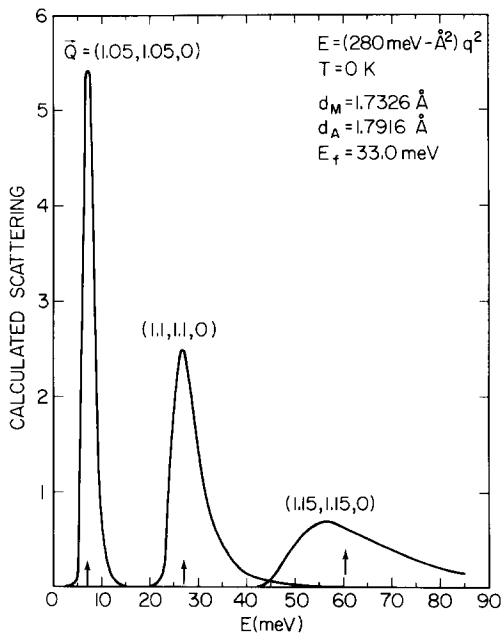The results for three different q's are shown in fig. 1. The calculations were performed for a fixed

Fig. 1. Calculated spin-wave scattering at $T = 0$ K for iron, at three values of q. As the slope of the dispersion relation becomes larger, the distribution of scattering is skewed to higher energies, with the peak position occurring below the spin-wave energy (indicated by the arrow). The widths of the peaks are also much larger than the energy resolution of the instrument.

exit energy of 33 meV, beryllium monochromator and analyzer, and horizontal collimations of 40'–20'–20'–60', which yields relatively good resolution as used for our original measurements [5]. At $Q = (1.05, 1.05, 0)$ the observed peak position occurs close to the true spin-wave position, but the observed width is considerably larger than the instrumental energy resolution even at this relatively modest spin-wave energy, as shown in table I. Note also that the distribution of scattering is skewed toward higher energies, which is caused by the curvature of the dispersion surface. At a larger value of q ($\zeta = 0.10$), where the slope of the dispersion relation is larger, we see that the width is about three times instrumental energy resolution ($E_{\rm res}$), and the skewing is more pronounced. In addition, a close inspection of the figure will reveal that the calculated peak position occurs at a significantly smaller energy than the true spin-wave energy (indicated by the arrow). At larger q ($\zeta = 0.15$) these effects are much more pronounced: the line shape is quite distorted, with a width which is about six times $E_{\rm res}$. These large widths originate from the wave vector resolution of the instrument, not the energy resolution. Note also that the calculated peak position occurs at an energy which is about 10% below the true spin-wave energy. We remark that at elevated temperatures the errors in the peak position will increase due to the spin wave population factor, which weights the cross section at lower energy more heavily than at higher energy. For comparison, under the identical experimental conditions, the constant-E technique yields the correct spin-wave positions to better than 1%.

More serious problems are found with the constant-q technique when integrated intensities are measured. Fig. 2 shows the results for the two techniques. We see that over most of the energy range the constant-E technique yields the correct spin-wave intensity (1.0 for this model). At low energies, however, the calculated intensities deviate from 1.0. This is the range where the slope of the dispersion curve is becoming small, and the constant-E technique yields substantial errors (~8% at 10 meV). The calculated intensity is also low at the highest energy shown (90 meV). This is because the complete peak cannot be measured

Table I
Data corresponding to figure one. Energies are in meV, widths are FWHM

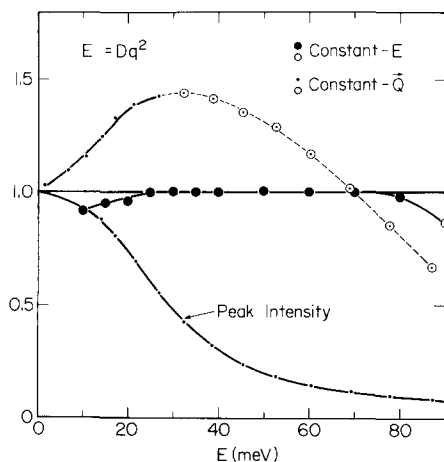| Q	E_{sw}	E_{obs}	Slope $(2Dq)$ (meV-Å)	E_{res}	Observed width
1.05, 1.05, 0	6.7	7.1	87	1.41	2.5
1.10, 1.10, 0	27	26	174	2.20	6.5
1.15, 1.15, 0	61	56	260	4.08	24.0

Fig. 2. Integrated spin-wave intensities are shown at the top of the figure for constant-E and constant-q scans. The results for constant-q do not agree very well with the correct result of 1.0. Also shown is the calculated peak height as a function of energy.

since some of the scattering lies outside the physically accessible range of (q, E); in order to measure in this range a higher exit energy must be chosen. We denote intensities where the entire peak cannot be measured by open circles on the figure. For constant-q we see that this is a very serious problem, and in fact over much of the q range a complete peak cannot be measured. Fig. 1 reveals the reason; the scattering is skewed to high energies, and for a large range of q's it extends into the region which is inaccessible. Thus intensity is lost, and the integrated intensity drops. Another problem is that the high energy tail of scattering adds an additional contribution to the integrated intensity, which under ideal conditions should not be there. Thus initially the integrated intensities appear to increase with increasing energy. The data of fig. 2 demonstrate that the constant-q technique will not yield reliable spin-wave intensities over the energy range of interest, except at quite small E.

One final point we wish to make is that the peak heights decrease as we move up the spin-wave dispersion relation, as shown in both figures, and hence the peak heights themselves should not be used as a measure of the relative strength of the scattering as a function of energy. This is an important point when making measurements in materials where the scattering is restricted in q-space, but is spread over a large range in energy. Examples of such systems are the phonons in 1d conductors such as KCP, and the paramagnetic scattering in the 3d magnets Cr, Fe, Co, and Ni. In the region where the scattering cross section is very dispersive the constant-q technique generally overestimates the scattering at low energies relative to the scattering at higher energies, and hence such scans can yield misleading information.

Acknowledgments

References

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