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Addendum to "Temperature dependence of the magnetic excitations in iron"

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Additional details and discussion of the neutron scattering data taken above T_c are given.

The spin dynamics of the $3d$ transition-metal ferromagnets Fe, Co, and Ni continues to attract considerable interest, and a number of neutron scattering studies of these materials near and above T_c have been carried out in recent years. For iron, Collins and co-workers[1,2] concentrated their efforts on the critical dynamics[3] at small (q,ω) while we concentrated[4,5] on the dynamics at higher energies and larger q. These studies avoided to a large extent the complications in the data collection and analyses at intermediate (q,ω) introduced by the presence of the lattice-dynamical scattering.

Since these studies were completed, considerable progress has been made theoretically. These theoretical studies have posed new questions, and it seems appropriate to discuss to what extent the original measurements can be used to answer these questions and what questions will require new experiments. We also would like to present some additional details of our data and analysis which should prove useful in comparing theory with experiment.

Most of the data of Ref. 4 (hereafter referred to as I) were taken on a large isotope single crystal of ^{54}Fe (12 at.% Si) with a triple-axis spectrometer operated in the "constant-E" mode. For energies above ~ 25 meV the instrumental background at each temperature was found to be independent of q and E, and agreed within statistical error with background at room temperature.[6] Higher backgrounds (for iron) were encountered at energies below 25 meV. They were still q independent over the range of interest, and room-temperature background values were used. Consequently, each scan was fit to a flat (q-independent) background, plus one Gaussian peak for each observed peak (e.g., Figs. 4 and 7 of I). The one-phonon scattering (at low energies) was sharply peaked and could be easily separated from the magnetic response, which was much broader than the instrumental resolution. The (Gaussian) resolution was then deconvoluted from the magnetic response by assuming that the latter was also Gaussian. This assumption was found to give a good fit to the data for both iron and nickel; in particular, a Lorentzian line shape (in q) did not give a good fit to the data.

Table I gives our results[7] from this analysis for the dynamic susceptibility $\chi(q,\omega)$ above T_c. The positions and widths were found not to be temperature dependent above T_c, and symmetry-related results have been averaged to obtain the final values shown. The relative amplitudes were not very sensitive to temperature but the absolute amplitudes were strongly temperature dependent as indicated in Figs. 3 and 5 of I. An estimate of the scattering function $S(q,\omega)$ can be obtained by multiplying by the appropriate thermal factors, although it should be kept in mind that the relative amplitudes do have some temperature dependence. The data of Table I were used to generate the isometric plot of $\chi(q,\omega)$ (Fig. 9 of I) as well as the $S(Q,\omega)$ plot shown in Fig. 10 of I.

The susceptibility $\chi(q,\omega)$ and the scattering function $S(q,\omega)$ are shown in Fig. 1 at a series of wave vectors. As previously discussed (I), the data show that the magnetic response evolves continuously from purely diffusive behavior at small q to a propagating character at large q. One question that is frequently asked is what value q_0 defines the "boundary" between the region of diffusive behavior at small q and the "spin-wave" region at large q. q_0 is, of course, model dependent; we have used the criterion of $\Delta E/E=1$, with ΔE being evaluated from the constant-E data by multiplying Δq by the measured dispersion as discussed in I. This "crossover" occurs at 0.25 Å^{-1}. The scattering is, of course, diffusive at this q, as already had been determined by Boronkay and Collins.[2] Another possible criterion is to have a reasonably well-defined peak at constant Q, which occurs for $q_0 \sim 0.5$ Å^{-1} with the proviso noted below.

If one wishes to compare the constant-Q curves of Fig. 1 with theory it is important to understand possible sources of experimental error and how these errors might affect the shapes of these curves. The statistical errors contributing to

TABLE I. Dynamic susceptibility above T_c. $\chi(q,E_0)=A_0e^{-(q-q_0)^2/2\sigma^2}$

E_0 (meV)	q_0 (Å^{-1})	σ (Å^{-1})	A_0 (arbitrary units)
8.27	0.262	0.110	100
12.41	0.333	0.116	98
16.54	0.380	0.124	96
20.68	0.425	0.127	94
24.81	0.455	0.130	92
28.95	0.475	0.147	90
33.08	0.505	0.153	88
37.22	0.525	0.157	86
41.35	0.550	0.160	84
45.59	0.575	0.165	82
53.76	0.605	0.167	78
62.03	0.635	0.168	74
70.03	0.670	0.170	70
78.56	0.70	0.173	66
86.84	0.73	0.176	62
95.10	0.76	0.178	54
103.4	0.78	0.181	28

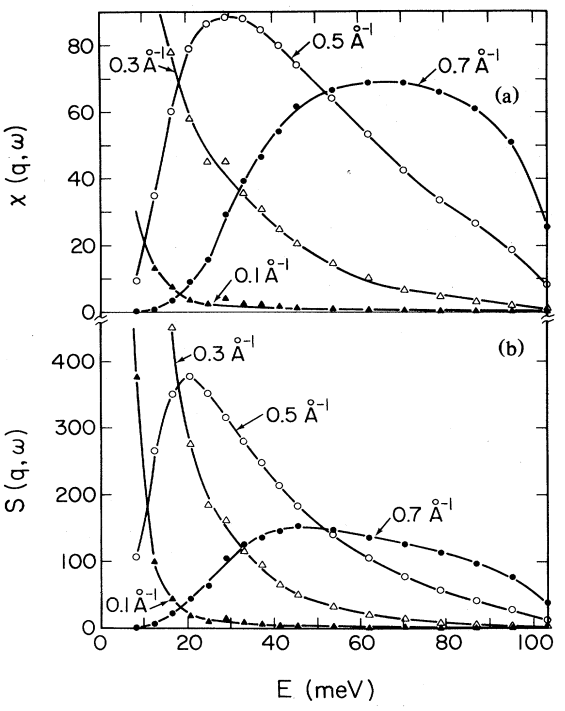

FIG. 1. (a) Susceptibility $\chi(q,\omega)$ at a series of wave vectors for iron above T_c. These curves have been taken directly from Table I. (b) Scattering function $S(q,\omega)$ at $T/T_c=1.10$, at a series of q values. The plots have been obtained from the susceptibility function of Table I by multiplying by the appropriate thermal factors.

the results are not very large, but there are possible systematic errors due to instrumental effects and background corrections. The scattering function is relatively broad in q and E compared with the instrumental resolution, but any error in the deconvolution procedure will distort the shapes of the curves in Fig. 1, particularly in the crossover region. The effects of the wave-vector resolution are particularly significant in these highly dispersive metallic ferromagnets, which is why the data were taken in the "constant-E" mode. The instrumental resolution is also strongly dependent on energy transfer. The resulting distortions of the observed line shapes as a function of energy can be severe, especially at higher temperatures where the strength of the scattering changes drastically with energy and wave vector. In addition, errors in the background determination could distort the curves below ~25 meV. This could affect the results quantitatively, but not qualitatively. Figure 2 shows an example of a constant-Q scan at a wave vector of 0.6 Å^{-1}. The open circles are the observed counts at $1.05T_c$, and the solid circles are the net (magnetic) scattering after subtraction of the room-temperature background. The data clearly show that $S(q,\omega)$ has a maximum at finite energy. It is also clear, however, that the line shape as a function of energy for fixed q is quite sensitive to the background correction. We emphasize, as we have in the past,[8] that these line shapes are only approximate. In our opinion, theoretical calculations should be compared with the positions and widths as given in Table I. These parameters were obtained directly from the constant-E measurements,

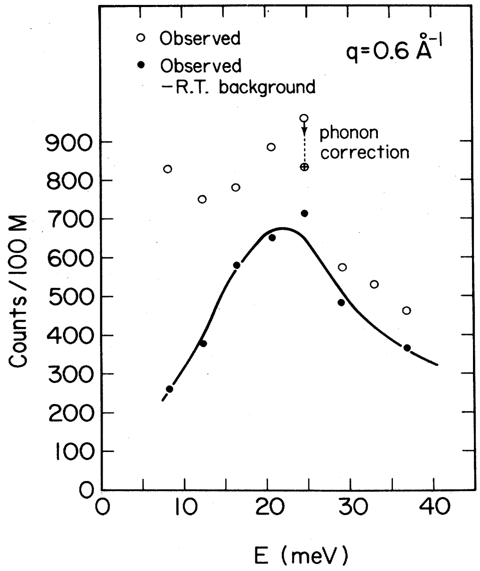

FIG. 2. Energy dependence of the observed counts at $q=0.6$ Å^{-1}. The open circles are the measured scattering at $1.05T_c$, and the solid circles are the net (magnetic) scattering after subtraction of room-temperature (R.T.) background.

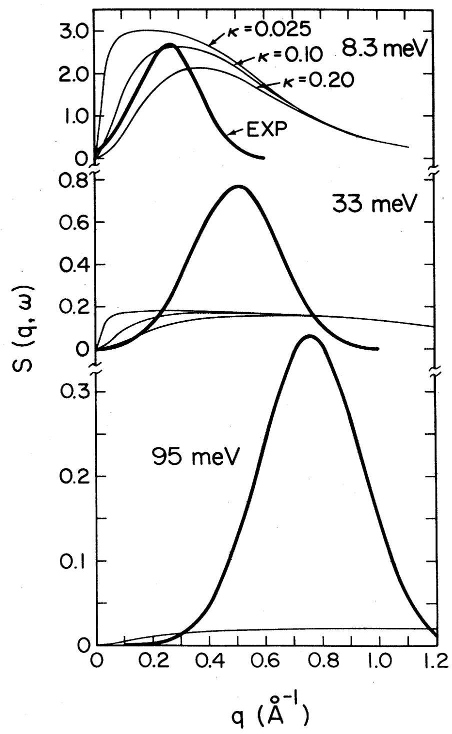

FIG. 3. Comparison of the hydrodynamic theory (using $\Lambda=20$ meV Å^2) with the data at three different energies. The discrepancy between the diffusive theory and experiment gets progressively worse with increasing energy until at high energies the scattering is qualitatively different than predicted.

in which the instrumental resolution and background are constant.

One important theoretical question which has emerged is how much magnetic scattering is there at large q and small energies. Clearly, the present data cannot address this question; little data were taken at low energies because of the large backgrounds (from the furnace as well as from nuclear scattering from the sample) and the data that were taken are subject to substantial background corrections. These experimental uncertainties will primarily affect the amplitudes at low energies in Table I, to a lesser extent the widths, while the positions should not be significantly affected at all. It will probably be necessary to use triple-axis polarized-beam techniques to study the details of the scattering in the large-q low-energy regime, and with recent advances in polarized-beam technology such measurements are beginning to be undertaken.[9,10]

Finally, we briefly remark on the comparison of our data with the predictions of hydrodynamic theory. It should be understood that all our data were taken outside the hydrodynamic regime and thus the comparison should not be regarded as a test of theory. It is nevertheless informative to see how large are the deviations from the theory. We have pointed out previously[4,5] that the discrepancies become more severe at higher energies. Figure 3 shows the calculations for several values of the inverse correlation range κ using the parameters available in the literature,[1,2,11] along with experiment. The overall scale factor has been adjusted so that the amplitudes agree at 8.27 meV for $\kappa = 0.1$. The agreement is not too bad at this energy, although we did not observe the predicted asymmetry of the scattering nor the expected temperature variation. The agreement gets progressively worse with increasing energy, and at 95 meV there is little resemblance to the experimental data. Here the observed peak in the scattering is more than an order of magnitude larger than calculated, and the observed width is much smaller.

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[2] S. Boronkay and M. F. Collins, Int. J. Magn. 4, 205 (1973).

[3] For nickel, see V. J. Minkiewicz, M. F. Collins, R. Nathans, and G. Shirane, Phys. Rev. 182, 624 (1969). For cobalt, see C. J. Glinka, V. J. Minkiewicz, and L. Passell, Phys. Rev. B 16, 4084 (1977).

[4] J. W. Lynn, Phys. Rev. B 11, 2624 (1975).

[5] For nickel, see H. A. Mook, J. W. Lynn, and R. M. Nicklow, Phys. Rev. Lett. 30, 556 (1973); J. W. Lynn and H. A. Mook, Phys. Rev. B 23, 198 (1981).

[6] With two exceptions. At the highest temperature measured, $1.4T_c$, there was some additional scattering due to multiphonons. Higher backgrounds were also encountered when high incident neutron energies and large energy transfers were employed, due to the corresponding small scattering angles (see Fig. 4 of I).

[7] Part of this table has already appeared in the literature in conjunction with a theoretical analysis; V. Korenman and R. E. Prange, Solid State Commun. 31, 909 (1979).

[8] See, for example, the panel discussion in *Physics of Transitions Metals,* edited by P. Rhodes (Arrowsmith Ltd., London, 1981), p. 669. It should be pointed out that the panelists did not have the opportunity to make corrections or changes in the draft of the (abbreviated) discussion before publication. Thus the published literature should be consulted for the proper details of the theories and experiments discussed.

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